

Appendix A

Publicly Available Protocols for the BCOP Test Method

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Appendix A1

INVITTOX Protocol 98. The Bovine Corneal Opacity and Permeability Assay – Method of Gautheron

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THE BOVINE CORNEAL OPACITY AND PERMEABILITY ASSAY - METHOD OF GAUTHERON

The effects of a test compound on the opacity and permeability of a freshly collected bovine cornea can be used as a measure of eye irritancy potential.

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NOTE

*The protocol presents the standard operation procedure used in the Home Office UK/EEC Validation Study for Alternatives to the Draize Test. It should be noted that this protocol might need to be modified in light of experience gained in the study. Additional information added in the course of producing this **INVITTOX** protocol, e.g. this note, is presented in italics.*

Critical Assessment

This technique has the advantage over the Draize test that both of the end-points used are objective and quantitative, in contrast to the subjective scoring used in the *in vivo* test. In contrast to cell-culture-based systems, the three-dimensional structure of the tissue is preserved, thus giving a closer approximation of the *in vivo* situation. The sacrifice of animals is not required, as slaughterhouse material is used. It does not require any special conditions or facilities for cell culture and is therefore inexpensive and relatively simple to implement.

The protocol includes a method to be used for the testing of solids, which may present some difficulties. Interference with opacity measurements may be caused by highly coloured test compounds which can stain the cornea.

General

This assay was developed in the Merck Sharp & Dohme Research Laboratories to assess the ocular irritancy potential of process intermediates. The test utilizes bovine corneas from eyes freshly collected in a local abattoir, and measures two end-points, namely opacity and permeability. The objective values obtained from both parameters are combined, and the *in vitro* irritancy scores are compared to a previously established scale of ocular irritancy. For in-house products, irritancy is classified into three broad categories: mild, moderate and severe.

Equipment

1. opacitometer, e.g. Electro-Design, RIOM, France
2. corneal holders (15) in polypropylene
3. dissection equipment (scissors, forceps, scalpels)
4. plastic containers for collection of eyes
5. electric screwdriver
6. vacuum pump
7. water-bath
8. spectrophotometer
9. mortar and pestle
10. common tissue culture and laboratory equipment

Materials

1. Hank's balanced salt solution with Ca^{++} , Mg^{++} , (HBSS, Sigma H-1387), supplemented with 0.350 g/l sodium bicarbonate according to the supplier's recommendation.
2. Fetal bovine serum (FBS)
3. Eagle's Minimum Essential Medium (MEM, Sigma M-3024). This is routinely prepared from powder, supplemented with 2.2 g/l sodium bicarbonate and 0.292 g/l (2 mM) glutamine, according to the supplier's recommendations, and stored refrigerated (one-week stock). In experiments, the medium also contains 1% FBS, prepared daily, and is used at 32°C. In this protocol, MEM medium always refers to complete medium which should be preheated to 32°C before use.
4. Dulbecco's phosphate-buffered saline (DPBS Sigma-D5780).
5. Na-fluorescein (Sigma F-6377). The dye is used as a 0.4 or 0.5% solution in DPBS (4 or 5 mg/ml).
6. Saline, always refers to 0.9% NaCl in distilled water.

Bovine eyes

Eyes, excised by an abattoir employee, are collected in a plastic jar containing one litre of HBSS for approximately 25 eyes. Buffer storage and transportation of eyes to the laboratory are performed at room temperature. The eyes are generally used within two hours after killing the animals.

Procedure Details

1. Preparation of corneas

During dissection, great care should be taken to avoid damage to corneal surfaces (epithelial and endothelial). All eyes are carefully examined, and those presenting defects, such as neovascularization, pigmentation, opacity or scratches are discarded. Eye balls are first dissected free of surrounding tissues (lids, conjunctiva, ocular muscles and glands) and placed in a jar containing fresh HBSS. Selected corneas are dissected with a 2-3 mm rim of sclera for easier handling, and stored in a petri dish containing HBSS until use. Corneas are then mounted in holders, the endothelial side being placed onto the O-ring of the posterior part of the holder. The anterior part of the holder is placed on the cornea and held in place with three screws. Compartments are then filled (the posterior part first) with MEM medium and corneas are incubated for one hour in a water-bath at 32°C.

2. Basal opacity

Immediately after incubation, anterior and posterior compartments are refilled with fresh medium, and opacity is determined (the method to measure opacity is described below). It should be very close to zero, thus permitting the elimination of any damaged or folded corneas: the limits for selecting good corneas are below or equal to 3 and above or equal to -3.

3. Treatment

Medium is removed from the anterior compartment, using a needle (with the point cut to remove the liquid completely) attached to a vacuum pump, and replaced by the test compound or an appropriate vehicle. Two treatment protocols are used, depending on the physical state (liquid or solid) of the product evaluated:

Protocol 1 : 10 min. treatment - **for liquids and surfactants**

Protocol 2 : 240 min, treatment - **for all solids**

In both protocols, substances are prewarmed at 32°C for a few minutes before being applied to the cornea. This is particularly important for liquids since the treatment time is only 10 minutes. For solids, this step is sometimes difficult; they are prepared in a mortar and very insoluble substances might be very sticky, preventing their transfer into a tube. In this case, place the mortar into warm (32°C) water for a few minutes.

3.1. Protocol 1

Liquid substances are applied neat (0.750 ml). If dilutions are requested, the solvent can be saline, for water-miscible products. PEG-600 or Triacetin can be used for immiscible liquids; triacetin may be preferred when possible (i.e. if miscible with the test liquid), because PEG-600 may enhance the penetration of some substances.

Surfactants are usually applied at 10% in saline, or at the dilution provided, and 0.750 ml is applied onto each cornea. Other concentrations (in saline) can also be tested as required.

Because some compounds, for example certain organic solvents, may be aggressive to plastic, it is recommended that glass syringes be used for all chemicals. In order to apply compounds uniformly onto the corneas, slightly rotate the holder, maintaining the cornea in a horizontal position (holes should be closed with the caps provided). Corneas are incubated in a horizontal position for 10 minutes at 32°C in a water bath. The holders should be completely immersed in water to ensure a uniform temperature.

The test substance is then removed, and the epithelium is washed at least three times, until the medium is clear, with approximately 4 ml of MEM. The anterior compartment is refilled with medium, and opacity is measured. Corneas are again incubated at 32°C for a period of 2 hours. Both compartments are refilled with fresh medium and opacity is again determined. The values obtained at this time-point (120 min) are the only ones used in calculations.

3.2. Protocol 2

Solutions or suspensions of solid products are prepared at 20% (in practice, 1 g plus 5 ml saline), using a mortar and pestle for homogenous preparations (start grinding in the mortar with a small volume of liquid). A volume of 0.750

ml is applied onto the epithelium with an appropriate syringe and needle. For sticky suspensions, it may be necessary to use a needle with a large diameter, or even to unscrew the anterior glass for pasty substances. Corneas are placed in a horizontal position for 4 hours at 32°C. The holders should be completely immersed in a water bath. The test compound is then removed and the epithelium is washed at least three times, until the cornea is free of particles; gentle swirling movements of the holders are sometimes necessary. It is also possible to remove the anterior glass if product is still present in the chamber. Both compartments are refilled with fresh medium and the opacity measurement is performed immediately without any further incubation.

N.B. This is the general procedure testing substances. In the EC/UK Study, however, all liquids and surfactants were tested neat and all solids at 20% in saline.

3.3. Number of corneas used

The number of corneas used per experiment is generally 15, but more or less may be used depending on the availability of eyes, holders and the number of test compounds. Each experiment includes a control group treated with saline (or with triacetin or PEG-600 if one of these has been used as solvent), a positive control group treated with a reference substance (see section "Positive controls") and several (generally 3) groups of corneas treated with the test substance. Each group is composed of three corneas.

4. Opacity measurement

The opacitometer determines changes in light transmission passing through the corneas, and displays a numerical opacity value (arbitrary units).

4.1. Calibration

This operation is performed with no cornea in the Opacitometer (Electro-Design, RIOM, France), but using the calibration devices. The electrical zero (balance between photocells) is adjusted with the "balance" knob, and the apparatus is set to "75" with a standardized opaque sheet of polyester.

4.2. Measurement

The lateral glasses of the holders should be dried. Changes in corneal opacity are determined by comparison with "basal opacity" measured before treatment (t=0 opacity).

Each corneal holder is placed in the experimental (positive) compartment of the apparatus with *no holder* in the control (negative) compartment. Thus, the value obtained (for control or treated corneas) represents the absolute opacity value for a given cornea, but not the difference between a treated and a control cornea, as was determined in previous studies.

5. Permeability

This second step of the assay is performed immediately after the measurement of opacity. The medium is removed from the anterior compartment, and replaced by 1 ml of fluorescein solution (0.4% for liquids and surfactants, 0.5% for solids). Corneas are incubated in a horizontal position for 90 minutes, immersed in a water-bath at 32°C. Medium from the posterior chamber is then removed, and its optical density (O.D.) determined with a spectrophotometer at 490 nm.

6. Data calculation

6.1. Opacity

Opacity values measured at a given time-point (120 minutes in protocol 1, 240 minutes in protocol 2) are *first* corrected (individually for each cornea in the experiment) for basal opacity ($t=0$), i.e. " $t=120 - t=0$ " and " $t=240 - t=0$ ". Then each individual cornea in the experimental groups, including the positive controls, is corrected for the mean value of saline-treated corneas (negative control) at this time-point. The values obtained are therefore the "corrected values" of opacity.

6.2. Permeability

The mean O.D. of saline-treated corneas is calculated, and then the individual value for each experimental cornea is corrected for this mean to give the "corrected value" of permeability.

6.3 In-vitro score

This score is calculated with corrected values of opacity and permeability *for each individual cornea*, using the formula:

$$\text{score} = \text{opacity} + (15 \times \text{O.D.})$$

For a given substance, the final in-vitro score will be the mean \pm SD of three corneas.

7. Quality control

7.1. Basal opacity

Only corneas with a basal opacity of ≤ 3 and ≥ -3 are selected for the experiment.

7.2. Fluorescein solution

Stock fluorescein solutions prepared at 4 mg/ml or 5 mg/ml in DPBS should be diluted to 10 $\mu\text{g/ml}$ in complete MEM (the medium used throughout the experiment to fill the posterior compartment), and O.D. determined before application to corneas. An acceptable range is between 1.610 and 1.910, otherwise the dilution should be performed again, and, if necessary, a new solution prepared. The actual value for each experiment has to be reported on the data sheets.

7.3. Positive controls

A group of three corneas treated with a known reference substance has to be included in each experiment. The substance selected will depend on the broad category of products to be evaluated:

- a) BENZALKONIUM CHLORIDE (=BAK) (Sigma, # B-1383) 5% solution in saline, for surfactants
- b) N,N,-DIMETHYLFORMAMIDE (=DMF) (Aldrich, # 15,481-4), 100%, for liquids.
- c) IMIDAZOLE (=IMDZ) (Aldrich, # I-20-2), 20% in saline, for solids.

The limits (mean of three corneas) for a valid experiment are as follows:

Compound	Opacity	Permeability	Score
Benzalkonium chloride	> 60	> 3.000	> 110
N,N-Dimethylformamide	> 70	> 1.500	> 100
Imidazole	> 35	> 2.000	> 70

8. Data interpretation (optional)

Based on experience at MS&D with reference and in-house compounds, and on data from collaborative studies, the following classification system was established:

In-vitro score:

from	0	to	25	=	mild irritant
from	25.1	to	55	=	moderate irritant
from	55.1	to	80	=	severe irritant
>=	80			=	very severe irritant

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Appendix A2

INVITTOX Protocol 124. Bovine Corneal Opacity and Permeability (BCOP) Assay – SOP of Microbiological Associates, United Kingdom

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BOVINE CORNEAL OPACITY AND PERMEABILITY (BCOP) ASSAY - SOP OF MICROBIOLOGICAL ASSOCIATES LTD., UK

The effects of a test compound on the opacity and permeability of a freshly collected bovine cornea can be used as a measure of eye irritancy potential.

Background

This protocol is based on the SOP developed by Gautheron (*INVITTOX N° 98*), which participated in the EC/HO Validation Study and did not meet the criteria set by the management team of this study for its use as a replacement of the Draize rabbit eye irritation test (Balls *et al.*, 1995). A subsequent study (BCOP assay Prevalidation Process; 1997-1998) has been carried out to overcome the previously encountered shortcomings. The new and optimised protocol version is herewith included. The Microbiological Associates Ltd., in collaboration with other laboratories, has refined and optimised the original protocol developed by Gautheron with the aim to assess the effects of some of the variables in the assay in order to eliminate sources of variation, optimise the methodology and reduce inter and intralaboratory variation.

Experimental Description

Endpoint and

Endpoint Detection : - Corneal opacity measured using an opacitometer.
- Corneal permeability determined using sodium fluorescein and measured spectrophotometrically (increase in OD).

Test System : Freshly isolated bovine cornea (intact, epithelium-removed, Descemet's membrane and endothelium-removed; stroma)

Bovine eyes recovered from a slaughterhouse are inspected and undamaged corneas are dissected and mounted in specially constructed holders.

After a 1 hour incubation in media, the basal opacity of each cornea is recorded using an opacitometer.

Two methodologies have been developed to adapt the protocol to the physico-chemical nature of the test compound. The first method (A) is used to test non-surfactant liquids and surfactants. Liquids are tested neat and surfactants, liquid and solid, are diluted at 10%. Both are applied for 10 minutes.

Before reading the final opacity, the corneas are rinsed and incubated for 2 hours in refilled media to equilibrate.

The second method (B) is used with solids, tested at 20% (w/w) solution or suspension in 0.9% NaCl. After 4 hours incubation, the corneas are rinsed and the final opacity measured.

Then the permeability of each cornea is determined with a fluorescein solution after an incubation of 90 minutes. Method A uses a fluorescein concentration of 4 mg/ml and method B uses 5 mg/ml.

Test Compounds

Ten chemicals were selected for use in Phase III of the BCOP prevalidation process: 3 surfactants (anionic and non-ionic), 1 aromatic amine, 1 alcohol, 1 ester, 1 ether, 1 ketone, 1 inorganic chemical and 1 aldehyde.

Prediction Model

The two endpoints, corneal opacity and permeability, are combined to give a final in vitro score and related to the five categories of irritancy: non irritant, mild, moderate, severe, very severe (see section "Evaluation of Test Results" of the present SOP). These in vitro index scores were then compared with in vivo scores (Modified Maximum Average Scores) obtained in the Draize eye test and assigned to appropriate categories.

Modifications of the Method

With respect to the original protocol developed by Gautheron the protocol refinements, carried out during the recent prevalidation study, refer to reagents and procedure adopted; the way of measuring permeability, calculation of the results, the treatment and dilution of test compounds and the kind of positive controls used.

Status

This protocol has successfully been tested in the "BCOP assay Prevalidation Process (1997-1998)". The participating laboratories concluded that the process was effective in improving the reproducibility of the assay.

The refinements introduced into the protocol contributed to an

improvement in the intralaboratory variability of the assay. However, the assay was found to overestimate the irritancy of two chemicals and to underpredict the irritancy of the others of the 10 chemicals tested.

NOTE: General comments of the BCOP Method Summary apply. It can be obtained from ecvam.sis@jrc.it

Last update: August 1999

Procedure Details, April 1997*

BOVINE CORNEAL OPACITY AND PERMEABILITY (BCOP) ASSAY - SOP OF MICROBIOLOGICAL ASSOCIATES LTD., UK

Note: This protocol presents the standard operating procedure used in the study "BCOP assay prevalidation project" (1997). It should be noted that this protocol might need to be modified in light of experience gained in the study.

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□ The herewith included SOP has been sent to the person responsible for the method to update or confirm it. As soon as new information will become available this version will be updated.

1. Procedure

1.1 SUMMARY

Bovine eyes obtained from the local slaughterhouse are inspected for scratches and defects etc. Undamaged corneas are dissected and mounted in specially constructed holders. After a 1 hour incubation in media, the basal opacity of each cornea is recorded using an opacitometer.

Two methodologies have been developed and are used depending on the physical / chemical nature of the test article. The nature of the test article to be tested will therefore determine the methodology employed.

Method A is used to test non surfactant liquids and surfactants. Liquids are tested neat and surfactants, both liquid and solid, are tested at a 10% dilution and applied to the cornea for 10 minutes. After the 10 minute incubation the corneas are rinsed, the holders refilled with media and the corneas incubated for a further 2 hours in media to equilibrate. The final opacity reading is taken.

Method B is used for the testing of solids which are tested as a 20% slurry for 4 hours. After a 4 hour incubation the corneas are rinsed and the final opacity measurement recorded.

The corneas are then exposed to a fluorescein solution, and the permeability of each cornea determined after an incubation of 90 minutes. Method A uses a fluorescein concentration of 4 mg/ml and Method B uses 5 mg/ml. An aliquot of the media from below the cornea is read in a spectrophotometer to determine the permeability of the cornea to the fluorescein solution. The opacity and permeability values are combined to obtain an in vitro score.

1.2 EQUIPMENT

- Opacitometer (see Appendix A)
- Cornea holders ~25
- Spectrophotometer (see Appendix B)
- Water bath 32°C
- Vacuum pump
- Scalpel
- Scissors
- Forceps
- Electric Screwdriver
- Mortar & Pestle
- Positive displacement pipette
- Micro pipettes
- 5ml Syringes
- 30ml Syringes
- Needles (19G11/21,1 x 40)
- Cuvettes

1.3 MEDIA AND REAGENTS:

Media: Clear media without phenol red is to be used throughout the study

MEM without Phenol Red [Life Technologies; Cat No.51200
]

or

Powdered MEM dissolved in sterile deionised H₂O

[Sigma; Cat No. M-3024]

with added sodium bicarbonate [Sigma; Cat No. S-5761]

L-glutamine [Gibco; Cat No.043-05030]

Foetal Bovine Serum (FBS) [PAA; Cat No.A15-652]

Preparation of complete MEM (cMEM):

To MEM add 1% L-glutamine and 1% FBS (To be freshly prepared at the beginning of each assay)

Hank's Balanced Salt Solution W/O Phenol Red (HBSS)

[Life Technologies; Cat No. 14025-050]

or

Powdered HBSS dissolved in sterile deionised H₂O

[Sigma; Cat No.H-1387]

Penicillin-Streptomycin (10000 IU/ml-10000 IU/ml) solution

[Life technologies; Cat No. 15140-114]

0.9% NaCl Solution [Sigma; Cat No. S-8776]
or
Deionised H₂O plus 0.9% NaCl (0.9g / 100 ml)
[Sigma; Cat No. S 7653]

Preparation of Stock Fluorescein solution; (see Appendix C)
cMEM plus Sodium Fluorescein [Sigma; Cat No. F-6377]

Ethanol [Sigma-Aldrich; Cat No. 27,074-1]

Benzalkonium Chloride [Sigma; Cat No. B1383]

Imidazole [Sigma-Aldrich; Cat No. I,20-2]

All chemicals and solutions to be disposed after 1 year of purchase or preparation unless an expiry date is stipulated on the original packaging.

2. Methodology

2.1 pH

An estimate of pH for each neat (liquid) test article or diluted test article (if diluted/suspended in 0.9% NaCl) will be determined and recorded using universal pH paper.

2.2 BOVINE EYES

Bovine eyes, excised by an abattoir employee, will be collected as soon after slaughter as possible. Care should be taken to avoid damaging the cornea during excision. Excised eyes will be contained and transported to the laboratory in HBSS containing 1% (v/v) Penicillin/Streptomycin Solution (enough to cover all eyes in the receptacle) at room temperature. The eyes will generally be used within 3 hours (± 1 hour) after slaughter.

2.3 PREPARATION OF CORNEAS

All eyes will be carefully examined macroscopically for defects (opacity, scratches, pigmentation, etc) and those exhibiting defects will be discarded. The tissue surrounding the eyeball will be carefully pulled away and the cornea will be dissected such that approximately 2 to 3mm of sclera is present around the cornea. The isolated corneas will be stored in a petri dish containing HBSS plus 1% Penicillin/streptomycin Solution until all corneas are dissected.

The corneas are mounted immediately in the corneal holders with the endothelial side against the O-ring of the posterior half of the holder. The cornea should be gently flattened over the O-ring and holder surface with a wetted, gloved finger to expel any air. The anterior half of the holder will then be positioned on top of the cornea and fixed in place with screws. Both compartments of the corneal holder will be filled with cMEM, using a 30ml syringe. The posterior compartment will always be filled first to return the cornea to its natural concave position. Care should be taken to make sure no air bubbles are present within the holders. The holders will be plugged and incubated for 1 hour \pm 5 min at 32°C \pm 2°C in a water bath.

2.4 TREATMENT GROUPS

Three corneas will be treated with each test article solution/suspension. Three corneas per assay will be treated with the positive control and three corneas with 0.9% NaCl as the negative control group.

One of two treatment methods (Method A or B) will be used depending on the physical nature and chemical characteristics (liquid or surfactant versus non-surfactant solid) of the test article. The controls used will depend on the method being used.

2.5 CONTROLS

Test Article Positive Control

Method A Liquid test articles ethanol

Surfactant test articles benzalkonium chloride (10%)

Method B Solid test articles imidazole (20%)

Negative Control 0.9% saline

2.6 TREATMENT OF CORNEAS

At the end of the one hour incubation period, the medium will be removed from both compartments using a suitable pipette tip or flat ended needle attached to a vacuum pump to ensure complete evacuation, and replaced with fresh cMEM. Again, care should be taken to make sure no air bubbles are present within the holders. The posterior compartment will be plugged and the anterior left unplugged for opacity determination.

2.7 OPACITY MEASUREMENT

The opacitometer will determine the light transmission through the centre of each mounted cornea. A numerical opacity value (arbitrary unit) will be displayed and recorded. The opacitometer will be calibrated

at the start of each experiment in each assay (see Appendix A) and the opacity of each of the corneas will be determined by reading each holder in the right hand chamber of a calibrated opacitometer.

Once the basal opacity of all corneas has been recorded, the mean value of all corneas can be taken and any corneas deviating from this by more than 3 units will be discarded. Sets of three corneas can be selected randomly for treatment with each test article, positive control compound and negative control.

Immediately prior to treatment the medium will be removed from the anterior compartment of the holder using a suitable pipette tip or flat ended needle attached to a vacuum pump, taking extra care to make sure all excess liquid has been removed. This will be replaced with the test article, positive control compound or negative control

2.7.1 Method A:

Non surfactant liquids and the positive control compound (ethanol) will be tested neat (100%). Known surfactants (either solids or liquids) and positive control (Benzalkonium Chloride) will be tested at a 10% (w/w) concentration in 0.9% NaCl.

Seven hundred and fifty μl of a test substance will be introduced into the anterior part of the holder using a suitable micro pipette, or if the test article is viscous, a suitable positive displacement pipette will be used. Control corneas will also be treated with 750 μl of the negative control (0.9% NaCl) and with the positive control.

The anterior compartment will be plugged. The holder will be turned to a horizontal position and slightly rotated to ensure uniform covering of the test substance over the cornea, and will be incubated in a horizontal position at $32\pm 2^{\circ}\text{C}$ for 10 minutes (± 30 seconds) in a water bath.

The test substance will then be removed and the epithelium will be washed at least 3 times (or until the wash medium is clear) with approximately 3 ml of cMEM using a syringe to add media. After each wash the medium will be removed using a pipette tip or flat ended needle attached to a vacuum pump. If the test article proves difficult to remove by this method, the front cover may be removed and the cornea carefully washed using a gentle stream of cMEM from a wash bottle.

The anterior compartment will then be refilled with cMEM using a syringe. Care should be taken to ensure that there are no air bubbles in the compartment. Once all air bubbles have been removed the anterior compartment is re-plugged, the corneas will then be incubated for 2 hours ± 10 minutes at $32\pm 2^{\circ}\text{C}$ in the water bath.

At the completion of the 2 hrs incubation period, the media will be removed from the anterior and the posterior compartments using a pipette tip or flat ended needle attached to a vacuum pump and replaced with fresh cMEM, again making sure no air bubbles are present. The posterior compartment will be re-plugged, and the opacity of each cornea will be recorded. The values obtained at this measurement will be recorded and used in calculating the corneal opacity.

The corneas will be observed for opaque spots or other irregularities and these will be noted on the workbook and raw data forms.

2.7.2 Method B:

Solid materials and the positive control compound (imidazole) will be tested at 20% (w/w) solution or suspension in 0.9% NaCl. Homogeneous preparations can be prepared in a mortar and pestle by grinding the test article with a small amount of 0.9% NaCl and slowly adding the remaining amount.

Seven hundred and fifty μ l of the test substance, negative control (0.9% NaCl) or positive control will be introduced into the anterior part of the holder using a suitable positive displacement pipette. The front cover may be removed to obtain even coverage of viscous solutions or pastes. The holder will be slightly rotated (with the corneas maintained in a horizontal position) to ensure uniform covering of the test substance over the cornea. Both compartments will be plugged and the corneas incubated in a horizontal position at $32\pm 2^{\circ}\text{C}$ for 4 hours \pm 5 minutes in a water bath.

After incubation, the test substance, negative control or positive control compound will be removed and the epithelium washed at least 3 times (or until the cornea is free of particles) with approximately 3 ml of cMEM each time using a syringe to add media and a vacuum to remove it. If the test article proves difficult to remove by this method, the front cover may be removed and the cornea gently washed with cMEM using a wash bottle.

The media in the anterior and the posterior compartments will then be removed and replaced with fresh cMEM, again making sure no air bubbles are present in the holder. The posterior compartment will be plugged and an opacity measurement performed immediately without any further incubation.

The corneas will be observed for opaque spots or other irregularities and these noted on the workbook and raw data forms.

2.8 PERMEABILITY DETERMINATIONS

When carrying out this assay for the first time, a calibration curve for the spectrophotometer to be used must be carried out. (see Appendix B).

Each assay also requires the preparation and reading of two samples of quality control solution (see Appendix C).

2.8.1 Method A:

After the final opacity measurement is performed, the medium will be removed from the anterior compartment using a suitable pipette tip or flat ended needle attached to a vacuum pump. One ml of a 4 mg/ml fluorescein solution (see Appendix C) will be added to the anterior compartment using a micro pipette.

2.8.2 Method B:

After the opacity measurement is performed, the medium will be removed from the anterior compartment using a suitable pipette tip or flat ended needle attached to a vacuum pump and replaced with 1ml of a 5 mg/ml fluorescein solution (see Appendix C).

2.8.3 Method A and B:

After the addition of the fluorescein solution to the anterior side of the holder, the compartment will be plugged and the corneas will be incubated in a horizontal position for 90 minutes \pm 5 minutes at $32\pm 2^{\circ}\text{C}$ in a water bath.

After incubation the medium in the posterior chamber will be mixed by drawing ~2.5ml gently up and down a 5ml syringe with a needle attached 3 times. An aliquot of the mixed medium from the posterior chamber will be removed using the syringe and needle, and transferred to a cuvette with a 1cm path length.

The spectrophotometer will be adjusted to read at OD₄₉₀ and a sample of cMEM read. The spectrophotometer will be blanked on this solution prior to reading the transferred solutions. Any solutions giving an OD₄₉₀ beyond the range of the spectrophotometer (see Appendix B) will be diluted 1:4 in cMEM.

2.9 HOLDER CLEANING

All holders should be stripped at the end of the assay by removing the screws, glass holder rings, glass and the centre O-ring. The separate parts should be washed, and preferably steeped in hot water containing a suitable detergent. Care should be taken to ensure all traces of Na-fluorescein are removed. All parts should then be rinsed in water to remove all detergent and allowed to dry.

3. Criteria for Determination of a Valid Test

The test will be accepted if the positive control causes an *In Vitro* Score that falls within two standard deviations of the current historical mean.

Ethanol: 36.0 to 56.0

Benzalkonium chloride: 98.8 to 209.2

Imidazole: 111.2 to 164.0

4. Evaluation of Test Results

The *In Vitro* Score is generated from the opacity and permeability measurements as described below. A suitable computer spreadsheet can be used to make the following calculations (See Appendix D).

4.1 OPACITY

The change in opacity value of each treated cornea or positive control and negative control corneas will be calculated by subtracting the initial basal opacity from the post treatment opacity reading, for each individual cornea.

The average change in opacity for the negative control corneas will be calculated and this value subtracted from the change in opacity of each treated cornea or positive control to obtain a corrected opacity.

The mean corrected opacity value of each treatment group will be calculated from the individual corrected opacity values of the treated corneas for each treatment condition.

4.2 PERMEABILITY

The corrected OD₄₉₀ value (permeability) of each treated or positive control cornea will be calculated by subtracting the average negative control cornea value from the original permeability value for each

cornea.

The mean corrected permeability values of each treatment group will be calculated from the individual corrected permeability values of the treated corneas for each treatment condition.

4.3 IN VITRO SCORE CALCULATION

The following formula is used to determine the *In Vitro* Score:

In Vitro Score = Corrected Opacity Value + (15 x Corrected OD490 Value)

The In Vitro Score will be calculated for each individual treatment and positive control cornea. The mean In Vitro Score value for each treatment group will be calculated from the individual In Vitro Score values.

4.4 DATA INTERPRETATION

The following classification system was established by Gautheron et al (1992) and refined by Vanparys et al 1994 for materials tested under standard conditions. Results from test situations should be compared to known materials tested under similar conditions.

Proposed Prediction Model

Draize <i>in vivo</i> Score	Draize Irritation Scale	<i>In Vitro</i> Score	Proposed <i>In Vitro</i> Irritation Scale
0 - 0.9	minimal	0 - 3	non eye irritant
1 - 25	minimal/slight	3.1-25	mild eye irritant
26 - 56	moderate	25.1-55	moderate eye irritant
57 - 84	marked	55.1-80	severe eye irritant
85 - 110	extreme	>80.1	very severe eye irritant

5. Regulatory Requirements/Good Laboratory Practice

This assay will be performed in compliance with the provisions of the

Good Laboratory Practice Regulations for Non clinical Laboratory Studies.

Appendix A

Calibration of Opacitometer

An opacitometer (formerly from Electro Design) can be obtained from STAG BIO at the following address:

STAG BIO
Rond Point La Pardieu 6
av. Michel Ange
BP 09F 63063
CLERMONT FD Cedex 01
FRANCE

The opacitometer will be calibrated at the beginning of every experiment on ever test day as follows:

- The unit will be switched on and allowed to warm up for at least 10 minutes prior to calibration.
- With both calibration blocks inserted into the reading chambers, the balance knob will be adjusted to give a reading of zero. Calibrator number 1 will be inserted into the right hand calibration block and a reading taken. Calibrator number 1 should be adjusted to read 75 with the calibration knob on the opacitometer.
- The other two calibrators can be checked in the right hand calibration block and should fall into the range of 145-155 (calibrator 2), 218-232 (calibrator 3).

Once calibrated, the unit should be left on for the duration of the test.

If the opacitometer does not read within these ranges, the unit should be recalibrated by the manufacturer, STAG BIO.

Protocol of BCOP only requires the use of the right hand chamber of the opacitometer for reading the opacity. A calibration block should be left in the left hand reading chamber of the opacitometer for the duration of the assay and the opacity of the treated corneas will be read in the right hand chamber only.

Appendix B

Spectrophotometer linearity

The linearity of the spectrophotometer to be used in these studies and its ability to replicate the readings obtained by other users of the BCOP must be determined. The following process is intended to identify any difference in individual spectrophotometers used in different laboratories.

The optical density (OD) of a series of dilutions of Na-fluorescein (NaF) solutions in cMEM should be recorded.

A (100X) stock solution of Na-fluorescein (NaF) is made by dissolving 0.2g NaF in 100ml cMEM; a second stock solution (1X) is then prepared by diluting 1ml of the first stock (100X) in 100ml of cMEM in a standard flask; a concentration of 20 μ g/ml is achieved.

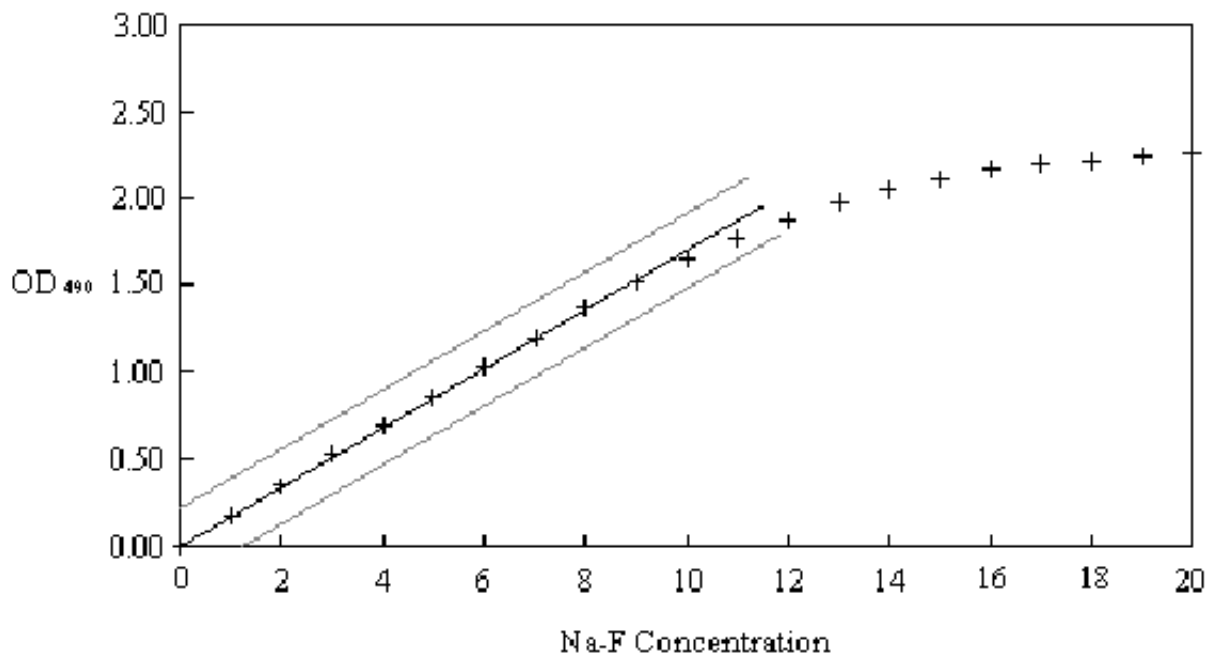
A series of 22 cuvettes will be prepared as described in Table 1. The OD determination is performed at 490 nm and results should closely follow those displayed in Figure 1.

Table 1: Preparation of the Standard Dilution Series of Na-fluorescein (NaF) in cMEM.

Cuvette No.	# μ l cMEM	# μ l stock 1x	Concentration (μ g/ml)
1	0	2,000	20
2	100	1,900	19
3	200	1,800	18
4	300	1,700	17
5	400	1,600	16
6	500	1,500	15
7	600	1,400	14
8	700	1,300	13
9	800	1,200	12
10	900	1,100	11
11	1,000	1,000	10
12	1,100	900	9

13	1,200	800	8
14	1,300	700	7
15	1,400	600	6
16	1,500	500	5
17	1,600	400	4
18	1,700	300	3
19	1,800	200	2
20	1,900	100	1
blank 21&22	2,000	0	0

Figure 1: Example of a Calibration curve of a Spectrophotometer using a serial dilution of Na-F Solution in cMEM



A graph similar to that shown in Figure 1 should be prepared and used to determine the linear range of each spectrophotometer and thus determine the upper limit of absorbance. Solutions recording absorbance above the linear portion should be diluted further.

Figure 1 demonstrates spectrophotometer linearity below an OD490 of 1.80, hence if the OD490 > 1.80, a dilution factor of 1:4 will be required.

Appendix C

Preparation & Quality Control of Na-fluorescein Solution for use in the BCOP Assay

Method A;

Liquid/surfactant test compounds

A stock solution of Na-fluorescein (1g dissolved in cMEM 250ml) is prepared.

This is diluted 1/400 in cMEM in two steps;

Step 1: 950 μ l cMEM + 50 μ l Na-F stock;

Step 2: 50 μ l of Step 1 solution + 950 μ l cMEM dilution is performed.

The same process should be repeated to obtain two separate solutions for testing. The final solution from Step 2 is measured on the spectrophotometer after blanking on 1 ml of cMEM. The two values obtained are averaged and this reading must be between 1.71 and 1.91.

If the final dilution is within the specified range, the stock solution can be aliquoted into suitable vials and stored at $-20^{\circ}\text{C} \pm 5^{\circ}\text{C}$ in the dark until required for use. To improve the consistency between assays, vials can be thawed and diluted for use on the day of assay. Any prepared solution not required should be discarded.

Method B;

Solid test compounds

A stock solution of Na-fluorescein (1.25g dissolved in cMEM 250ml) is prepared.

This is diluted 1/500 in cMEM in two steps.

Step1: 950 μ l cMEM + 50 μ l Na-F stock;

Step2: 40 μ l of Step 1 solution + 960 μ l cMEM dilution is performed.

The same dilution sequence should be repeated to obtain two separate solutions for testing. The final solution from Step 2 is measured on the spectrophotometer after blanking on 1 ml of cMEM. The two values obtained are averaged and this reading must be between 1.71 and 1.91.

If the final dilution is within the specified range, the stock solution can be aliquoted into suitable vials and stored at $-20^{\circ}\text{C} \pm 5^{\circ}\text{C}$ in the dark until required for use. To improve the consistency between assays, vials can be thawed and diluted for use on the day of assay. Any prepared solution not required should be discarded..

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Appendix A3

Table of BCOP Protocols from the Reviewed Literature

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Table of BCOP Protocols from Reviewed Literature

REFERENCE	INVITTOX Protocol #124 (BCOP Prevalidation - SOP of Microbiological Associates Ltd., UK)	INVITTOX Protocol #98 (EC/HO Validation Study; Balls et al. 1995)	Bailey et al. (2004)	Bruner et al. (1998)	Cassidy and Stanton (1997)
TEST METHOD COMPONENT					
Collection of bovine eyes	Eyes excised by an abattoir employee and collected as soon as possible after slaughter	Eyes are excised by an abattoir employee and collected in a plastic jar that holds approximately 25 eyes		Eyes excised by an abattoir employee and collected as soon as possible after slaughter	Bovine eyes obtained from a local abattoir
Transport conditions	Eyes transported to the lab in a container with Hanks Balanced Salt Solution containing 1% (v/v) penicillin/streptomycin solution	Storage jar contains 1 L of Hanks Balanced Salt Solution with Ca ⁺⁺ , Mg ⁺⁺ , supplemented with 0.350 g/L sodium bicarbonate	Transported in a receptacle containing Hank's Balanced Salt Solution with Ca ⁺⁺ and Mg ⁺⁺ , and with 100 IU/mL penicillin and 100 µg/mL streptomycin (HBSS)	Eyes transported to the lab in a container with Hanks Balanced Salt Solution containing 1% (v/v) penicillin/streptomycin solution	Not noted
Temperature	Transported at ambient temperature	Transported at ambient temperature	Transported on ice	Not noted	Not noted
Time after slaughter until use	3 (± 1) hours after slaughter	Within 2 hours after slaughter	Eyes arrive in the laboratory within 4-5 hours of removing first eyes in a batch from cattle	Eyes used within 12 hours after receipt at laboratory	Not noted
Cornea preparation	At lab, eyes carefully examined for defects; unacceptable eyes rejected	At lab, eyes carefully examined for defects; unacceptable eyes rejected	At lab eyes are examined carefully and those with defects such as neovascularization, pigmentation, opacity, or scratches are rejected for testing.	At lab, eyes carefully examined for defects; unacceptable eyes rejected	At lab, eyes carefully examined for defects; unacceptable eyes rejected
Description of cornea dissection	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea with care taken to avoid damage to corneal epithelium and endothelium	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that a rim of sclera surrounds cornea
Storage of isolated corneas until use	Isolated corneas stored in petri dish with HBSS 1% penicillin/streptomycin solution until all dissections completed	Isolated corneas stored in petri dish with HBSS until use	Isolated corneas stored in petri dish with HBSS/penicillin/streptomycin solution until mounted in holders	Rinsed in HBSS	Not described
Type of cornea holder used	Conventional cornea holder for opacitometer with anterior (epithelial side) and posterior (endothelial side) chambers	Conventional cornea holder for opacitometer	Cornea holder for opacitometer with anterior (epithelial side) and posterior (endothelial side) chambers	Stag Bio, Clermont, France	Specially designed holder for the assay with anterior (epithelial side) and posterior (endothelial side) chambers

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TEST METHOD COMPONENT					
Pretreatment incubation/equilibration in corneal holder	After positioning cornea in holder and fixing in place with screws, posterior then anterior compartments of the holder are filled with assay medium. Air bubbles should not be present in the chambers.	After positioning cornea in holder and fixing in place with screws, posterior then anterior compartments of the holder are filled with assay medium.	Holders and medium are prewarmed to 32°C before mounting corneas. Endothelial side of the cornea is placed against O-ring of posterior chamber. Anterior chamber is placed over the cornea and chambers are joined together. Posterior then anterior chambers are filled with assay medium, avoiding formation of air bubbles and minimizing shear forces on the corneal endothelium.	After positioning cornea in holder and fixing in place with screws, posterior then anterior compartments of the holder are filled with assay medium.	Corneas free of defects were mounted in holders. Both posterior and anterior holder compartments were filled with assay medium.
Duration	1 hour (±5min)	1 hour	1 hour	1 hour	1 hour
Temperature	32°C (±2°C)	32°C	32°C (±1°C) maintained in a forced air incubator	32°C (±1°C)	32°C
Medium used for incubation	Freshly prepared complete (c) MEM (MEM + 1% L-glutamine + fetal bovine serum; clear medium without phenol red is to be used)	Eagle's Minimum Essential Medium (MEM) supplemented with 2.2 g/L sodium bicarbonate and 0.292 g/L (2 mM) glutamine (stored refrigerated up to 7 days); 1% fetal bovine serum is added to MEM for experiments (prepared daily); complete (c)MEM is preheated to 32°C for experiments	Eagle's Minimum Essential Medium (MEM) without phenol red containing 1% fetal bovine serum (complete MEM)	Minimum essential medium (MEM) containing 1% fetal bovine serum	Complete minimum essential medium (MEM)
Basal (pretreatment) opacity measurement taken	An initial opacity measurement was made immediately after 1 hour equilibration period and replacement of incubation media with fresh complete MEM	An initial opacity measurement was made immediately after 1 hour equilibration period and replacement of incubation media with fresh complete MEM	After the 1 hour incubation period, the medium is removed from both chambers of each holder (anterior chamber first) and replaced with fresh complete MEM. Then an initial opacity reading is taken and recorded for each cornea.	An initial opacity measurement was made after equilibration period	An initial opacity measurement was made after equilibration period
Instrument used to measure opacity	Opacitometer, which determines light transmission through the center of each mounted cornea	Opacitometer, which determines light transmission through the center of each mounted cornea	Opacitometer (Spectro Designs OP-KIT), which determines light transmission through the center of each mounted cornea	Opacitometer	Spectro-Designs OP-KIT opacitometer
Instrument calibrated prior to test (y/n)	Yes	Not noted	Not noted	Not noted	Not noted
Criteria for acceptable corneas for testing after equilibration period	Basal opacity of all corneas in the test is recorded; mean opacity value is determined; corneas deviating from mean by >3 units are discarded	Basal opacity values should be between 3 and -3	Corneas that display an initial opacity reading greater than 10 units from the average opacity for all of the corneas are not used in the assay	Not noted	Not noted
Treatment groups used (No. of corneas used/test substance)	3 corneas per test article	3 corneas per treatment group	3 to 5 corneas per test article	5 corneas per treatment group (3 for permeability and 2 for histopathology)	5 corneas per treatment group
Controls	3 corneas for each control	3 corneas for each control	2 or 3 corneas	5 corneas for each control (3 for permeability and 2 for histopathology)	2 or 3 corneas used depending on the type of control

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TEST METHOD COMPONENT					
Positive control(s), if used	Varies for test substance. For liquids, the control is ethanol; for surfactants, benzalkonium chloride (10%); for solids, imidazole (20%)	Varies for test substance. For liquids, the control is N,N-dimethylformamide; for surfactants, benzalkonium chloride (5% in saline); for solids, imidazole (20% in saline)	Liquids and surfactants: undiluted ethanol; solid test articles: 20% (w/v) solution of imidazole in complete MEM (without phenol red)	Pre-treatment exposure of 5 corneas to 100% ethanol for 10 minutes; post-treatment exposure of 5 other corneas that went through 24 hour treatment regimen with complete MEM to 100% ethanol for 10 minutes	2 corneas were treated with ethanol
Negative/untreated control	0.9% saline	Saline	Corneas that have opacity values close to the average opacity for all corneas are chosen as the negative (or solvent) control corneas. The negative control is sterile, deionized water.	MEM	3 corneas with opacity readings close to the median opacity for all the corneas were treated with complete MEM
Other controls, if used		Triacetin or PEG-600 when used as the solvent for dilutions	When alternate solvents are used, such as saline or phosphate buffered saline, solvent controls are run through the assay		
Treatment of corneas	Just prior to treatment, the anterior chamber is completely emptied of cMEM using an appropriately sized pipette tip or needle attached to a vacuum pump	Just prior to treatment, the anterior chamber is completely emptied of cMEM using an appropriately sized pipette tip or needle attached to a vacuum pump		Corneas receive four consecutive 6 hour exposures to test article over 24 hours. Just prior to first treatment, the anterior chamber is emptied.	Just prior to treatment, the anterior chamber is completely emptied of complete MEM
<i>Liquid substances</i>	Test substances are added to anterior chamber of holder, which is turned to a horizontal position and rocked gently to ensure complete coverage of cornea	Test substances are prewarmed at 32°C for a few minutes then added to anterior chamber of holder	Nonviscous and semiviscous liquids tested using "closed chamber method". Semiviscous and viscous liquids tested using "open chamber method".	Cosmetic formulations are tested by addition to the anterior chamber of the cornea holder	Liquid silicone polymers were tested by addition to the anterior chamber of the cornea holder
Concentration tested	100% (neat)	Usually 100% (neat); if dilutions are required, saline is used for water soluble substances and PEG-600 or triacetin are used for water insoluble substances	Generally tested at 100% (neat); dilutions performed as needed or requested	100% (neat)	100%
Amount tested	750 µL (test substances and controls)	750 µL (test substances and controls)	750 µL (test substances and controls)	750 µL (test substances and controls)	750 µL (test substances and controls)
Incubation time	10 minutes (±30 seconds)	10 minutes	Standard exposure time is 10 minutes; shorter or longer exposure times are also used	6 hours x 4 exposure periods for a total of 24 hours	10 minutes
Incubation temperature	32°C (±2°C) water bath	32°C water bath	32°C (±1°C) for exposure times > 3 minutes; ≤3 minutes incubated at room temperature	32°C (±1°C) water bath	32°C incubator

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TEST METHOD COMPONENT					
Rinsing procedure	Epithelium is washed 3 or more times with 3 mL of cMEM from a syringe or until the wash medium is clear	Epithelium is washed 3 or more times with 4 mL of cMEM from a syringe or until the wash medium is clear	Epithelium is washed 3 or more times with 2-3 mL of cMEM (with phenol red) from a syringe. Once the rinsing medium is clear, one last rinse of the epithelium is performed using fresh complete MEM (without phenol red).	At the end of each 6 hour incubation, the test article was washed from the cornea with MEM, fresh MEM was added to both chambers, and opacity was measured. Fresh test article was added to the front chamber after the first three exposure periods.	Epithelium is washed 3 or more times with complete MEM until test material is completely removed. The anterior compartment was refilled with complete MEM and relative opacity determined.
Post-treatment incubation (time, temp.)	cMEM is added to anterior chamber of holder and corneas are incubated for 2 hours (± 10 minutes) in a 32°C ($\pm 2^\circ\text{C}$) water bath; fresh cMEM is added to both chambers and final opacity measurement is taken	cMEM is added to anterior chamber of holder and corneas are incubated for 2 hours in a 32°C water bath; fresh cMEM is added to both chambers and final opacity measurement is taken	The anterior chamber is refilled with fresh complete MEM. A post-treatment opacity reading is taken and recorded for each cornea. Visual observations are performed for each cornea. Holders are incubated in a vertical position at 32°C ($\pm 1^\circ\text{C}$) for up to 3 hours. For test articles with exposure times >10 minutes, the exposure time is subtracted from the 2-hour post-exposure incubation period. Other post-exposure incubation times may be used. If corneas are incubated for >4 hours, the incubation medium is supplemented with antibiotics, and changed every 6 hours.	Not performed	Corneas returned to incubator for approximately 2 hours, after which a second measure of relative opacity was taken (report does not state that fresh MEM is added before final opacity measurements)
<i>Surfactants</i>		Test substances are prewarmed at 32°C for a few minutes then added to anterior chamber of holder		Not applicable	Not applicable
Concentration tested	10% (w/w) in 0.9% saline	10% in saline; other concentrations (in saline) can be tested as required			
Amount tested	750 μL (test substance and controls)	750 μL (test substance and controls)			
Incubation time	10 minutes (± 30 seconds)	10 minutes			
Incubation temperature	32°C ($\pm 2^\circ\text{C}$) water bath	32°C water bath			
Rinsing procedure	Epithelium is washed 3 or more times with 3 mL of cMEM each time from a syringe or until the wash medium is clear	Epithelium is washed 3 or more times with 4 mL of cMEM from a syringe or until the wash medium is clear			
Post-treatment incubation (time, temp.)	cMEM is added to anterior chamber of holder and corneas are incubated for 2 hours (± 10 minutes) in a 32°C ($\pm 2^\circ\text{C}$) water bath; fresh cMEM is added to both chambers and final opacity measurement is taken	cMEM is added to anterior chamber of holder and corneas are incubated for 2 hours in a 32°C water bath; fresh cMEM is added to both chambers and final opacity measurement is taken			
<i>Solid substances</i>		Test substances are prewarmed at 32°C for a few minutes then added to anterior chamber of holder		Not applicable	Not applicable

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TEST METHOD COMPONENT					
Concentration tested	20% (w/w) solution or suspension in 0.9% NaCl	20% solution or suspension in saline (usually 1g test substance + 5 mL saline)	20% (w/w) solution or suspension in sterile deionized water, complete MEM, or saline (or other appropriate solvent)		
Amount tested	750 µL (test substance and controls)	750 µL (test substance and controls)	750 µL (test substance and controls)		
Incubation time	4 hours (±5 minutes)	4 hours	4 hours (±5 minutes)		
Incubation temperature	32°C (±2°C) water bath	32°C water bath (holders completely immersed)	32°C (±2°C) water bath		
Rinsing procedure	Epithelium is washed 3 or more times with 3 mL of cMEM each time from a syringe or until all particles are removed; fresh cMEM is added to both chambers and final opacity measurement is taken	Epithelium is washed 3 or more times with cMEM until all particles are removed; fresh cMEM is added to both chambers and final opacity measurement is taken	Epithelium is washed 3 or more times with 3 mL of cMEM each time from a syringe or until all particles are removed; fresh cMEM is added to both chambers and final opacity measurement is taken		
Post-treatment incubation (time, temp.)	Not performed	Not performed			
Endpoints assessed					
<i>Corneal opacity</i>					
Data collected for opacity	Numerical opacity value (arbitrary unit) displayed by opacitometer; opaque spots or other irregularities are noted	Numerical opacity value (arbitrary unit) displayed by opacitometer	Numerical opacity value (arbitrary unit) displayed by opacitometer	Opacity measurements were recorded directly from the output display of the opacitometer; each opacity measurement was made relative to an air blank	Opacity value not described, but likely a numerical opacity value with an arbitrary unit displayed by opacitometer
<i>Permeability</i>					
Amount and concentration of sodium fluorescein solution used	Medium is removed from the anterior chamber, which is refilled with sodium fluorescein solution; amount of dye that reaches posterior chamber is evaluated as an indicator of increased permeability or damage to the cornea	Medium is removed from the anterior chamber, which is refilled with sodium fluorescein solution; amount of dye that reaches posterior chamber is evaluated as an indicator of increased permeability or damage to the cornea	Medium is removed from the anterior chamber, which is refilled with sodium fluorescein solution; amount of dye that reaches posterior chamber is evaluated as an indicator of increased permeability or damage to the cornea	3 of the 5 treated corneas are used for permeability measurements. After the final 24 hour opacity reading, MEM was removed from the front chamber.	After the final opacity reading, medium was removed from both chambers of the holder. The posterior chamber was refilled with complete MEM.
Amount and concentration of sodium fluorescein solution used	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	1 mL of a 4 mg/mL fluorescein solution was added to the anterior chamber	1 mL of a 4 mg/mL fluorescein solution was added to the anterior chamber
Incubation time for fluorescein solution	90 minutes ±5 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes ±5 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally
Incubation temperature for fluorescein	32°C (±2°C) water bath	32°C water bath (holders completely immersed)	32°C (±1°C)	32°C (±1°C) water bath	32°C
Instrumentation used	Spectrophotometer set at 490 nm; cuvette with a 1 cm path length is used	Spectrophotometer set at 490 nm	Microplate reader	Beckman DU-640 spectrophotometer which is zeroed with a sample of MEM	Spectrophotometer set at 490 nm
Instrument calibrated (y/n)	Yes	Not noted	Yes	Not noted	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	INVITTOX Protocol #124 (BCOP Prevalidation - SOP of Microbiological Associates Ltd., UK)	INVITTOX Protocol #98 (EC/HO Validation Study; Balls et al. 1995)	Bailey et al. (2004)	Bruner et al. (1998)	Cassidy and Stanton (1997)
TEST METHOD COMPONENT					
Data collected for permeability	Optical density reading at 490 nm	Optical density reading at 490 nm	Optical density reading at 490 nm	Optical density reading at 490 nm	Optical density reading at 490 nm
Aliquot taken from posterior chamber for OD 490 nm reading	1 mL	Not noted	Most of medium is removed from posterior chamber, then mixed in a sample tube. A 360 µL aliquot is taken from the sample tube and transferred to a 96-well plate. Standard plate map provides 2 wells for each cornea in case a dilution is required.	1 mL	Not noted
Other observations			During the final, post-treatment opacity reading, visual observations are performed for each cornea and, if necessary, are recorded. Special attention is taken to observe dissimilar opacity patterns, tissue peeling, or residual test article.	Histopathological examination of 2 corneas per treatment and control groups	Histological examination of all corneas
Evaluation of test results					
<i>Corneal opacity</i>					
Basal (pretreatment) opacity subtracted from opacity of each treated cornea?	Yes	Yes	Yes	Yes	Opacity changes for each cornea were calculated by subtracting the initial opacity value from the final opacity value
Opacity for each treated cornea corrected for average value of negative/solvent controls?	Yes	Yes	Yes	Yes	Yes
Mean corrected opacity value calculated for each treatment group?	Yes	No	Yes		Yes
<i>Permeability</i>					
OD value for each treated cornea corrected for average value of negative/solvent controls?	Yes	Yes	Yes	Yes	Yes
Mean corrected permeability value calculated for each treatment group?	Yes	No	Yes		Yes

Table of BCOP Protocols from Reviewed Literature

REFERENCE	INVITTOX Protocol #124 (BCOP Prevalidation - SOP of Microbiological Associates Ltd., UK)	INVITTOX Protocol #98 (EC/HO Validation Study; Balls et al. 1995)	Bailey et al. (2004)	Bruner et al. (1998)	Cassidy and Stanton (1997)
TEST METHOD COMPONENT					
Formula used to calculate <i>In Vitro</i> Score	<i>In vitro</i> score = corrected opacity value + (15 x corrected OD ₄₉₀ value); the <i>in vitro</i> score is calculated for each cornea and the mean <i>in vitro</i> score is calculated from the individual <i>in vitro</i> score values	<i>In vitro</i> score = corrected opacity value + (15 x corrected OD ₄₉₀ value); the <i>in vitro</i> score is calculated for each cornea and the mean <i>in vitro</i> score is calculated from the individual <i>in vitro</i> score values	<i>In vitro</i> score = mean corrected opacity value + (15 x mean corrected OD ₄₉₀ value)	<i>In vitro</i> score calculated only for ethanol controls = corrected opacity value + (15 x corrected OD ₄₉₀ value)	<i>In vitro</i> score = mean opacity value + (15 x mean OD ₄₉₀ value)
<i>In vitro</i> classification of ocular irritancy	BCOP score 0 -3 = nonirritant; 3.1 - 25 = mild eye irritant; 25.1 - 55 moderate; 55.1 - 80 = severe; > 80.1 = very severe	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate; 55.1 - 80 = severe; > 80 = very severe	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate irritant; 55.1 and above = severe irritant.	Not discussed	BCOP score 0 - 25 = nonirritating to mild eye irritant; 25.1 - 55 moderate; ≥ 55.1 = severe
Criteria for an acceptable test	Test is accepted if positive control gives an <i>in vitro</i> score that falls within 2 SDs of the current historical mean: ethanol (36.0 - 56.0); benzalkonium chloride (98.8 - 209.2); imidazole (111.2 - 164.0)	Test is accepted if positive control values fall within following limits: benzalkonium chloride (opacity > 60, permeability >3,000, score > 110); N,N-dimethylformamide (opacity >70, permeability > 1,500, score > 100); imidazole (opacity >35, permeability > 2,000, score > 70)	Test is accepted if positive control gives an <i>in vitro</i> score that falls within 2 SDs of the current historical mean, which is updated every 3 months.	The acceptable range for the <i>in vitro</i> score for the ethanol positive control was 22.1 to 44.7 (historical mean ±SD)	The acceptable range for the <i>in vitro</i> score for the ethanol positive control was 33.7 to 69.6 (historical mean ± 2SD)
Conducted in compliance with GLPs	Yes	Not noted	Yes	Not noted	Not noted
Other useful information				Dose-response curves were presented in the publication for the formulations tested showing changes in opacity over 24 hours. Photomicrographs of some histological data also are presented.	Photomicrographs of some histological data are presented in the publication.

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Casterton et al. (1996)	Cerven and Moreno (1998)	Chamberlain et al. (1997) -- IRAG Evaluation (8 data sets)	Cooper et al. (2001)	Gautheron et al. (1994) (fresh and preserved corneas)
TEST METHOD COMPONENT					
Collection of bovine eyes	Bovine eyes are collected and stored in a plastic cooler containing Hanks' Balanced Salt Solution with Ca ⁺⁺ and Mg ⁺⁺	Bovine eyes were received from a local supplier	Bovine eyes were collected from a local slaughterhouse	Bovine eyes were obtained from a local abattoir where the eyes were excised	Bovine eyes were collected from a commercial abattoir in a plastic jar for about 25 eyes
Transport conditions	Not described	Eyes were transported to the laboratory in Hanks Balanced Salt Solution in a refrigerated container.	Eyes were immersed in pH-adjusted (7.2-7.4) Hanks salt solution within 2 hours after the animals were killed	Eyes transported in a container with Hanks balanced salt solution supplemented with penicillin/streptomycin	1 L of Hanks balanced salt solution (HBSS) with Ca ⁺⁺ and Mg ⁺⁺
Temperature	Ambient temperature	Not noted	Not noted	Transported to laboratory over ice packs	Ambient temperature
Time after slaughter until use	Immediately after receipt and no more than 3 hours after removal from carcass	Eyes were examined within 1 hour after receipt	Not noted	Not noted	Eyes were used within 2 hours of killing the animals
Cornea preparation	At lab, eyes carefully examined for defects; unacceptable eyes rejected	At lab, eyes carefully examined for defects; unacceptable eyes rejected	At lab, eyes carefully examined for defects; unacceptable eyes rejected	Corneas were grossly examined for damage and those exhibiting defects were discarded	At lab, eyes carefully examined for defects; unacceptable eyes rejected
Description of cornea dissection	Cornea dissected such that approximately 1 - 2 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea; iris and lens were removed	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea
Storage of isolated corneas until use	Isolated corneas stored in petri dish with Eagle's Minimum Essential Medium (MEM) until use	Not noted	Not noted	Isolated corneas stored in petri dish with HBSS until they were mounted in a corneal holder	<i>Fresh corneas</i> : isolated corneas stored in petri dish with HBSS until they were used. <i>Preserved corneas</i> : corneas were washed 3x, each for 15 minutes, in HBSS supplemented with antibiotics (penicillin/streptomycin); after rinsing in normal HBSS, they were placed individually into wells of 6-well culture plates, each containing 12 mL preservative medium; plates were then placed in the refrigerator at 4-5°C until the next day; for use, the preserved corneas were removed from the refrigerator, left on the bench for 30 minutes at room temperature, and thereafter treated the same way as fresh corneas
Type of cornea holder used	Cornea holder with anterior and posterior chambers, and custom-fitted rack for spectrophotometer	Specially designed holders segmented into anterior and posterior chambers	Specially made holder with two 5 mL chambers that interface with the epithelial and endothelial surfaces of the cornea	Not noted	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Casterton et al. (1996)	Cerven and Moreno (1998)	Chamberlain et al. (1997) -- IRAG Evaluation (8 data sets)	Cooper et al. (2001)	Gautheron et al. (1994) (fresh and preserved corneas)
TEST METHOD COMPONENT					
Pretreatment incubation/equilibration in corneal holder	After positioning cornea in holder and fixing in place with screws, posterior then anterior compartments of the holder are filled with warmed MEM.	After positioning cornea in holder and fixing in place with screws, posterior then anterior compartments of the holder are filled with assay medium. Cornea was inspected afterwards to ensure it was still intact.	After mounting cornea in holder, both chambers were filled with medium.	Each cornea was mounted in a holder with the endothelial side against the O-ring of the posterior half of the holder; the anterior half of the holder was then positioned on top of the cornea and screws were tightened; posterior then anterior chambers were filled with medium	Corneas were mounted in holders, which were subsequently filled with medium
Duration	1 hour	At least 1 hour, but not longer than 2 hours	1 hour	1 hour	1 hour
Temperature	32°C water bath	32°C water bath	32°C water bath	32°C (±1°C)	32°C (±1°C)
Medium used for incubation	Eagle's MEM supplemented with sodium bicarbonate, L-glutamine, and fetal bovine serum; continually warmed at 32°C during use; free of phenol red	Minimal essential media supplemented with 1% fetal bovine serum (MEM).	Eagle's minimal essential medium (MEM) supplemented with 1% fetal bovine serum	Eagle's minimum essential medium (MEM) without phenol red, with 1% fetal bovine serum (complete MEM)	Minimum essential medium (MEM) supplemented with glutamine and sodium bicarbonate as indicated by the supplier; the pH was adjusted to 7.4 and the medium was freshly used or stored refrigerated (1 week stock); in daily experiments it was supplemented with 1% fetal bovine serum and used prewarmed at 32°C
Basal (pretreatment) opacity measurement taken	For initial absorbance readings, each cornea is read against a blank in the reference beam	An initial opacity measurement was made immediately after equilibration period and replacement of incubation media with fresh MEM	The report states that the first opacity measurement was taken after the cornea was exposed to test substance	An initial opacity measurement was made immediately after 1 hour equilibration period and replacement of incubation media with fresh complete MEM	Not noted
Instrument used to measure opacity	Cary 219 UV-VIS spectrophotometer set at 570 nm	OP-KIT opacimeter produced by Electro-Design Corp. of Riom, France	Specially-designed opacimeter to determine the difference in light transmission between treated and control corneas	Spectro Designs OP-KIT opacimeter (Stag Bio, Clermont, Ferrand, France)	Opacimeter (Electro-Design, Riom, France), which determines the difference in light transmission between a treated and a control cornea
Instrument calibrated prior to test (y/n)	Calibration not described; instrument is balanced on two blank holders (filled only with MEM)	Not noted	Not noted	Not noted	The instrument was previously calibrated with standardized opaque sheets of polyester
Criteria for acceptable corneas for testing after equilibration period	Corneas with absorbance values > 0.1 are removed from the study	Not noted	Not noted	Not noted	Not noted
Treatment groups used (No. of corneas used/test substance)	At least 4 corneas per test material	Five corneas	3 to 6 corneas for each treatment group	5 corneas per formulation tested	6 corneas per test substance
Controls	3 corneas	2 corneas (at each opacity reading, each treated cornea was scored in comparison with the 2 control corneas)	3 to 6 corneas for each control	3 corneas for negative control and 5 corneas for positive control	3 corneas

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TEST METHOD COMPONENT					
Positive control(s), if used	Not described		3 labs reported use of acetone as a positive control for liquids; one lab reported use of imidazole as a positive control for solids	Ethanol	Not noted
Negative/untreated control	3 corneas with the lowest absorbance values are selected as controls		Not described	3 corneas with opacity readings close to the median opacity for all the corneas were treated with complete MEM	3 corneas treated with MEM
Other controls, if used					
Treatment of corneas	The anterior chamber is aspirated of MEM	Just prior to treatment, the anterior chamber is completely emptied of MEM.			The medium was removed from both chambers of the holders using a needle attached to a vacuum pump or a syringe. The posterior chamber was refilled with fresh MEM
<i>Liquid substances</i>	Prewarmed (32°C) test material is added to anterior chamber; corneas incubated in a horizontal position to completely bath the corneal surface with test material	Test substances are added to anterior chamber of holder, which is turned to a horizontal position	Test substances are added to anterior chamber of holder, which is turned to a horizontal position	Shampoo formulations were tested	Test substances are added to anterior chamber of holder, which is turned to a horizontal position
Concentration tested	100%	100%	100%	100% and 10% (w/v) prepared in complete MEM	100%
Amount tested	1.00 mL	750 µL (test substances)	500 µL (test substances)	750 µL (test substances and controls)	750 µL (test substances and controls)
Incubation time	10 minutes	10 minutes (± 1 minute)	10 minutes (3 labs), 30 minutes (3 labs), or 60 minutes (1 lab); 1 lab used both 10 and 30 minute exposures; 1 lab did not report an exposure time	For most materials, incubation time was 10 minutes for undiluted materials and 60 minutes for 10% dilutions; in a separate study, 2 materials were tested undiluted for 10, 30, and 60 minutes AND as 10% dilutions for 10, 30, 60 and 120 minutes.	10 minutes
Incubation temperature	Room temperature	32°C water bath	32°C	32°C (±1°C) water bath	32°C

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REFERENCE	Casterton et al. (1996)	Cerven and Moreno (1998)	Chamberlain et al. (1997) -- IRAG Evaluation (8 data sets)	Cooper et al. (2001)	Gautheron et al. (1994) (fresh and preserved corneas)
TEST METHOD COMPONENT					
Rinsing procedure	Epithelium is washed 3 or more times with HBSS until the wash medium is clear. After last rinse, both chambers are aspirated and filled with fresh MEM.	Test substance removed from chamber by washing with MEM. Both chambers then refilled with fresh MEM. NOTE: For test materials containing alcohol, an additional opacity measurement was taken following the 10 minute exposure time and addition of fresh medium to both chambers	At the end of the exposure, the epithelial side was washed, the anterior compartment was refilled with MEM + 1% fetal bovine serum and a first opacity measurement taken	Epithelium is washed 3 or more times with complete MEM containing phenol red to ensure complete removal of test material; corneas given a final rinse with complete MEM without phenol red; anterior chamber was refilled with complete MEM and opacity determined	Epithelium is washed 3 or more times with 4 mL of MEM until the wash medium is clear. Anterior chamber was refilled with medium, and first opacity measurement taken.
Post-treatment incubation (time, temp.)	Corneas are incubated for 2 more hours in a 32°C water bath	Corneas are incubated for 2 hours in a 32°C water bath; the MEM was changed and opacity measured, comparing each of the 5 treated corneas to the 2 control corneas	Corneas are incubated for 2 more hours in a 32°C water bath, followed by a second opacity reading, which was the reported value	Corneas are incubated in a 32±1°C water bath until total incubation time reaches 120 minutes. Post-treatment incubation varies depending on initial exposure time from 110 minutes to 90 minutes to 60 minutes or no further incubation. A second opacity reading was taken for all corneas except for those with a 120 minute exposure time.	After treatment, corneas were incubated for 2 hours at 32°C; a second opacity measurement was taken, which was used for calculations
Surfactants	Not described	Not applicable	Although surfactants were tested by some labs, a specific protocol for surfactants was not included in report	Not tested	
Concentration tested					10% in MEM
Amount tested					750 µL (test substance and controls)
Incubation time					10 minutes
Incubation temperature					32°C
Rinsing procedure					Epithelium is washed 3 or more times with 4 mL of MEM until the wash medium is clear. Anterior chamber was refilled with medium, and first opacity measurement taken.
Post-treatment incubation (time, temp.)					After treatment, corneas were incubated for 2 hours at 32°C; a second opacity measurement was taken, which was used for calculations
Solid substances	Solids are applied directly to the corneal surface. The glass window of the anterior chamber of the corneal holder is removed to facilitate application of solids.			Not tested	

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Casterton et al. (1996)	Cerven and Moreno (1998)	Chamberlain et al. (1997) -- IRAG Evaluation (8 data sets)	Cooper et al. (2001)	Gautheron et al. (1994) (fresh and preserved corneas)
TEST METHOD COMPONENT					
Concentration tested	100%	Solids dissolved in MEM at a 20% dilution	20% (200 mg/mL) in MEM + 1% fetal bovine serum; many compounds were tested as suspensions		Approximate 20% solution or suspension (200 mg + 1 mL) in MEM
Amount tested	Enough to cover the corneal thoroughly (about 1/8 teaspoon)	750 µL (test substance)	500 µL (test substance)		750 µL (test substance and controls)
Incubation time	1 hour		4 hours		4 hours
Incubation temperature	32°C water bath	32°C water bath	room temperature		32°C
Rinsing procedure	Epithelium is washed 3 or more times with HBSS until the wash medium is clear. After last rinse, both chambers are aspirated and filled with fresh MEM.	Test substance removed from chamber by washing with MEM. Both chambers then refilled with fresh MEM. Opacity was measured, comparing each of the 5 treated corneas to the 2 control corneas.	The epithelial side was washed, fresh medium was added, and opacity was measured		Epithelium is washed 3 or more times with 3 mL of cMEM each time from a syringe or until all particles are removed; fresh cMEM is added to both chambers and opacity measurement is taken
Post-treatment incubation (time, temp.)	1 hour	Not performed	Not performed		Not performed
Endpoints assessed					
<i>Corneal opacity</i>					
Data collected for opacity	UV-VIS spectrophotometer absorbance readings at 570 nm	A pre-exposure determination of opacity was made for each control by measuring each against the blanks supplied with the opacitometer; a pre-exposure determination of opacity was made for each of the test corneas by measuring against each control cornea	Not described	The opacity values obtained at the second opacity measurement (except for the 120 minute exposure group) were used to calculate the corneal opacity	Numerical opacity value (arbitrary unit) displayed by opacitometer
<i>Permeability</i>	After the final absorbance readings, both chambers are aspirated and the posterior side is filled with fresh MEM.	Immediately following the 2 hour opacity measurement, the MEM was changed in the posterior chamber of both the control and test corneas.	Fresh medium is added to the posterior compartment	After the final opacity measurement, the medium was removed from both chambers of the holder. The posterior chamber was refilled with fresh complete MEM.	After the final opacity measurement, the medium was removed from both chambers of the holder. The posterior chamber was refilled with fresh MEM.
Amount and concentration of sodium fluorescein solution used	1 mL of fluorescein solution (0.4% in Dulbecco's phosphate buffered saline) was added to the anterior chamber	1.0 mL of 0.4% sodium fluorescein solution	1 mL of a 5 mg/mL solution of sodium fluorescein in Dulbecco's phosphate buffered saline was added to the anterior compartment	1 mL of a 4 mg/mL fluorescein solution was added to the anterior chamber	1 mL of a 0.4% fluorescein solution is used for liquids and surfactants; 1 mL of a 0.5% fluorescein solution is used for solids
Incubation time for fluorescein solution	90 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally
Incubation temperature for fluorescein	32°C water bath	32°C water bath	Not specified	32±1°C water bath	32°C
Instrumentation used	Dynatech MR5000 microplate reader	Spectronic 20 spectrophotometer	Spectrophotometer	Molecular Devices Vmax kinetic microplate reader (Molecular Devices Corp., Menlo Park, CA, USA)	Spectrophotometer set at 490 nm
Instrument calibrated (y/n)	Not described	Not described	Not described	Not described	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Casterton et al. (1996)	Cerven and Moreno (1998)	Chamberlain et al. (1997) -- IRAG Evaluation (8 data sets)	Cooper et al. (2001)	Gautheron et al. (1994) (fresh and preserved corneas)
TEST METHOD COMPONENT					
Data collected for permeability	Optical density reading at 490 nm	Optical density reading at 450 nm	Optical density reading at 490 nm	Optical density reading at 490 nm	Optical density reading at 490 nm
Aliquot taken from posterior chamber for OD 490 nm reading	100 µL	Not described	Not specified	360 µL added to designated well of a 96-well plate	Not noted
Other observations					
				Corneal swelling (wet weight of 8 mm tissue punch) and histology	
Evaluation of test results					
<i>Corneal opacity</i>					
Basal (pretreatment) opacity subtracted from opacity of each treated cornea?	Pretreatment absorbance values for each treated cornea are subtracted from the corresponding 2 hour post-treatment absorbance values	A pre-exposure determination of opacity was made for each control by measuring each against the blanks supplied with the opacitometer; a pre-exposure determination of opacity was made for each of the test corneas by measuring against each control cornea	Not described	Yes	Basal opacity not performed
Opacity for each treated cornea corrected for average value of negative/solvent controls?	The absorbance for each treated cornea is corrected by the mean absorbance value for the three control corneas	The corrected mean opacity score was calculated, using the control and treated cornea opacity values as determined from the OP-KIT opacitometer	The difference in light transmission between treated and control corneas was determined with the opacitometer	The corrected opacity value of each cornea was calculated by subtracting the average change in opacity of the negative control corneas from that of each treated cornea	The difference in light transmission between treated and control corneas was determined with the opacitometer
Mean corrected opacity value calculated for each treatment group?	No	The corrected mean opacity score was calculated, using the control and treated cornea opacity values as determined from the OP-KIT opacitometer	The mean value of opacity ± SD was calculated for each substance	The mean opacity value of each treatment group was calculated by averaging the mean corrected opacity values of the treated corneas for each treatment group	For each substance evaluated, the mean value of opacity ± SD was calculated
<i>Permeability</i>					
OD value for each treated cornea corrected for average value of negative/solvent controls?	The instrument setup allows calculations to take into account both the blank and the control values; therefore, the resulting readings require no further correction	The corrected mean OD 450 nm score was calculated using the control and treated OD values	The amount of dye penetration through the control corneas was subtracted from the amount of dye penetration through treated corneas	The corrected OD ₄₉₀ was calculated by subtracting the mean OD ₄₉₀ value of the negative control corneas from the OD ₄₉₀ of each treated cornea	Not noted
Mean corrected permeability value calculated for each treatment group?	Instrument setup takes into account number of replicates per test material; the obtained value represents the mean corrected optical permeability that results from exposure of the corneal surface to a test material	The corrected mean OD 450 nm score was calculated using the control and treated OD values	The mean absorbance value ± SD was calculated for each substance	The mean OD ₄₉₀ value of each treatment group was calculated by averaging the corrected OD ₄₉₀ values of the treated corneas	The mean OD ₄₉₀ value of each treatment group was calculated by averaging the OD ₄₉₀ values of the treated corneas

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Casterton et al. (1996)	Cerven and Moreno (1998)	Chamberlain et al. (1997) -- IRAG Evaluation (8 data sets)	Cooper et al. (2001)	Gautheron et al. (1994) (fresh and preserved corneas)
TEST METHOD COMPONENT					
Formula used to calculate <i>In Vitro</i> Score	The two endpoints, opacity and permeability, are evaluated separately.	<i>In vitro</i> score = corrected mean opacity value + (15 x mean corrected OD ₄₅₀ value)	For some submissions, <i>in vitro</i> score = opacity value + (15 x OD ₄₉₀ value). In other submissions, the opacity and permeability values are considered separately, with the irritancy classification based on the greater of the two values.	<i>In vitro</i> score = mean opacity value + (15 x mean OD ₄₉₀ value)	<i>In vitro</i> score = mean opacity value + (15 x mean OD ₄₉₀ value)
<i>In vitro</i> classification of ocular irritancy	The irritation class is based on the endpoint that equates to the greater irritation potential: mild (opacity <0.400 or permeability <0.175); moderate (0.400 ≤ opacity < 1.300 or 0.175 ≤ permeability < 0.600); severe (opacity >1.300 or permeability >0.600)	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate; 55.1 and greater = severe	Not noted	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate; 55.1 and greater = severe (applied to both undiluted and diluted test materials)	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate; 55.1 and greater = severe
Criteria for an acceptable test	Not noted	Not noted	Not noted	Not described	Not noted
Conducted in compliance with GLPs	Not noted	Not noted	Not noted	Not described	Not noted
Other useful information			A generalized BCOP protocol was provided in the IRAG report for the eight BCOP data sets evaluated by the IRAG working group. Although some protocol differences were noted between the testing laboratories (e.g., exposure time and data analysis), some generalizations do not reflect a majority of other published protocols (e.g., amount of substance tested, use of assay medium, measuring basal corneal opacity prior to exposure period). Note that the generalized protocol description was not very detailed, and that individual protocols for each of the 8 data sets were not provided.		

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Collection of bovine eyes		Bovine eyes were obtained from a local abattoir where the eyes were excised	Bovine eyes were collected in a plastic container	Bovine eyes obtained from a local abattoir	Eyes collected from a local slaughterhouse
Transport conditions	Transported in a receptacle containing Hank's Balanced Salt Solution with Ca ⁺⁺ and Mg ⁺⁺ , and with 100 IU/mL penicillin and 100 µg/mL streptomycin (HBSS)	Eyes transported in a container with Hanks balanced salt solution supplemented with penicillin/streptomycin	Eyes transported in Hanks balanced salt solution	Eyes transported to the laboratory in a saline solution (Hanks)	Eyes transported to the laboratory immersed in pH-adjusted (7.2 - 7.4) Hanks salt solution
Temperature	Transported on ice	Transported to laboratory over ice packs	Room temperature	Not noted	Not noted
Time after slaughter until use	Eyes arrive in the laboratory within 4-5 hours of removing first eyes in a batch from cattle	Not noted	Collection of eyes and transportation to testing laboratory was completed within 2 hours	Not noted	Eyes were collected and transported to the laboratory within 2 hours of killing the animals
Cornea preparation	At lab eyes are examined carefully and those with defects such as neovascularization, pigmentation, opacity, or scratches are rejected for testing.	Corneas were grossly examined for damage and those exhibiting defects were discarded	All eyes were carefully examined visually, or with a stereomicroscope, if needed, and eyes presenting defects were rejected	Eyes were carefully examined for their quality at the laboratory	At lab, eyes carefully examined for defects; unacceptable eyes rejected
Description of cornea dissection	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Iris and lens were removed, and cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Not noted	Selected corneas were dissected with a 2-3 mm rim of sclera attached; the iris and the lens were removed
Storage of isolated corneas until use	Isolated corneas stored in petri dish with HBSS/penicillin/streptomycin solution until mounted in holders	Isolated corneas stored in petri dish with HBSS until they were mounted in a corneal holder	Isolated corneas stored in petri dish with HBSS until they were mounted in a corneal holder	Not applicable. After dissection, corneas were quickly mounted in holders	Corneas were mounted in holders immediately after dissection
Type of cornea holder used	Cornea holder for opacitometer with anterior (epithelial side) and posterior (endothelial side) chambers	Not noted	Conventional cornea holder for opacitometer with anterior (epithelial side) and posterior (endothelial side) chambers	Composed of specially designed plastic chambers with two separate compartments	Holder consisted of two 5 mL chambers

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Pretreatment incubation/equilibration in corneal holder	Holders and medium are prewarmed to 32°C before mounting corneas. Endothelial side of the cornea is placed against O-ring of posterior chamber. Anterior chamber is placed over the cornea and chambers are joined together. Posterior then anterior chambers are filled with assay medium, avoiding formation of air bubbles and minimizing shear forces on the corneal endothelium.	Each cornea was mounted in a holder filled with medium	Each cornea was mounted in a holder with the endothelial side against the O-ring of the posterior half of the holder; the anterior half of the holder was then positioned on top of the cornea and screws were tightened; posterior then anterior chambers were filled with medium	Corneas were firmly clamped in between the anterior and posterior compartments	
Duration	1 hour	1 hour	1 hour	1 hour	1 hour
Temperature	32°C (±1°C) maintained in a forced air incubator	32°C (±1°C)	32°C (±1°C)	32°C	32°C
Medium used for incubation	Eagle's Minimum Essential Medium (MEM) without phenol red containing 1% fetal bovine serum (complete MEM)	Eagle's minimum essential medium (MEM) without phenol red, with 1% fetal bovine serum (complete MEM)	Prewarmed Eagle's minimum essential medium	Eagle's minimum essential medium supplemented with 1% fetal calf serum	Eagle's minimum essential medium (pH 7.2-7.4) supplemented with 1% fetal bovine serum
Basal (pretreatment) opacity measurement taken	After the 1 hour incubation period, the medium is removed from both chambers of each holder (anterior chamber first) and replaced with fresh complete MEM. Then an initial opacity reading is taken and recorded for each cornea.	An initial opacity measurement was made immediately after 1 hour equilibration period and replacement of incubation media with fresh complete MEM	An initial opacity measurement was made immediately after 1 hour equilibration period	Not noted	No
Instrument used to measure opacity	Opacitometer (Spectro Designs OP-KIT), which determines light transmission through the center of each mounted cornea	Spectro Designs OP-KIT opacitometer (Stag Bio, Clermont, Ferrand, France)	Opacitometer	Opacitometer	Specially-designed opacitometer; light passes simultaneously through a control and treated cornea held in separate chambers and the transmitted light is detected by photocells in each chamber
Instrument calibrated prior to test (y/n)	Not noted	Not noted	Not noted	Not noted	Instrument was calibrated but it's not clear if this was done prior to each test
Criteria for acceptable corneas for testing after equilibration period	Corneas that display an initial opacity reading greater than 10 units from the average opacity for all of the corneas are not used in the assay	Not noted	Not noted	Not noted	Not noted
Treatment groups used (No. of corneas used/test substance)	3 to 5 corneas per test article	5 corneas per formulation tested	3 corneas per formulation tested (cosmetics and personal care products)	Not noted	4 corneas per test compound
Controls	2 or 3 corneas	3 corneas for negative control and 2 corneas for positive control	3 corneas with the lowest opacity scores were selected as negative controls	Vehicle controls used, but specific number not noted	1 cornea for the "control" slot in the opacitometer

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Positive control(s), if used	Acetone was the concurrent positive control (10 minute exposure)	Ethanol			Not noted
Negative/untreated control	Corneas that have opacity values close to the average opacity for all corneas are chosen as the negative (or solvent) control corneas. The negative control is sterile, deionized water.	3 corneas with opacity readings close to the median opacity for all the corneas were treated with complete MEM	Eagle's MEM	Eagle's MEM	On each experimental day, two corneas were exposed to the vehicle and the one remaining the clearest was used as the control for the opacitometer
Other controls, if used					
Treatment of corneas			The MEM was removed from both compartments, anterior compartment first, and the posterior compartment refilled with fresh MEM.	After equilibration, fresh medium was added to the posterior compartment (endothelial side) and test material or vehicle was added to the anterior compartment (epithelial side)	To start the experiment, fresh MEM with 1% FBS was added to the posterior compartment
<i>Liquid substances</i>	<i>Nonviscous and semiviscous liquids</i> tested using "closed chamber method". <i>Semiviscous and viscous liquids</i> tested using "open chamber method".		The test material was added to the anterior compartment	Cosmetic formulations were tested	Test substances were added to the anterior compartment (epithelium side)
Concentration tested	10% (w/v) solution	100% for conditioners; shampoos were tested at both 100% and 10% (w/v) prepared in complete MEM	100%	Not noted	100%
Amount tested	750 µL (test substances and controls)	750 µL (test substances and controls)	750 µL (test substances and control)	Not noted	500 µL
Incubation time	1 hour	Undiluted materials were incubated for 10 minutes and 10% dilutions were incubated for 60 minutes	10 minutes	10 minutes	30 minutes
Incubation temperature	32°C (±1°C)	32°C (±1°C)	32°C (±2°C) water bath	Not noted	Room temperature

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Rinsing procedure	Epithelium is washed 3 or more times with 2-3 mL of cMEM (with phenol red) from a syringe. Once the rinsing medium is clear, one last rinse of the epithelium is performed using fresh complete MEM (without phenol red).	Epithelium is washed 3 or more times with complete MEM containing phenol red to ensure complete removal of test material; corneas given a final rinse with complete MEM without phenol red; anterior chamber was refilled with complete MEM and opacity determined	The epithelium was washed at least three times, until the medium was clear, with MEM	The epithelial side was washed; no details provided	The epithelial side was washed; no details provided
Post-treatment incubation (time, temp.)	The anterior chamber is refilled with fresh complete MEM. A post-treatment opacity reading is taken and recorded for each cornea. Visual observations are performed for each cornea. Holders are incubated in a vertical position at 32°C ($\pm 1^\circ\text{C}$) for 1 hour.	After treatment, corneas were incubated for 2 hours at 32(± 1)°C; a second opacity measurement was taken, which was used for calculations	The anterior compartment was refilled with MEM, and an initial opacity measurement taken. Corneas were incubated for 2 hours at 32(± 1)°C, and a second opacity measurement was taken, which was used for calculations	The anterior compartment was refilled with fresh medium. Corneas were incubated for 2 hours, temperature not noted	The anterior compartment was refilled with MEM + 1%FBS and a first opacity reading was performed; corneas were incubated at 32°C for another 2 hours followed by a second opacity reading which was the reported value
<i>Surfactants</i>		Not tested	Not tested		
Concentration tested				Not noted	
Amount tested				Not noted	
Incubation time				10 minutes	
Incubation temperature				Not noted	
Rinsing procedure				The epithelial side was washed; no details provided	
Post-treatment incubation (time, temp.)				The anterior compartment was refilled with fresh medium. Corneas were incubated for 2 hours, temperature not noted	
<i>Solid substances</i>		Not tested		Not tested	

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Concentration tested			Concentration not noted, although solids were tested as solutions or suspensions		20% (200 mg/mL) in MEM + 1%FBS as solutions or suspensions
Amount tested			750 μ L (test substance and vehicle control)		500 μ L
Incubation time			4 hours		4 hours
Incubation temperature			32°C (\pm 2°C) water bath		Room temperature
Rinsing procedure			Epithelium was washed at least three times with MEM until the medium was clear and particulate free. Gentle swirling movements were necessary to remove particulates from the surface of the cornea. The posterior then the anterior chambers were refilled with fresh MEM, and a final opacity measurement taken.		Epithelial side was washed, but no details provided; opacity was measured
Post-treatment incubation (time, temp.)			Not performed		Not performed
Endpoints assessed					
<i>Corneal opacity</i>					
Data collected for opacity	Numerical opacity value (arbitrary unit) displayed by opacitometer	The opacity values obtained at the second opacity measurement (except for the 120 minute exposure group) were used to calculate the corneal opacity	Opacity was measured by placing each control cornea in the "control" compartment of the opacitometer. Each treated cornea was placed the "treated" compartment and the values displayed were recorded. The glass portion of each holder was dried prior to opacity measurement.	No details provided	The opacity reading is expressed as arbitrary units on a scale which is determined by calibrating the instrument with increasing thicknesses of a standard opaque material (provided by the manufacturer)
<i>Permeability</i>	Medium is removed from the anterior chamber, which is refilled with sodium fluorescein solution; amount of dye that reaches posterior chamber is evaluated as an indicator of increased permeability or damage to the cornea	After the final opacity measurement, the medium was removed from both chambers of the holder. The posterior chamber was refilled with fresh complete MEM.	Medium was removed from both chambers of each holder, anterior chamber first. Fresh MEM was added to the posterior chamber.	Medium was removed from both compartments. Fresh medium was added to the posterior compartment.	After the final opacity readings were completed, medium was removed from the holders. Fresh medium was added to the posterior compartment.
Amount and concentration of sodium fluorescein solution used	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	1 mL of a 4 mg/mL fluorescein solution was added to the anterior chamber	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	Sodium fluorescein solution was added to the anterior compartment; no details provided	1 mL of 5 mg/mL Na-fluorescein solution in Dulbecco's phosphate-buffered saline was added to the anterior compartment
Incubation time for fluorescein solution	90 minutes \pm 5 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally	90 minutes	90 minutes; holder incubated horizontally
Incubation temperature for fluorescein	32°C (\pm 1°C)	32 \pm 1°C water bath	32°C (\pm 2°C) water bath	Not noted	Not noted
Instrumentation used	Microplate reader	Molecular Devices Vmax kinetic microplate reader (Molecular Devices Corp., Menlo Park, CA, USA)	Optical density was measured spectrophotometrically in a plate reader using 200 μ L MEM as a blank	Not specified	Measured spectrophotometrically at 490 nm (peak wavelength for Na-fluorescein absorbance)
Instrument calibrated (y/n)	Yes	Not described	Not noted	Not noted	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Data collected for permeability	Optical density reading at 490 nm	Optical density reading at 490 nm	Optical density reading at 490 nm	Absorbance values determined spectrophotometrically at 490 nm	Optical density reading at 490 nm
Aliquot taken from posterior chamber for OD 490 nm reading	Most of medium is removed from posterior chamber, then mixed in a sample tube. A 360 µL aliquot is taken from the sample tube and transferred to a 96-well plate. Standard plate map provides 2 wells for each cornea in case a dilution is required.	Not noted	200 µL	Not noted	Not noted
Other observations	During the final, post-treatment opacity reading, visual observations are performed for each cornea and, if necessary, are recorded. Special attention is taken to observe dissimilar opacity patterns, tissue peeling, or residual test article.	Corneal swelling (dry weight of 8 mm tissue punch) and histology			
Evaluation of test results					
<i>Corneal opacity</i>					
Basal (pretreatment) opacity subtracted from opacity of each treated cornea?	Yes	Yes	Not noted	Not noted	Basal opacity not measured for each cornea
Opacity for each treated cornea corrected for average value of negative/solvent controls?	Yes	The corrected opacity value of each cornea was calculated by subtracting the average change in opacity of the negative control corneas from that of each treated cornea	The difference in light transmission between treated and control corneas was determined with the opacimeter	Not noted	Opacimeter determines the difference in light transmission between treated and control corneas
Mean corrected opacity value calculated for each treatment group?	Yes	The mean corrected opacity value of each treatment group was calculated	Not noted	Not noted	Mean opacity value ± SD was calculated for each treatment group
<i>Permeability</i>					
OD value for each treated cornea corrected for average value of negative/solvent controls?	Yes	The corrected OD ₄₉₀ was calculated by subtracting the mean OD ₄₉₀ value of the negative control corneas from the OD ₄₉₀ of each treated cornea	Not noted	Not noted	No
Mean corrected permeability value calculated for each treatment group?	Yes	The mean OD ₄₉₀ value of each treatment group was calculated	Not noted	Not noted	Mean OD value ± SD was calculated

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Gettings et al. (1996)	Jones et al. (2001)	Rachui et al. (1994)	Rougier et al. (1994)	Sina et al. (1995)
TEST METHOD COMPONENT					
Formula used to calculate <i>In Vitro</i> Score	<i>In vitro</i> score = mean corrected opacity value + (15 x mean corrected OD ₄₉₀ value)	<i>In vitro</i> score = mean opacity value + (15 x mean OD ₄₉₀ value)	<i>In vitro</i> score = opacity value + (15 x OD ₄₉₀ value)	<i>In vitro</i> score = opacity value + (15 x absorbance value)	It was not clearly stated that mean values were used in the formulas. <i>In vitro</i> score = opacity value + (15 x OD ₄₉₀ value). This formula was derived empirically during in-house and interlaboratory evaluation studies. Data generated for 36 compounds in a multilaboratory study were subjected to a multivariate analysis to determine the equation of best fit between the <i>in vivo</i> and <i>in vitro</i> data.
<i>In vitro</i> classification of ocular irritancy	The surfactant-based formulations induced little opacity, so the permeability value was used to assign an <i>in vitro</i> classification (>0.600 = severe irritant)	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate; 55.1 and greater = substantial	For each test substance an average was taken of <i>in vitro</i> scores obtained for 3 corneas. BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 mild/moderate; 55.1 and greater = severe	Not noted; likely the same one used by Gautheron et al. (1994)	BCOP score 0 - 15 = nonirritant/mild; >15 - 25 = mild eye irritant; >25 - 55 moderate; >55 = severe
Criteria for an acceptable test	Test is accepted if positive control gives an <i>in vitro</i> score that falls within 2 SDs of the current historical mean, which is updated every 3 months.	Not described	Not described	Not noted	Not noted
Conducted in compliance with GLPs	Yes	Not noted	Not noted		Not noted
Other useful information					

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
<i>TEST METHOD COMPONENT</i>			
Collection of bovine eyes			Bovine eyes were excised in the slaughterhouse shortly after slaughter.
Transport conditions	Transported in a receptacle containing Hank's Balanced Salt Solution with Ca ⁺⁺ and Mg ⁺⁺ , and with 100 IU/mL penicillin and 100 µg/mL streptomycin (HBSS)	Transported in a receptacle containing Hank's Balanced Salt Solution with Ca ⁺⁺ and Mg ⁺⁺ , and with 100 IU/mL penicillin and 100 µg/mL streptomycin (HBSS)	Eyes were transported immersed in Hanks' balanced salt solution
Temperature	Transported on ice	Transported on ice	Not noted
Time after slaughter until use	Eyes arrive in the laboratory within 4-5 hours of removing first eyes in a batch from cattle	Eyes arrive in the laboratory within 4-5 hours of removing first eyes in a batch from cattle	Not noted
Cornea preparation	At lab eyes are examined carefully and those with defects such as neovascularization, pigmentation, opacity, or scratches are rejected for testing.	At lab eyes are examined carefully and those with defects such as neovascularization, pigmentation, opacity, or scratches are rejected for testing.	
Description of cornea dissection	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Cornea dissected such that approximately 2 - 3 mm rim of sclera surrounds cornea	Corneas were dissected from eyes leaving a small sclera rim (about 2 mm), after which they were rinsed twice in HBSS before mounting in corneal holders
Storage of isolated corneas until use	Isolated corneas stored in petri dish with HBSS/penicillin/streptomycin solution until mounted in holders	Isolated corneas stored in petri dish with HBSS/penicillin/streptomycin solution until mounted in holders	Not noted
Type of cornea holder used	Cornea holder for opacitometer with anterior (epithelial side) and posterior (endothelial side) chambers	Cornea holder for opacitometer with anterior (epithelial side) and posterior (endothelial side) chambers	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
TEST METHOD COMPONENT			
Pretreatment incubation/equilibration in corneal holder	Holders and medium are prewarmed to 32°C before mounting corneas. Endothelial side of the cornea is placed against O-ring of posterior chamber. Anterior chamber is placed over the cornea and chambers are joined together. Posterior then anterior chambers are filled with assay medium, avoiding formation of air bubbles and minimizing shear forces on the corneal endothelium.	Holders and medium are prewarmed to 32°C before mounting corneas. Endothelial side of the cornea is placed against O-ring of posterior chamber. Anterior chamber is placed over the cornea and chambers are joined together. Posterior then anterior chambers are filled with assay medium, avoiding formation of air bubbles and minimizing shear forces on the corneal endothelium.	
Duration	1 hour	1 hour	1 hour
Temperature	32°C (±1°C) maintained in a forced air incubator	32°C (±1°C) maintained in a forced air incubator	32°C
Medium used for incubation	Eagle's Minimum Essential Medium (MEM) without phenol red containing 1% fetal bovine serum (complete MEM)	Eagle's Minimum Essential Medium (MEM) without phenol red containing 1% fetal bovine serum (complete MEM)	Eagle's Minimal Essential Medium (MEM, Sigma) supplemented with serum and sodium hydrogen carbonate pH adjusted to 7.2 (complete MEM).
Basal (pretreatment) opacity measurement taken	After the 1 hour incubation period, the medium is removed from both chambers of each holder (anterior chamber first) and replaced with fresh complete MEM. Then an initial opacity reading is taken and recorded for each cornea.	After the 1 hour incubation period, the medium is removed from both chambers of each holder (anterior chamber first) and replaced with fresh complete MEM. Then an initial opacity reading is taken and recorded for each cornea.	An initial opacity measurement was made immediately after 1 hour equilibration period and replacement of incubation media with fresh complete MEM
Instrument used to measure opacity	Opacitometer (Spectro Designs OP-KIT), which determines light transmission through the center of each mounted cornea	Opacitometer (Spectro Designs OP-KIT), which determines light transmission through the center of each mounted cornea	OP-KIT, Electro Design, Riom, France
Instrument calibrated prior to test (y/n)	Not noted	Not noted	
Criteria for acceptable corneas for testing after equilibration period	Corneas that display an initial opacity reading greater than 10 units from the average opacity for all of the corneas are not used in the assay	Corneas that display an initial opacity reading greater than 10 units from the average opacity for all of the corneas are not used in the assay	Corneas were rejected if their background opacity grade was greater than 3
Treatment groups used (No. of corneas used/test substance)	3 to 5 corneas per test article	3 to 5 corneas per test article	6 corneas per test compound
Controls	2 or 3 corneas	2 or 3 corneas	3 corneas

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
TEST METHOD COMPONENT			
Positive control(s), if used	Liquids and surfactants: undiluted ethanol; solid test articles: 20% (w/v) solution of imidazole in complete MEM (without phenol red)	Liquids and surfactants: undiluted ethanol; solid test articles: 20% (w/v) solution of imidazole in complete MEM (without phenol red)	Not noted
Negative/untreated control	Corneas that have opacity values close to the average opacity for all corneas are chosen as the negative (or solvent) control corneas. The negative control is sterile, deionized water.	Corneas that have opacity values close to the average opacity for all corneas are chosen as the negative (or solvent) control corneas. The negative control is sterile, deionized water.	Complete MEM
Other controls, if used			
Treatment of corneas			Just prior to treatment, the anterior chamber is completely emptied of MEM
Liquid substances	Nonviscous and semiviscous liquids tested using "closed chamber method". Semiviscous and viscous liquids tested using "open chamber method".	Nonviscous and semiviscous liquids tested using "closed chamber method". Semiviscous and viscous liquids tested using "open chamber method".	Test substances were added to the anterior compartment (epithelium side)
Concentration tested	Generally tested at 100% (neat); dilutions performed as needed or requested	Generally tested at 100% (neat); dilutions performed as needed or requested	100%
Amount tested	750 µL (test substances and controls)	750 µL (test substances and controls)	750 µL
Incubation time	10 minutes (±30 seconds)	10 minutes (±30 seconds)	10 minutes
Incubation temperature	32°C (±1°C)	32°C (±1°C)	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
TEST METHOD COMPONENT			
Rinsing procedure	Epithelium is washed 3 or more times with 2-3 mL of cMEM (with phenol red) from a syringe. Once the rinsing medium is clear, one last rinse of the epithelium is performed using fresh complete MEM (without phenol red).	Epithelium is washed 3 or more times with 2-3 mL of cMEM (with phenol red) from a syringe. Once the rinsing medium is clear, one last rinse of the epithelium is performed using fresh complete MEM (without phenol red).	Not noted
Post-treatment incubation (time, temp.)	The anterior chamber is refilled with fresh complete MEM. A post-treatment opacity reading is taken and recorded for each cornea. Visual observations are performed for each cornea. Holders are incubated in a vertical position at 32°C (±1°C) for 2 hours.	The anterior chamber is refilled with fresh complete MEM. A post-treatment opacity reading is taken and recorded for each cornea. Visual observations are performed for each cornea. Holders are incubated in a vertical position at 32°C (±1°C) for 2 hours.	Corneas were incubated for 2 hours; however, no other details provided
<i>Surfactants</i>			Not tested
Concentration tested			
Amount tested			
Incubation time			
Incubation temperature			
Rinsing procedure			
Post-treatment incubation (time, temp.)			
<i>Solid substances</i>			

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
TEST METHOD COMPONENT			
Concentration tested	20% (w/w) solution or suspension in sterile deionized water, complete MEM, or saline (or other appropriate solvent)	20% (w/w) solution or suspension in sterile deionized water, complete MEM, or saline (or other appropriate solvent)	20% solutions or suspensions were prepared in complete MEM
Amount tested	750 µL (test substance and controls)	750 µL (test substance and controls)	750 µL
Incubation time	4 hours (±5 minutes)	4 hours (±5 minutes)	4 hours
Incubation temperature	32°C (±2°C) water bath	32°C (±2°C) water bath	Not noted
Rinsing procedure	Epithelium is washed 3 or more times with 3 mL of cMEM each time from a syringe or until all particles are removed; fresh cMEM is added to both chambers and final opacity measurement is taken	Epithelium is washed 3 or more times with 3 mL of cMEM each time from a syringe or until all particles are removed; fresh cMEM is added to both chambers and final opacity measurement is taken	Not noted
Post-treatment incubation (time, temp.)			Not performed
Endpoints assessed			
<i>Corneal opacity</i>			
Data collected for opacity	Numerical opacity value (arbitrary unit) displayed by opacitometer	Numerical opacity value (arbitrary unit) displayed by opacitometer	Numerical opacity value (arbitrary unit) displayed by opacitometer
<i>Permeability</i>	Medium is removed from the anterior chamber, which is refilled with sodium fluorescein solution; amount of dye that reaches posterior chamber is evaluated as an indicator of increased permeability or damage to the cornea	Medium is removed from the anterior chamber, which is refilled with sodium fluorescein solution; amount of dye that reaches posterior chamber is evaluated as an indicator of increased permeability or damage to the cornea	Medium was removed from both chambers of the corneal holder and the posterior chamber was refilled with fresh complete MEM.
Amount and concentration of sodium fluorescein solution used	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	1 mL of a 4 mg/mL fluorescein solution is used for liquids and surfactants; 1 mL of a 5 mg/mL fluorescein solution is used for solids	0.4% or 0.5% sodium fluorescein solution for liquids or solids, respectively; dye diluted in Dulbecco's phosphate buffered saline (Sigma)
Incubation time for fluorescein solution	90 minutes ±5 minutes; holder is incubated horizontally	90 minutes ±5 minutes; holder is incubated horizontally	90 minutes; holder is incubated horizontally
Incubation temperature for fluorescein	32°C (±1°C)	32°C (±1°C)	Not noted
Instrumentation used	Microplate reader	Microplate reader	Cary 1 UV-visible spectrophotometer set at 490 nm
Instrument calibrated (y/n)	Yes	Yes	Not noted

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
TEST METHOD COMPONENT			
Data collected for permeability	Optical density reading at 490 nm	Optical density reading at 490 nm	Optical density reading at 490 nm
Aliquot taken from posterior chamber for OD 490 nm reading	Most of medium is removed from posterior chamber, then mixed in a sample tube. A 360 µL aliquot is taken from the sample tube and transferred to a 96-well plate. Standard plate map provides 2 wells for each cornea in case a dilution is required.	Most of medium is removed from posterior chamber, then mixed in a sample tube. A 360 µL aliquot is taken from the sample tube and transferred to a 96-well plate. Standard plate map provides 2 wells for each cornea in case a dilution is required.	Not noted
Other observations	During the final, post-treatment opacity reading, visual observations are performed for each cornea and, if necessary, are recorded. Special attention is taken to observe dissimilar opacity patterns, tissue peeling, or residual test article.	During the final, post-treatment opacity reading, visual observations are performed for each cornea and, if necessary, are recorded. Special attention is taken to observe dissimilar opacity patterns, tissue peeling, or residual test article.	
Evaluation of test results			
<i>Corneal opacity</i>			
Basal (pretreatment) opacity subtracted from opacity of each treated cornea?	Yes	Yes	Initial opacity of each cornea was subtracted from the chemically induced value
Opacity for each treated cornea corrected for average value of negative/solvent controls?	Yes	Yes	Not noted
Mean corrected opacity value calculated for each treatment group?	Yes	Yes	Yes
<i>Permeability</i>			
OD value for each treated cornea corrected for average value of negative/solvent controls?	Yes	Yes	Not noted
Mean corrected permeability value calculated for each treatment group?	Yes	Yes	Yes

Table of BCOP Protocols from Reviewed Literature

REFERENCE	Swanson et al. (1995)	Swanson and Harbell (2000)	Vanparys et al. (1993)
TEST METHOD COMPONENT			
Formula used to calculate <i>In Vitro</i> Score	<i>In vitro</i> score = mean corrected opacity value + (15 x mean corrected OD ₄₉₀ value)	<i>In vitro</i> score = mean corrected opacity value + (15 x mean corrected OD ₄₉₀ value)	<i>In vitro</i> score = mean opacity value + (15 x mean OD ₄₉₀ value)
<i>In vitro</i> classification of ocular irritancy	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate irritant; 55.1 and above = severe irritant.	BCOP score 0 - 25 = mild eye irritant; 25.1 - 55 moderate irritant; 55.1 and above = severe irritant.	BCOP score 0 -3 = nonirritant; 3.1 - 25 = mild eye irritant; 25.1 - 55 moderate; > 55 = severe
Criteria for an acceptable test	Test is accepted if positive control gives an <i>in vitro</i> score that falls within 2 SDs of the current historical mean, which is updated every 3 months.	Test is accepted if positive control gives an <i>in vitro</i> score that falls within 2 SDs of the current historical mean, which is updated every 3 months.	Not noted
Conducted in compliance with GLPs	Yes	Yes	Not noted
Other useful information			

Appendix B

Characterization of the Substances Tested in the BCOP Test Method

B1	Chemical and Product Classes of Substances Tested in the BCOP Assay	B-3
B2	Components of Formulations Tested in Gettings et al. (1996)	B-13
B3	Components of Formulations Tested in Swanson et al. (1995)	B-17
B4	Components of Formulations Tested in Swanson and Harbell (2000).....	B-23

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Appendix B1

Chemical and Product Classes of Substances Tested in the BCOP Assay

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Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
1-1 (#1)	-	Formulation	Insect repellent
1-2 (#2)	-	Formulation	Insect repellent
1-3 (#3)	-	Formulation	Insect repellent
2-4 (#4)	-	Formulation	Insect repellent
2-7 (#7)	-	Formulation	Insect repellent
2-8 (#8)	-	Formulation	Insect repellent
Acetone	67-64-1	Ketone	Solvent; Antiseptic; Chemical intermediate; Raw material
Alkyl phosphoric acid ester/amine salt	-	Organic salt, Ester, Amine	Petroleum product
All Purpose Cleaner (#5)	-	Formulation	Cleaner
All Purpose Cleaner (#7)	-	Formulation	Cleaner
Allyl alcohol	107-18-6	Alcohol	Pesticide
Aluminum hydroxide	21645-51-2	Alkali, Aluminum compound	Chemical intermediate, Dessicant
2-Aminophenol	95-55-6		Chemical intermediate
Ammonium nitrate	6484-52-2	Inorganic salt, Onium compound	Fertilizer; Chemical intermediate; Industrial explosive
Amway all fabric bleach	-	Formulation	Detergent
Amway automatic dishwashing compound for soft water	-	Formulation	Detergent
Amway automatic dishwashing compound, standard formula	-	Formulation	Detergent
Amway concrete floor cleaner	-	Formulation	Cleaner
Amway Dish Drops dishwashing liquid	-	Formulation	Detergent
Amway dry chlorine bleach	-	Formulation	Bleach
Amway fabric softener	-	Formulation	Fabric softener
Amway Kool Wash delicate fabric detergent	-	Formulation	Detergent
Amway LOC all purpose cleaner	-	Formulation	Cleaner
Amway prewash liquid	-	Formulation	Detergent
Amway Pursue disinfectant cleaner	-	Formulation	Cleaner
Amway Redu dye stain remover	-	Formulation	Stain remover
Amway SA8 laundry liquid	-	Formulation	Detergent
Amway SA8 limited phos laundry powder	-	Formulation	Detergent
Anthracene	120-12-7	Polycyclic	Dye manufacturing agent
Anti-Dandruff Shampoo (HZY) 100%	-	Formulation	Surfactant-containing formulation

Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
Aromatic hydrocarbon #1	-	Hydrocarbon (cyclic)	Solvent/industrial chemical; Petrochemical product
Aromatic hydrocarbon #2	-	Hydrocarbon (cyclic)	Solvent/industrial chemical; Petrochemical product
Aryl phosphonates	-	Not classified	Lubricant additive; Petrochemical product
L-Aspartic acid	70-47-3	Amino acid	Organic intermediate; Fungicides; Germicides
Baby Shampoo No. 1 (HZP)	-	Formulation	Surfactant-containing formulation
Baby Shampoo No. 2 (HZF)	-	Formulation	Surfactant-containing formulation
Bathroom Cleaner (#6)	-	Formulation	Cleaner
Benchmark-Group 1 (#12)	-	Formulation	Insect repellent
Benchmark-Group 2 (#13)	-	Formulation	Insect repellent
Benzalkonium chloride (100%)	8001-54-5	Onium compound	Surfactant (cationic); Bactericide; Fungicide; Preservative
Benzalkonium chloride (1 %)	8001-54-5	Inorganic salt, Onium compound	Fertilizer; Chemical intermediate; Industrial explosive
Benzalkonium chloride (10%)	8001-54-5	Onium compound	Surfactant (cationic); Bactericide; Fungicide; Preservative
Benzalkonium chloride (5%)	8001-54-5	Onium compound	Surfactant (cationic); Bactericide; Fungicide; Preservative
Benzethonium chloride	121-54-0	Amine, Onium compound	Bactericide
Benzoyl-L-tartaric acid	2743-38-6	Carboxylic acid, Ester	Optical resolution agent
Betaine monohydrate	590-47-6	Amino acid, Onium compound	Not classified
BRIJ-35	9002-92-0	Alcohol	Emulsifier
4-Bromophenetole	589-10-6	Ether	Not classified
Bubble Bath (HZK) 100%	-	Formulation	Surfactant-containing formulation
n-Butanol	71-36-3	Ketone	Solvent; Synthetic flavor; Drycleaning
2-Butoxyethanol	111-76-2	Alcohol	Solvent
Butyl acetate	123-86-4	Ester	Solvent; Synthetic flavor ingredient
Butyl cellosolve	111-76-2	Alcohol, Ester	Solvent
Butyrolactone	96-48-0	Lactone, Heterocycle	Synthetic intermediate; Solvent
gamma-Butyrolactone	96-48-0	Heterocyclic, Lactone	Synthetic intermediate; Solvent
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Not classified
Carboxylic acid amides	-	Formulation	Lubricant additive; Petrochemical product
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Onium compound	Surfactant (cationic); Germicide; Laboratory reagent
Cetylpyridinium bromide (1%)	140-72-7	Surfactant, cationic	Germicide; Laboratory reagent

Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Onium compound	Surfactant (cationic); Germicide; Laboratory reagent
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Onium compound	Surfactant (cationic); Germicide; Laboratory reagent
Chlorhexidine	55-56-1	Amine/Amidine	Disinfectant; Mouthwash; Anti-infective agent
2-Chloro-2,4,4-trimethylpentane	-	Hydrocarbon (halogenated)	Solvent/industrial chemical; Petrochemical product
Clarified slurry oil	-	Hydrocarbon (cyclic)	Petrochemical product
Cleaner/Degreaser (#13)	-	Formulation	Cleaner
Cleansing Gel (HZQ) 100%	-	Formulation	Surfactant-containing formulation
Cutting fluid (conc.) #1	-	Formulation	Cutting fluid; Petrochemical product
Cutting fluid (conc.) #2	-	Formulation	Cutting fluid; Petrochemical product
Cyclohexanol	108-93-0	Alcohol	Solvent; Chemical intermediate
Cyclohexanone	108-94-1	Ketone, Hydrocarbon (cyclic)	Solvent, Chemical intermediate
Degreaser (#16)	-	Formulation	Degreaser
Deoxycholic acid, sodium salt	302-95-4	Alcohol, Carboxylic acid (salt)	Detergent/Surfactant, Chemical intermediate
Diacetone alcohol	123-42-2	Ketone, Alcohol	Solvent
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified
2,6-Dichlorobenzoyl chloride	4659-45-4	Acyl halide	Anti-infective; Anti-fungal; Preservative
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	Amide, Organic sulfur compound	Intermediate for pharmaceuticals, pesticides, perfumes
2,4-Difluoronitrobenzene	446-35-5	Acyl halide	Anti-infective; Anti-fungal; Preservative
1,3-Diisopropylbenzene	99-62-7	Hydrocarbon (cyclic)	Not classified
Dimethylbiguanide	657-24-9	Amidine	Pharmaceutical
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes
Dimethyl sulfoxide	67-68-5	Organic sulfur compound	Solvent
Dodecane	112-40-3	Hydrocarbon (acyclic)	Not classified
EDTA, di-potassium salt	25102-12-9	Amine, Carboxylic acid (salt)	Chelator
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent
Ethanol (#14)	64-17-5	Alcohol	Solvent
2-Ethoxyethanol	110-80-5	Alcohol	Solvent
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring
Ethyl acetoacetate	141-97-9	Carboxylic acid, Ketone	Chemical intermediate, Flavoring agent
2-Ethylhexanol	104-76-7	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer

Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
Ethylhexyl acid phosphate ester	-	Ester, Carboxylic acid	Lubricant additive; Petrochemical product
5-Ethylidene-2-norbornene	16219-75-3	Not classified	Solvent/industrial chemical; Petrochemical product
Ethyl-2-methylacetoacetate	609-14-3	Ketone, Ester	Not classified
3-Ethyltoluene	620-14-4	Hydrocarbon (cyclic)	Not classified
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent
Eye Make-Up Remover (HZH) 100%	-	Formulation	Surfactant-containing formulation
Facial Cleaning Foam (HZR) 25%	-	Formulation	Surfactant-containing formulation
Facial Cleanser (HZZ) 100%	-	Formulation	Surfactant-containing formulation
Floor Cleaner (#10)	-	Formulation	Cleaner
Floor Cleaner (#2)	-	Formulation	Cleaner
Floor Stripper (#14)	-	Formulation	Floor stripper
Floor Stripper (#17)	-	Formulation	Floor stripper
Floor Stripper (#18)	-	Formulation	Floor stripper
Foam Bath (HZZ) 100%	-	Formulation	Surfactant-containing formulation
Fomesafen	72128-02-0	Imide, Ether, Nitro compound	Pesticide
Furan	110-00-9	Heterocyclic	Chemical intermediate
Gel Cleanser (HZE) 100%	-	Formulation	Surfactant-containing formulation
General Cleaner (#11)	-	Formulation	Cleaner
General Cleaner (#12)	-	Formulation	Cleaner
Glass Cleaner (#19)	-	Formulation	Cleaner
Gluconolactone	90-80-2	Carboxylic acid, Lactone, Carbohydrate	Food additive
DL-Glutamic acid	19285-83-7	Amino acid	Not classified
Glycerol	56-81-5	Alcohol	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle
3-Glycidoxypolytrimethoxysilane	2530-83-8	Organosilicon compound	Adhesive
Hand Soap (HZU) 25%	-	Formulation	Surfactant-containing formulation
Heavy Duty Cleaner (#15)	-	Formulation	Cleaner
Heavy Duty Cleaner/Degreaser (#9)	-	Formulation	Cleaner
Hexadecyltrimethylammonium bromide	57-09-0	Organic salt, Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent
1,5-Hexadiene	592-42-7	Hydrocarbon (acyclic)	Not classified
Hexane	110-54-3	Hydrocarbon (acyclic)	Solvent
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor
Iminodibenzyl	494-19-9	Heterocyclic	Personal care product

Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulations (ingredient)
N-Lauroylsarcosine, sodium salt	7631-98-3	Amide, Amino acid (salt)	Surfactant (anionic)
Laurylsulfobetaine	14933-08-5	Amine, Onium compound	Detergent, Surfactant (zwitterionic)
Liquid Soap No. 2 (HZW) 25%	-	Formulation	Surfactant-containing formulation
Liquid Soap No. 1 (HZB) 25%	-	Formulation	Surfactant-containing formulation
Magnesium carbonate	56378-72-4	Inorganic salt	Chemical intermediate
Maneb	12427-38-2	Amine/Amidine, Organic salt, Urea compound	Pesticide
Meat Room Degreaser (#3)	-	Formulation	Degreaser
2-Mercaptopyrimidine	1450-85-7	Acyl halide	Anti-infective; Anti-fungal; Preservative
Metal Cleaner (#20)	-	Formulation	Cleaner
Methanol	67-56-1	Alcohol	Solvent
2-Methoxyethanol	109-86-4	Alcohol	Solvent; Plasticizer
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient
Methyl cyanoacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate
Methyl cyclopentadiene dimer	-	Cyclic hydrocarbon	Solvent/industrial chemical; Petrochemical product
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Drycleaning
1-Methylpropyl benzene	135-98-8	Hydrocarbon (cyclic)	Not classified
Mild Shampoo (HZJ) 25%	-	Ketone	Solvent; Synthetic flavor; Drycleaning
MYRJ-45	-	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals
1-Naphthalene acetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide
1-Naphthalene acetic acid, Na salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide
1-Nitropropane	108-03-2	Hydrocarbon (acyclic), Nitro compound	Solvent, Chemical intermediate
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance
Parafluoriline	371-40-4	Amine/Amidine	Intermediate for herbicides; Dyes
2,4-Pentanedione	123-54-6	Ketone	Solvent; Plasticizer
Petroleum ether	8032-32-4	Hydrocarbon (acyclic)	Solvent
Petroleum wax	-	Wax	Petrochemical product

Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
Phenylbutazone	50-33-9	Heterocyclic	Pharmaceutical
1-Phenyl-3-pyrazolidone	92-43-3	Heterocyclic	Photographic agent
Polishing Scrub (HZT) 100%	-	Formulation	Surfactant-containing formulation
Polyalkenylsuccinate ester/amine salt	-	Amidine	Lubricant additive; Petrochemical product
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent
Polyethylene glycol 600	-	Alcohol, Polyether	Surfactant (nonionic)
Pot and Pan Cleaner (#8)	-	Formulation	Cleaner
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate
Process oil	-	Oil	Petrochemical product
Promethazine hydrochloride	58-33-3	Amine/Amidine, Heterocyclic, Organic sulfur compound	Antihistamine; Anti-nausea drug
Propylene glycol	57-55-6	Alcohol	Solvent
Propyl-4-hydroxybenzoate	94-13-3	Carboxylic acid, Phenol	Antimicrobial
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides
Quinacrine	69-05-6	Heterocyclic	Drug/Therapeutic agent
Shampoo No. 1 (HZC) 25%	-	Formulation	Surfactant-containing formulation
Shampoo No. 2 (HZX)	-	Formulation	Surfactant-containing formulation
Shampoo No. 3 (HZM) 25%	-	Formulation	Surfactant-containing formulation
Shampoo No. 4 (HZV) 25%	-	Formulation	Surfactant-containing formulation
Shampoo No. 5 (HZD) 25%	-	Formulation	Surfactant-containing formulation
Shampoo No. 6 (HZN) 25%	-	Formulation	Surfactant-containing formulation
Shampoo No. 7 (HZA)	-	Formulation	Surfactant-containing formulation
Shampoo No. 8 (HZG) 25%	-	Formulation	Surfactant-containing formulation
Shower Gel (HZS) 100%	-	Formulation	Surfactant-containing formulation
Skin Cleanser (HZI) 100%	-	Formulation	Surfactant-containing formulation
Sodium hydroxide (1%)	1310-73-2	Alkali	Caustic agent
Sodium hydroxide (10%)	1310-73-2	Alkali	Caustic agent
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent
Sodium lauryl sulfate (30 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic, Industrial byproduct
Sodium perborate	10486-00-7	Inorganic salt, Boron compound	Household cleaner; Detergent

Chemical and Product Classes of Substances Tested in the BCOP Assay

Substance	CASRN ¹	Chemical Class	Product Class
Tetraaminopyrimidine sulfate	5392-28-9	Amine, Heterocycle, Inorganic salt	Not classified
Thiadiazole alkyl derivative	-		Lubricant additive; Petrochemical product
Thiourea	62-56-6	Organic sulfur compound	Photographic agent; Flame-retardant; Chelation reagent and catalyst; Chemical intermediate; Pesticide; Drug/Therapeutic agent
Toilet Bowl Cleaner (#1)	-	Formulation	Cleaner
Toilet Bowl Cleaner (#4)	-	Formulation	Cleaner
Toluene	108-88-3	Hydrocarbon (cyclic)	Solvent
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide
1,2,3-Trichloropropane	96-18-4	Hydrocarbon (halogenated)	Solvent
Triethanolamine	102-71-6	Amine, Alcohol	Antimicrobial, Chemical intermediate
1,2,4-Trimethylbenzene	95-63-6	Hydrocarbon (cyclic)	Chemical intermediate
Triton X-100 (1%)	9002-93-1	Ether	Surfactant (nonionic)
Triton X-100 (10 %)	9002-93-1	Ether	Surfactant (nonionic), Detergent, Emulsifier
Triton X-100 (5%)	9002-93-1	Ether	Surfactant (nonionic)
Triton X-155	9010-44-0	Ether	Surfactant (nonionic)
Tween 20	9005-64-5	Ester, Polyether	Surfactant (nonionic); Detergent
Xylene	1330-20-7	Hydrocarbon (cyclic)	Agricultural chemical

¹CASRN = Chemical Abstracts Service Registry Number

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Appendix B2

Components of Formulations Tested in Gettings et al. (1996)

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Components of Formulations Tested in Gettings et al. (1996)

Formulation	Formulation Components	% (W/W)	Formulation	Formulation Components	% (W/W)
HZA-Shampoo No. 7	Water	53.86	HZN-Shampoo No. 6	Water	44.381
	Sodium lauryl sulfate (30%)	25.00		Sodium laureth (2EO) sulfate (28%)	43.634
	Disodium laureth sulfocuccinate (40%)	15.00		Cocamidopropyl betaine (30%)	11.760
	Lauramide DEA	0.50		Tetrasodium EDTA	0.125
	Butylene glycol	5.00		Formalin	0.100
	Methyl and propylparabens	0.25			
	Carageenan	0.35			
	Methyl and methylchloroisothiazolinone	0.04			
HZB-Liquid Soap No. 1	Water and volatiles	65-85	HZP-Baby Shampoo No. 1	Water	49.54
	Ammonium lauryl sulfate	1-10		PEG-80 sorbitan laurate (50%)	23.60
	Sodium laureth sulfate	1-10		Sodium trideceth sulfate (50%)	17.40
	Lauramide DEA	1-10		Lauroamphocarboxyglycinate (50%)	5.40
	Glycerine	1-10		PEG-150 distearate (50%)	5.00
	Isosteamidopropyl morpholine lactate	0.1-1.0		Cocamidodrolyl hydroxysultane (50%)	4.00
	Disodium ricinoleamide MEA-sulfosuccinate	0.1-1.0		Sodium laureth-13 carboxylate (50%)	1.00
	DMDM hydantoin	0.1-1.0		Quaternium 15	0.03
	Citric acid	0.1-1.0		Benzyl alcohol	0.05
	Triclosan	0.1-1.0		FD&C Yellow No. 5 (1.0%)	0.25
	Tetrasodium EDTA	<0.1		FD&C Yellow No. 6 (1.0%)	0.05
	FD&C Yellow No. 5	<0.1		Citric acid	0.08
	FD&C Red No. 4	<0.1			
HZA-Shampoo No. 1	Water	14.037	HZQ-Cleansing Gel	Water	68.93
	Laurylamidopropyl betaine (30%)	60.000		Lauroamphocarboxyglycinate (25%)	10.40
	Cetrimonium chloride	16.000		Sodium trideceth sulfate (16%)	10.60
	PEG-3 cocamide	4.500		TEA-lauryl sulfate (40%)	3.50
	Citric acid	3.500		Lauramide DEA	0.50
	Sodium chloride	1.000		PEG-150 distearate	2.80
	Ditallowdimonium chloride (73%)	0.700		Propylene glycol	1.40
	Lauryl alcohol	0.250		Hexylene glycol	1.05
	Methyl and chlorisothiazolinone (1.5%)	0.033		Citric acid	0.28
				Diazolidinyl urea	0.20
		Methylparaben	0.20		
		Sodium citrate	0.14		
HZD-Shampoo No. 5	Water	54.120	HZR-Facial Cleansing Foam	Water	32.97
	Sodium laureth sulfate (26%)	38.00		Sodium cocoyl isethionate	20.00
	Cocamide DEA	3.000		Sodium lauroyl sarcosinate (30%)	25.00
	Cocamide propyl betaine (37%)	1.750		PPG-5-ceteth-10 phosphate	4.00
	Disodium EDTA	0.050		Linoleamide DEA	2.00
	Methylparaben	0.150		Sorbitol (70%)	2.75
	Propylparaben	0.100		Glycol stearate	5.50
	Citric acid	0.250		Glycerin	2.00
	FD&C Yellow No. 5 (1%)	0.050		Diglycerol	2.00
	D&C Red No. 33 (0.5%)	0.015		Cetearyl alcohol	2.75
	DMDM hydantoin (54%)	0.300		Mineral oil	0.50
	BHT	0.050		Methylparaben	0.15
	Sodium glutamate	2.000		Propylparaben	0.10
	Sodium chloride	0.170		Trisodium EDTA	0.10
		Beeswax	0.10		
		Ceresin	0.06		
		Sodium borate	0.02		
HZE-Gel Cleanser	Water	59.974	HZZ-Shower Gel	Water	27.567
	Acylglutamate CT-12 (30%)	15.000		Sodium lauroyl sarcosinate (30%)	25.000
	Cocamphodiacetate (50%)	15.000		Laurimidopropyl betaine (30%)	25.000
	Sodium nonoxynol-6 phosphate (88.5%)	6.000		Cocamidopropyl hydroxysultaine (50%)	15.000
	Quaternium-26 (58%)	1.500		Linoleamide DEA	4.500
	PEG-120-methyl glucose dioleate	1.500		Glycol stearate	1.000
	Citric acid	0.100		Polyquaternium-2	1.000
	Sodium citrate	0.500		Phosphoric acid (86.5%)	0.600
	Disodium EDTA	0.050		Tetrasodium EDTA	0.200
	Methylparaben	0.150		BHT	0.050
	DMDM hydantoin (55%)	0.200		PPG-12-buteth-16	0.050
	FD&C Yellow No. 10 (1%)	0.001		Methyl and chlorisothiazolinone (1.5%)	0.033
	D&C Blue No. 1 (0.746%)	0.025			
HZF-Baby Shampoo No. 2	Water	57.653	HZT-Polishing Scrub	Water	33.85
	Sodium laureth (2EO) sulfate (28%)	21.430		Mineral oil	10.00
	Disodium laureth-3-sulfosuccinate (40%)	9.090		Lauroamphocarboxyglycinate (25%)	8.80
	Cocamidopropyl betaine (30%)	10.000		Sodium trideceth sulfate (16%)	9.40
	Lauramide DEA	1.500		Petrolatum	6.60
	Kathon CG (1.5%)	0.067		Isopropyl palmitate	6.60
	Tetrasodium EDTA (30%)	0.260		Propylene glycol	5.00
				Cetyl palmitate	4.40
		Glyceryl stearate and PEG-100 stearate	4.40		
		Aluminum silicate	3.00		
		Cetyl alcohol	2.50		
		Polypropylene	2.50		
		Magnesium aluminum silicate	1.00		
		Titanium dioxide	0.50		
		Hexylene glycol	0.40		
		Imidazolidinyl urea	0.30		
		Methylparaben	0.30		
		Lactic acid	0.25		
		Propylparaben	0.20		

Components of Formulations Tested in Gettings et al. (1996)

Formulation	Formulation Components	% (W/W)	Formulation	Formulation Components	% (W/W)
HZG-Shampoo No. 8	Water	48.43	HZU-Hand Soap	Water	37.95
	Sodium laureth sulfate (28%)	20.00		Sodium C14-16 olefin sulfonate (36%)	20.25
	Sodium lauryl sulfate (30%)	25.00		Sodium lauroyl sarcosinate	20.00
	Lauramide-DEA	5.00		Cocamidopropyl hydroxysulfate	8.00
	Hydroxyethyl tallow glycinate	1.00		Propylene glycol	3.00
	Citric acid	0.20		Glycerol stearate	3.00
	PEG-45M	0.20		PPG-12-PEG-50 lanolin	3.00
	Methyl and propylparabens	0.13		Polyquaternium-7	2.00
	Methyl and chloromethyl-isothiazolinone	0.04		Citric acid	1.00
HZH-Eye Make-Up Remover	Water	96.242	HZV-Shampoo No. 4	Water	80-90
	Sodium laureth sulfate (21%)	0.900		Ammonium lauryl sulfate	5-10
	Cocamphocarboxyglycinate (40%)	1.100		Lauramide DEA	1-5
	Hexylene glycol	1.000		Cocamidopropyl sulfate	<1.0
	Dipotassium phosphate	0.394		Ammonium chloride USP	<1.0
	Potassium phosphate	0.102		Citric acid	<1.0
	Allantoin	0.050		DMDM hydantoin	<1.0
	Methyl paraben	0.150		Tetrasodium EDTA	<1.0
	EDTA	0.150		Methylparaben	<1.0
Rose water	0.008	FD&C Yellow No. 5	<1.0		
Thimerosal	0.003	D&C Yellow No. 10	<1.0		
HZI-Skin Cleanser	Water	44.0	HZW-Liquid Soap No. 2	Water and volatiles	60-80
	Sodium laureth sulfate (30%)	50.0		TEA-lauryl sulfate	1-10
	Cocamide MEA	5.0		Sodium laureth sulfate	1-10
	Sodium chloride	0.4		Sodium lauroyl sarcosinate	1-10
	Disodium EDTA	0.2		Lauramide DEA	1-10
	Imidazolidinyl urea	0.2		Glycol distearate	1-10
	Methylparaben	0.2		Isostearamideopropyl morpholine lactate	0.1-1.0
	Benzoic acid	0.1		Disodium ricinoleamide MEA-sulfosuccinate	0.1-1.0
				DMDM hydantoin	0.1-1.0
		Citric acid	0.1-1.0		
		Tetrasodium EDTA	<0.1		
HZJ-Mild Shampoo	Water	52.09	HZX-Shampoo No. 2	Water	69.1895
	Tween 20	12.63		Ammonium lauryl sulfate (25%)	25.0000
	Cocamphodiacetate (24%)	21.25		Cocamide DEA	3.0000
	PEG 6000	2.60		Hydroxypropyl methylcellulose	1.4500
	Cedepal TD403 (75%)	6.53		EDTA	0.6000
	Hydrochloric acid (15%)	1.68		Formaldehyde	0.2000
	Arlacel 20	0.92		Benzyl alcohol	0.2000
	Benzyl alcohol	0.10		Benzophenone-4 sodium hydroxide	0.0400
	Dowicel 200	0.10		Citric acid	0.0100
D&C Yellow No. 10 (0.2%)	1.70	Ammonium chloride	0.0100		
D&C Orange No. 4 (0.2%)	0.20	FD&C Blue No. 1	0.0005		
HZK-Bubble Bath	Water	68.75	HZY-Anti-Dandruff Shampoo	Water	27.13
	Sodium laureth sulfate (60%)	25.00		Sodium lauroyl sarcosinate (30%)	15.00
	Lauramide DEA	4.50		Lauramide DEA	4.50
	SD Alcohol 3-A	3.75		TEA-lauryl sulfate (40%)	45.00
	Sodium chloride	0.80		Glycol distearate	3.00
	Triethanolamine	0.40		Zinc pyrithione	2.10
	Phosphoric acid (86.5%)	0.35		Sodium chloride	1.20
	Sorbic acid	0.20		Citric acid	0.90
				Imidazolidinyl urea	0.50
		Methylparaben	0.30		
		Propylparaben	0.10		
		Xanthan gum	0.27		
HZL-Foam Bath	Water	47.760	HZZ-Facial Cleanser	Water	32.55
	Sodium laureth sulfate (26%)	46.000		Mineral oil	40.00
	Cocamido propyl betaine (30%)	2.500		Beeswax	2.30
	Sodium chloride	2.400		PEG-16 soya sterol	5.00
	Glycol monostearate	0.400		PEG-8 dilaurate	2.00
	Color solution	0.300		Cetaryl alcohol (70%)	0.80
	DMDM hydantoin (54%)	0.250		Ceteareth 20 (30%)	0.80
	Methylparaben	0.200		Beheme acid	0.80
	Propylparaben	0.100		Sodium borate	0.75
	BHT	0.050		Ceresin	0.50
	Aloe vera gel	0.015		Carbopol dispersion (25%)	15.00
	Citric acid	0.016		Methylparaben	0.15
	Tetrasodium EDTA	0.010		Propylparaben	0.10
		Disodium EDTA	0.05		
HZM-Shampoo No. 3	Water	80-90			
	Ammonium lauryl sulfate	5-10			
	Lauramide DEA	1-5			
	Cocamidopropyl sultaine	1-5			
	Citric acid	<1.0			
	Ammonium chloride	<1.0			
	DMDM Hydantoin	<1.0			
	Tetrasodium EDTA	<1.0			
	Methylparaben	<1.0			
	FD&C Yellow No. 5	<0.1			
	D&C Yellow No. 10	<0.1			
	FD&C Red No. 4	<0.1			
	PPG-9				

Appendix B3

Components of Formulations Tested in Swanson et al. (1995)

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Components of Formulations Tested in Swanson et al. (1995)

Code	Formulation	Formulation Components	Percentage	pH
1	Toilet Bowl Cleaner	Water	90-95	8.8
		Nonionic Surfactant	1-5	
		Anionic Surfactant	1-5	
		Preservative	< 1	
		Thickener	< 1	
		Dye	< 1	
		Fragrance	< 1	
		Phosphate	< 1	
2	Floor Cleaner	Water	90-95	10.8
		Anionic Surfactant	1-5	
		Nonionic Surfactant	1-5	
		MEA	< 1	
		Fragrance	< 1	
		Dye	< 1	
3	Meat Room Degreaser	Water	80-85	12.65
		Anionic surfactant	1-5	
		Nonionic surfactant	1-5	
		Chelator	1-5	
		Glycol ether	1-5	
		Inorganic salt	1-5	
		KOH	< 1	
4	Toilet Bowl Cleaner	Water	90-95	2.5
		Organic acid	1-5	
		Anionic surfactant	1-5	
		Thickener	< 1	
		Dye	< 1	
		Fragrance	< 1	
5	All Purpose Cleaner	Water	90-95	13
		Nonionic surfactant	1-5	
		Inorganic salt	1-5	
		NaOH	1-5	
		Chelator	< 1	
		KOH	< 1	
		Anionic surfactant	< 1	
		Fragrance	< 1	
		Dye	< 1	
6	Bathroom Cleaner	Water	80-85	13
		Chelator	10-15	
		Glycol ether	1-5	
		Nonionic surfactant	1-5	
		Quaternary compound	< 1	

Components of Formulations Tested in Swanson et al. (1995)

Code	Formulation	Formulation Components	Percentage	pH
7	All Purpose Cleaner	Water	80-85	14
		Inorganic salt	5-10	
		NaOH	1-5	
		Nonionic surfactant	1-5	
		Anionic surfactant	1-5	
		KOH	< 1	
		Chelator	< 1	
		Amphoteric surfactant	< 1	
		Fragrance	< 1	
		Dye	< 1	
8	Pot and pan cleaner	Water	60-65	7.8
		Anionic surfactant	25-30	
		Nonionic surfactant	5-10	
		Glycol ether	1-5	
		Preservative	< 1	
		Dye	< 1	
9	Heavy-duty cleaner/degreaser	Water	75-80	13.6
		Inorganic salts	10-15	
		Chelator	1-5	
		NaOH	1-5	
		Nonionic surfactant	1-5	
		Amphoteric surfactant	1-5	
		Dye	< 1	
10	Floor cleaner	Water	85-90	11.7
		MEA	1-5	
		Anionic surfactant	1-5	
		Glycol ether	1-5	
		Ammonium hydroxide	1-5	
		Nonionic surfactant	< 1	
		Chelator	< 1	
		Fragrance	< 1	
		Dye	< 1	
		11	General Cleaner	
Inorganic acid	15-20			
Nonionic surfactant	1-5			
Amphoteric surfactant	< 1			
Fragrance	< 1			
Dye	< 1			

Components of Formulations Tested in Swanson et al. (1995)

Code	Formulation	Formulation Components	Percentage	pH
12	General Cleaner	Water	75-80	14
		Anionic surfactant	10-15	
		Nonionic surfactant	5-10	
		Chelator	1-5	
		Inorganic salt	1-5	
13	Cleaner/Degreaser	Water	65-70	12
		Glycol ether	10-15	
		Anionic surfactant	1-5	
		Inorganic salt	1-5	
		Chelator	1-5	
		Nonionic surfactant	5-10	
		NaOH	1-5	
Dye	< 1			
14	Floor stripper	Water	50-55	11.5
		Glycol ether	30-35	
		MEA	10-15	
		Organic solvent	1-5	
		Ammonium hydroxide	1-5	
		Anionic surfactant	1-5	
15	Heavy Duty cleaner	Water	65-70	13.5
		Inorganic salts	10-15	
		Anionic surfactant	5-10	
		Chelator	1-5	
		NaOH	1-5	
		Nonionic surfactant	1-5	
		Amphoteric surfactant	1-5	
16	Degreaser	Water	65-70	12.9
		Anionic surfactant	5-10	
		Chelator	5-10	
		Nonionic surfactant	5-10	
		KOH	1-5	
		Inorganic salt	1-5	
		Glycol ether	1-5	

Components of Formulations Tested in Swanson et al. (1995)

Code	Formulation	Formulation Components	Percentage	pH
17	Floor stripper	Water	60-65	13.1
		Glycol ether	10-15	
		Anionic surfactant	10-15	
		MEA	5-10	
		Organic solvent	1-5	
		Inorganic salt	1-5	
		NaOH	1-5	
		Chelator	< 1	
		Flurochemical	< 1	
		Fragrance	< 1	
18	Floor stripper	Water	55-60	14
		Glycol ether	10-15	
		Inorganic salt	5-10	
		Amphoteric surfactant	5-10	
		MEA	1-5	
		NaOH	1-5	
		Chelator	1-5	
		Nonionic surfactants	< 1	
		Fragrance	< 1	
19	Glass cleaner	Water	65-70	12.1
		Glycol ether	20-25	
		Ammonium hydroxide	1-5	
		Anionic surfactant	1-5	
		Chelator	1-5	
		Dye	< 1	
20	Metal cleaner	Water	65-70	14
		Chelator	5-10	
		NaOH	5-10	
		Nonionic surfactant	5-10	
		KOH	< 1	

Appendix B4

Components of Formulations Tested in Swanson and Harbell (2000)

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Components of Formulations Tested in Swanson and Harbell (2000)

Substance	Group	Formulation Component	Percentage
1	1-1	Cyclomethicone	50-55
		Alcohol	40-45
		Active	10-15
2	1-2	Dimethicone (alkoxylated derivative)	50-55
		Alcohol	40-45
		Active	10-15
3	1-3	Alcohol	40-45
		Cyclomethicone	30-35
		Dimethicone (alkoxylated derivative)	20-25
		Active	10-15
4	2-4	Isoparaffinic hydrocarbon	80-85
		Active	10-15
		Cyclic polysiloxane	5-10
		Emollient	< 1
5	2-5	Isoparaffinic hydrocarbon	80-85
		Active	10-15
		Cyclic polysiloxane	5-10
		Alcohol	1-5
		Emollient	< 1
6	2-6	Isoparaffinic hydrocarbon	75-80
		Active	10-15
		Cyclic polysiloxane	5-10
		Alcohol	5-10
		Emollient	< 1
7	2-7	Isoparaffinic hydrocarbon	70-75
		Active	10-15
		Alcohol	10-15
		Cyclic polysiloxane	5-10
		Emollient	< 1
8	2-8	Isoparaffinic hydrocarbon	65-70
		Alcohol	15-20
		Active	10-15
		Cyclic polysiloxane	5-10
		Emollient	< 1
9	3-9	Alcohol	60-65
		Water	25-30
		Active	10-15
		Fragrance	< 1

Components of Formulations Tested in Swanson and Harbell (2000)

Substance	Group	Formulation Component	Percentage
10	3-10	Water	45-50
		Alcohol	40-45
		Active	10-15
		Fragrance	< 1
11	3-11	Water	55-60
		Alcohol	30-35
		Active	10-15
		Fragrance	< 1
12, 13	Benchmark	Alcohol	85-90
		Active	10-15
		Dimethicone	1-5
		Fragrance	< 1
14, 15	Ethanol	Ethanol	100
16	Vehicle control	Alcohol	85-90
		Water	10-15
		Dimethicone	1-5
		Fragrance	< 1

Appendix C

***In Vitro* Data for Substances Tested in the BCOP Assay**

C1	BCOP Data Sorted by Reference	C-3
C2	BCOP Data Sorted by Substance Name	C-29

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Appendix C1

BCOP Data Sorted by Reference

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In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	ⁿ	SD - Opacity	Mean OD ₂₀₀	ⁿ	SD - OD ₂₀₀	In Vitro Score ¹	ⁿ	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Alkyl phosphoric acid ester/amine salt	-	liquid	moderate	100%	n.p.	-	37.7			3.577			91.3			Severe	Severe	Bailey et al. (2004)
Aromatic hydrocarbon #1	-	liquid	negligible	100%	n.p.	-	2.7			0.000			2.7			Mild	Mild	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	negligible	100%	n.p.	-	4.3			0.017			4.6			Mild	Mild	Bailey et al. (2004)
Aryl phosphonates	-	liquid	moderate	100%	n.p.	-	20.3			1.399			41.3			Moderate	Moderate	Bailey et al. (2004)
Carboxylic acid amides	-	solid	moderate	100%	n.p.	-	10.7			1.125			27.5			Moderate	Moderate	Bailey et al. (2004)
2-Chloro-2,4,4-trimethylpentane	-	liquid	negligible	100%	n.p.	-	4.0			0.004			4.1			Mild	Mild	Bailey et al. (2004)
Clarified slurry oil	-	liquid	negligible	100%	n.p.	-	2.3			0.000			2.3			Mild	Mild	Bailey et al. (2004)
Cutting fluid (conc.) #1	-	liquid	emulsifies	100%	n.p.	-	3.3			0.001			3.5			Mild	Mild	Bailey et al. (2004)
Cutting fluid (conc.) #2	-	liquid	emulsifies	100%	n.p.	-	4.3			0.038			4.9			Mild	Mild	Bailey et al. (2004)
Ethylhexyl acid phosphate ester	-	liquid	moderate	100%	n.p.	-	117.3			0.880			130.5			Severe	Severe	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	negligible	100%	n.p.	-	5.7			0.207			8.8			Mild	Mild	Bailey et al. (2004)
Methyl cyclopentadiene dimer	-	liquid	negligible	100%	n.p.	-	0.7			0.001			0.7			Mild	Mild	Bailey et al. (2004)
Petroleum wax	-	solid	negligible	100%	n.p.	-	0.3			-0.001			0.3			Mild	Mild	Bailey et al. (2004)
Polyalkenylsuccinate ester/amine salt	-	liquid	moderate	100%	n.p.	-	2.3			0.000			2.3			Mild	Mild	Bailey et al. (2004)
Process oil	-	liquid	negligible	100%	n.p.	-	2.7			0.004			2.7			Mild	Mild	Bailey et al. (2004)
Thiadiazole alkyl derivative	-	liquid	negligible	100%	n.p.	-	7.3			0.237			10.9			Moderate	Moderate	Bailey et al. (2004)
Acetone	67-64-1	liquid	water soluble	100%	99	1	90.3			3.676			145.5			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	2	83.7			2.389			119.5			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	3	55.7			4.315			120.4			Very severe	Very Severe	Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	4	94.33			2.492			131.72			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	5	69.3			1.942			98.4			Very severe		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	1	6.3			0.132			8.3			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	2	6			0.026			6.4			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	3	6			0.079			7.2			Mild	Mild	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	4	11.34			0.698			21.82			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	5	4.7			0.034			5.2			Mild		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	1	2			-0.011			1.8			Mild		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	2	1.7			-0.107			0.1			Mild		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	3	2.7			-0.003			2.6			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	4	0.33			0.03			0.788			Mild		Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	5	0			0.082			1.2			Mild		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	1	75.3			4.456			142.2			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	2	79.3			5.223			157.7			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	3	61.7			4.142			123.8			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	4	63			4.967			137.5			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	5	74.7			3.096			121.1			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	1	126.6			3.264			126.6			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	2	163.7			6.599			163.7			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	3	110.7			3.891			110.7			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	4	130.41			4.338			130.41			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	5	111.1			3.117			111.1			Very severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	1	59			3.588			112.8			Very severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	2	37			3.566			90.5			Very severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	3	34.3			4.336			99.4			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	4	22			2.699			62.49			Severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	5	38			2.706			78.6			Severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	1	169.7			0.218			173			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	2	286.7			0.134			288.7			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	3	90			0.073			91.1			Very severe	Very Severe	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	4	147			0.191			149.86			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	5	141.3			0.266			145.3			Very severe		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	99	1	9			2.7			49.5			Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	99	2	7.7			1.989			37.5			Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	99	3	5.7			2.546			43.9			Moderate	Moderate	Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	99	4	5			1.257			23.86			Mild		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	99	5	2.3			1.051			18.1			Mild		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	ⁿ	SD - Opacity	Mean OD ₂₀₀	ⁿ	SD - OD ₂₀₀	In Vitro Score ¹	ⁿ	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	1	37.3			3.553			90.6			Very severe	Severe	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	2	22.7			0.682			32.9			Moderate	Severe	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	3	22			0.63			31.5			Moderate	Severe	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	4	48.67			2.192			81.55			Very severe	Severe	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	5	31.7			2.357			67.1			Severe	Severe	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	water soluble	20%	90	1	28			-0.008			27.8			Moderate	Moderate	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	water soluble	20%	90	2	26.3			0.055			27.2			Moderate	Moderate	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	water soluble	20%	90	3	34.7			0.007			34.8			Moderate	Moderate	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	water soluble	20%	90	4	102			0.061			102.918			Very severe	Moderate	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	water soluble	20%	90	5	26.3			0.004			26.4			Moderate	Moderate	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	1	97.3			0.02			97.6			Very severe	Severe	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	2	96.3			0.116			98.1			Very severe	Severe	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	3	57.3			0.012			57.5			Severe	Severe	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	4	64			0.022			64.33			Severe	Severe	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	5	72			0.128			73.9			Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	98	1	31.7			2.705			72.2			Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	98	2	38.3			3.195			86.3			Very severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	98	3	18.3			3.015			63.6			Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	98	4	25.33			2.892			68.72			Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	98	5	34			2.097			65.4			Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	98	1	22.7			1.389			43.5			Moderate	Very Severe	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	98	2	27.7			4.128			89.6			Very severe	Very Severe	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	98	3	24.7			3.759			81			Very severe	Very Severe	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	98	4	17			3.97			71.22			Severe	Very Severe	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	98	5	23			3.58			76.7			Severe	Very Severe	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	98	1	6.7			0.293			11			Mild	Mild	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	98	2	1.7			0.163			4.1			Mild	Mild	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	98	3	3			0.606			12.1			Mild	Mild	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	98	4	3.33			0.066			4.33			Mild	Mild	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	98	5	6.3			0.543			14.5			Mild	Mild	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	1	141			0.399			147			Very severe	Very Severe	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	2	124			-0.071			122.9			Very severe	Very Severe	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	3	96.3			0.062			97.3			Very severe	Very Severe	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	4	97.66			0.277			101.78			Very severe	Very Severe	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	5	98.7			0.189			101.5			Very severe	Very Severe	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	water soluble	100%	97	1	18.3			4.442			85			Very severe	Moderate	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	water soluble	100%	97	2	7.3			2.838			49.9			Moderate	Moderate	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	water soluble	100%	97	3	12			3.87			70.1			Severe	Moderate	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	water soluble	100%	97	4	11.66			2.71			52.24			Moderate	Moderate	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	water soluble	100%	97	5	7			2.392			43.2			Moderate	Moderate	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	1	304.3			-0.017			304.1			Very severe	Very Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	2	389.3			0.117			391.1			Very severe	Very Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	3	418			-0.002			418			Very severe	Very Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	4	467			-0.016			467.09			Very severe	Very Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	5	304			0.234			307.5			Very severe	Very Severe	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	1	9			0.058			9.9			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	2	10.3			0.059			11.2			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	3	9.7			0.078			10.8			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	4	14.33			0.007			14.43			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	5	5.4			0.012			5.6			Mild	Mild	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	1	65			2.583			103.8			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	2	58.3			3.78			115			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	3	62.7			4.601			131.7			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	4	84			3.803			130.26			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	5	37			2.783			78.8			Severe	Very Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	1	12			0.415			18.2			Mild	Mild	Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	2	10.7			0.979			25.3			Moderate		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	3	6.7			0.925			20.5			Mild	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	4	21.33			0.68			31.533			Moderate		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	5	4.7			0.245			8.3			Mild		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1	31			2.893			74.4			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2	21.3			2.123			53.2			Moderate		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3	16.3			3.134			63.3			Severe	Severe	Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	4	36			4.134			98.01			Very severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	5	30			2.277			64.2			Severe		Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	99	1	8.7			0.737			19.7			Mild		Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	99	2	5.7			1.513			28.4			Moderate		Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	99	3	9			2.543			47.1			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	99	4	13.33			2.065			44.31			Moderate		Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	99	5	11			0.64			20.6			Mild		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	99	1	8.3			3.58			62			Severe		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	99	2	9			1.279			28.2			Moderate		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	99	3	4.3			1.761			30.7			Moderate	Nonsevere	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	99	4	7			3.347			58.71			Severe		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	99	5	7			0.837			19.6			Mild		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	97	1	26.7			0.052			27.5			Moderate		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	97	2	14.3			-0.014			14.1			Mild		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	97	3	5.7			-0.012			5.5			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	97	4	5.33			0.014			5.543			Mild		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	97	5	18.7			0.061			19.6			Mild		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	99	1	10.3			1.136			27.4			Moderate		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	99	2	5			1.916			33.7			Moderate		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	99	3	1.3			0.609			10.5			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	99	4	5.33			0.22			8.633			Mild		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	99	5	3.6			0.357			9			Mild		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	1	2.6			2.859			45.5			Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	2	4.3			9.837			151.9			Very severe		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	3	6.3			3.904			64.9			Severe	Nonsevere	Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	4	13			0.668			23.023			Mild		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	5	5.7			0.834			18.2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1	-2			-0.001			-2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2	-0.7			0.029			-0.2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3	0			0.018			0.3			Mild	Mild	Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	4	3			0.005			3.08			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	5	0			0.01			0.1			Mild		Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	1	17.7			3.591			71.5			Severe		Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	2	16			4.509			83.6			Very severe		Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	3	7			3.746			63.2			Severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	4	15.33			2.191			48.19			Moderate		Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	5	10.7			2.145			42.9			Moderate		Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	1	68.3			3.232			116.8			Very severe		Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	2	93			2.724			133.9			Very severe		Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	3	62.3			2.741			103.4			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	4	97.34			1.424			118.7			Very severe		Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	5	54.3			2.431			90.8			Very severe		Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	1	17			2.494			54.4			Moderate		Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	2	20			3.598			74			Severe		Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	3	19			3.248			67.7			Severe	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	4	26			1.052			41.78			Moderate		Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	5	21.4			1.39			42.2			Moderate		Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	1	11.7			1.868			39.7			Moderate		Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	2	23.3			2.409			59.5			Severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	ⁿ	SD - Opacity	Mean OD ₂₀₀	ⁿ	SD - OD ₂₀₀	In Vitro Score ¹	ⁿ	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	3	16			3.755			72.3			Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	4	30.66			3.189			78.5			Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	5	18.3			1.4			39.3			Moderate	Severe	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	1	67.6			-0.045			67			Severe	Nonsevere	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	2	17			-0.008			16.9			Mild	Nonsevere	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	3	21			-0.002			21			Mild	Nonsevere	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	4	56.33			0.495			63.76			Severe	Nonsevere	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	5	33.3			0.029			33.8			Moderate	Nonsevere	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	1	51.6			1.301			71.2			Severe	Moderate	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	2	42			0.299			46.5			Moderate	Moderate	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	3	38.3			0.887			51.6			Moderate	Moderate	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	4	43.1			0.72			53.9			Moderate	Moderate	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	5	45.3			0.384			51.1			Moderate	Moderate	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	1	16.3			0.002			16.3			Mild	Mild	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	2	6.7			-0.052			5.9			Mild	Mild	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	3	10.3			-0.015			10.1			Mild	Mild	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	4	17.33			0.013			17.53			Mild	Mild	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	5	11			-0.003			11			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	1	1.3			0.169			3.8			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	2	2.3			0.152			4.6			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	3	0.3			0.071			1.4			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	4	1			0.047			1.71			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	5	0.3			0.161			2.7			Mild	Mild	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1	68			1.665			93			Very severe	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2	51.3			1.069			67.4			Severe	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3	34			1.212			52.2			Moderate	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	4	58			1.38			78.71			Severe	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	5	51.7			0.607			60.8			Severe	Severe	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	1	4.7			0.273			8.8			Mild	Mild	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	2	8.7			0.759			20.1			Mild	Mild	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	3	5.7			0.307			10.3			Mild	Mild	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	4	8			0.35			13.25			Mild	Mild	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	5	5.7			0.305			10.3			Mild	Mild	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	1	119.4			0.095			120.8			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	2	65.7			0.045			66.3			Severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	3	41			0.065			42			Moderate	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	4	86.67			0.137			88.73			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	5	70			0.168			72.5			Severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	1	73.3			4.177			136			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	2	83			4.124			144.9			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	3	73			5.864			161			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	4	108			3.55			161.2			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	5	94.7			3.222			143			Very severe	Very Severe	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	1	11			2.159			43.4			Moderate	Moderate	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	2	13			4.392			78.9			Severe	Moderate	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	3	10			1.984			39.8			Moderate	Moderate	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	4	6			0.569			14.54			Mild	Moderate	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	5	6			1.464			28			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1	17.3			0.809			29.5			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2	11.3			1.006			26.4			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3	18.7			1.474			40.8			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	4	18			0.8996			31.82			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	5	13.3			0.679			23.5			Moderate	Moderate	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	1	0.3			0.019			0.6			Mild	Mild	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	2	2			0.036			2.5			Mild	Mild	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	3	-1.7			0.021			-1.3			Nonirritant	Mild	Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	ⁿ	SD - Opacity	Mean OD ₂₀₀	ⁿ	SD - OD ₂₀₀	In Vitro Score ¹	ⁿ	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	4	1			0.005			1.08			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	5	2.7			0.01			2.8			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	1	8.7			0.499			16.2			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	2	11			0.793			22.9			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	3	8.3			0.248			12			Mild	Mild	Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	4	7			0.692			17.38			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	5	3			0.234			6.5			Mild		Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	1	120.7			-0.022			120.3			Very severe		Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	2	87.7			-0.234			84.2			Very severe		Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	3	125			0.044			125.7			Very severe	Very Severe	Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	4	121.33			0.051			123.09			Very severe		Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	5	153.7			0.011			153.8			Very severe		Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	1	73.7			4.468			140.7			Very severe		Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	2	83.7			4.117			145.4			Very severe		Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	3	61			4.763			132.4			Very severe	Very Severe	Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	4	87.33			7.445			199.02			Very severe		Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	5	74.7			3.204			122.7			Very severe		Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	1	1			-0.047			0.3			Mild		Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	2	0.3			0.002			0.4			Mild		Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	3	1.7			0.028			2.1			Mild	Mild	Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	4	2.34			-0.033			1.85			Mild		Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	5	2			0.07			3.1			Mild		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	1	232.3			3.53			285.2			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	2	173.3			3.382			224.1			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	3	197			3.849			254.7			Very severe	Very Severe	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	4	283			4.329			348.27			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	5	197.3			3.321			247.2			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	1	100.3			4.471			167.4			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	2	80.7			3.504			133.2			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	3	88.7			3.856			146.5			Very severe	Very Severe	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	4	116.66			3.628			171.08			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	5	88			2.888			132.3			Very severe		Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	1	12.3			1.29			31.7			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	2	3.3			1.892			31.7			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	3	0.3			1.801			27.3			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	4	6			1.348			26.22			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	5	0			0.82			12.3			Mild		Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	surfactant	15%	98	1	4			2.884			47.3			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	surfactant	15%	98	2	6			5.801			93			Very severe		Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	surfactant	15%	98	3	3.3			3.988			63.2			Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	surfactant	15%	98	4	1.66			3.862			59.61			Severe		Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	surfactant	15%	98	5	7.7			3.042			53.3			Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	1	1.3			0.054			2.1			Mild		Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	2	6.7			0.059			7.6			Mild		Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	3	3			0.187			5.8			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	4	43			0.556			49.59			Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	5	4			0.081			4.9			Mild		Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	1	10			8.908			143.6			Very severe		Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	2	13.7			6.982			118.4			Very severe		Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	3	10			5.749			96.2			Very severe	Very Severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	4	11			3.568			64.531			Severe		Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	5	9.7			3.547			62.9			Severe		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	1	24			-0.023			23.6			Mild		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	2	8.3			-0.027			7.9			Mild		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	3	14.3			-0.008			14.2			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	4	21.33			-0.045			20.65			Mild		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	5	6			0.19			8.9			Mild		Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	1	88			4.095			149.4			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	2	106.3			2.19			139.2			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	3	82			3.572			135.6			Very severe	Very Severe	Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	4	81.01			3.76			137.44			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	5	74			1.671			99.1			Very severe		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	1	9.3			2.26			43.3			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	2	6			1.813			33.2			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	3	5.3			2.122			37.2			Moderate	Moderate	Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	4	2			2.427			38.41			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	5	4			1.473			26.1			Moderate		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	1	228			2.93			272			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	2	154.7			4.687			225			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	3	245.3			3.44			296.9			Very severe	Very Severe	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	4	277			3.072			323.08			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	5	157			3.115			203.7			Very severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	1	79.3			0.173			81.9			Very severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	2	49			0.053			49.8			Moderate		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	3	73.7			0.111			75.3			Severe	Severe/Very Severe	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	4	92.33			0.042			92.97			Very severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	5	78.4			0.067			79.3			Severe		Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	surfactant	5%	98	1	5.3			4.6			74.3			Severe		Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	surfactant	5%	98	2	8.3			6.553			106.6			Very severe		Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	surfactant	5%	98	3	3.7			5.099			80.2			Very severe	Very Severe	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	surfactant	5%	98	4	5			4.79			76.79			Very severe		Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	surfactant	5%	98	5	7.7			3.06			53.6			Moderate		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	1	6			5.312			85.7			Very severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	2	6.7			4.624			76			Severe	Severe/Very Severe	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	3	6			5.337			86.1			Very severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	4	3.33			3.617			57.58			Severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	5	7.7			2.567			46.2			Moderate		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	1	-0.7			0.006			-0.6			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	2	-0.3			-0.052			-1.1			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	3	-2			0.026			-1.6			Mild	Mild	Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	4	2.67			0.0003			2.711			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	5	0.1			0.026			0.4			Mild		Balls et al. (1995)
Anti-Dandruff Shampoo (HZY)	-	n.p.	n.p.	100%	n.p.	-	-0.092			0.182						Moderate	Moderate	Casterton et al. (1996)
Baby Shampoo No. 1 (HZP)	-	n.p.	n.p.	100%	n.p.	-	-0.02			0.062						Mild	Mild	Casterton et al. (1996)
Baby Shampoo No. 2 (HZF)	-	n.p.	n.p.	100%	n.p.	-	0.067			0.265						Moderate	Moderate	Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	n.p.	100%	n.p.	-	0.007			0.103						Moderate	Moderate	Casterton et al. (1996)
Cleansing Gel (HZQ)	-	n.p.	n.p.	100%	n.p.	-	0.034			0.073						Mild	Mild	Casterton et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	n.p.	100%	n.p.	-	0.034			0.068						Mild	Mild	Casterton et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	n.p.	100%	n.p.	-	0.067			0.001						Mild	Mild	Casterton et al. (1996)
Foam Bath (HZZ)	-	n.p.	n.p.	100%	n.p.	-	0.094			0.238						Moderate	Moderate	Casterton et al. (1996)
Gel Cleanser (HZE)	-	n.p.	n.p.	100%	n.p.	-	0.009			0.124						Mild	Mild	Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	n.p.	100%	n.p.	-	-0.007			0.01						Mild	Mild	Casterton et al. (1996)
Polishing Scrub (HZT)	-	n.p.	n.p.	100%	n.p.	-	0.027			0.015						Mild	Mild	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	n.p.	100%	n.p.	-	0.087			0.184						Moderate	Moderate	Casterton et al. (1996)
Shampoo No. 7 (HZA)	-	n.p.	n.p.	100%	n.p.	-	0.113			0.205						Moderate	Moderate	Casterton et al. (1996)
Shower Gel (HZS)	-	n.p.	n.p.	100%	n.p.	-	0.189			0.303						Moderate	Moderate	Casterton et al. (1996)
Skin Cleanser (HZL)	-	n.p.	n.p.	100%	n.p.	-	0.127			0.261						Moderate	Moderate	Casterton et al. (1996)
Acetone	67-64-1	liquid	water soluble	100%	n.p.	-	1.38			0.653						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (1%)	8001-54-5	liquid	surfactant	1%	n.p.	-	0.970			0.764						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	n.p.	-	1.612			1.180						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	n.p.	-	1.332			0.776						Severe	Severe	Casterton et al. (1996)
4-Bromophenotole	-	n.p.	n.p.	100%	n.p.	-	0.079			0.018						Mild	Mild	Casterton et al. (1996)

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n-Butanol	71-36-3	liquid	n.p.	100%	n.p.	-	0.414			0.671						Severe	Severe	Casterton et al. (1996)
2-Butoxyethanol	111-76-2	liquid	n.p.	100%	n.p.	-	0.394			1.160						Severe	Severe	Casterton et al. (1996)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	100%	n.p.	-	0.331			0.002						Mild	Mild	Casterton et al. (1996)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0%	n.p.	-	0.082			0.089						Mild	Mild	Casterton et al. (1996)
Cetylpyridinium bromide (1%)	140-72-7	liquid	surfactant	1%	n.p.	-	0.425			0.364						Moderate	Moderate	Casterton et al. (1996)
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	-	0.855			0.705						Severe	Severe	Casterton et al. (1996)
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	-	0.908			0.775						Severe	Severe	Casterton et al. (1996)
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	-	0.312			0.647						Severe	Severe	Casterton et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	n.p.	-	0.124			0.106						Mild	Mild	Casterton et al. (1996)
2,4-Difluoronitrobenzene	446-35-5	liquid	n.p.	100%	n.p.	-	0.049			0.008						Mild	Mild	Casterton et al. (1996)
1,3-Diisopropylbenzene	99-62-7	liquid	n.p.	100%	n.p.	-	0.029			0.000						Mild	Mild	Casterton et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	n.p.	-	1.30			1.11						Severe	Severe	Casterton et al. (1996)
Dodecane	112-40-3	liquid	n.p.	100%	n.p.	-	0.086			0.006						Mild	Mild	Casterton et al. (1996)
2-Ethylhexanol	104-76-7	liquid	water soluble	100%	n.p.	-	0.321			0.352						Moderate	Moderate	Casterton et al. (1996)
3-Ethyltoluene	620-14-4	liquid	n.p.	100%	n.p.	-	0.029			0.009						Mild	Mild	Casterton et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	-	0.330			0.257						Moderate	Moderate	Casterton et al. (1996)
Glycerol	56-81-5	liquid	water soluble	100%	n.p.	-	-0.020			0.013						Mild	Mild	Casterton et al. (1996)
1,5-Hexadiene	592-42-7	liquid	n.p.	100%	n.p.	-	0.164			0.085						Mild	Mild	Casterton et al. (1996)
Isobutanol	78-83-1	liquid	water insoluble*	100%	n.p.	-	0.453			0.688						Severe	Severe	Casterton et al. (1996)
Isopropanol	67-63-0	liquid	water soluble	100%	n.p.	-	0.593			0.526						Moderate	Moderate	Casterton et al. (1996)
Methyl acetate	79-20-9	liquid	water soluble	100%	n.p.	-	1.07			0.236						Moderate	Moderate	Casterton et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	n.p.	-	1.110			0.395						Moderate	Moderate	Casterton et al. (1996)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	n.p.	-	0.413			0.172						Moderate	Moderate	Casterton et al. (1996)
1-Methylpropyl benzene	135-98-8	liquid	n.p.	100%	n.p.	-	0.041			0.005						Mild	Mild	Casterton et al. (1996)
Parafluoramine	371-40-4	liquid	water insoluble	100%	n.p.	-	0.413			0.106						Moderate	Moderate	Casterton et al. (1996)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	-	-0.015			0.008						Mild	Mild	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	surfactant	100%	n.p.	-	-0.013			0.008						Mild	Mild	Casterton et al. (1996)
Propylene glycol	57-55-6	liquid	n.p.	100%	n.p.	-	0.076			0.024						Mild	Mild	Casterton et al. (1996)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	n.p.	-	1.69			1.28						Severe	Severe	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	-	1.97			1.23						Severe	Severe	Casterton et al. (1996)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	n.p.	-	0.163			0.424						Moderate	Moderate	Casterton et al. (1996)
Sodium lauryl sulfate (3%)	151-21-3	liquid	surfactant	3%	n.p.	-	0.040			0.113						Mild	Mild	Casterton et al. (1996)
Sodium lauryl sulfate (30%)	151-21-3	liquid	surfactant	30%	n.p.	-	0.095			0.312						Moderate	Moderate	Casterton et al. (1996)
Toluene	108-88-3	liquid	water insoluble*	100%	n.p.	-	0.420			0.805						Severe	Severe	Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	n.p.	-	0.029			0.011						Mild	Mild	Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	n.p.	-	1.43			0.031						Severe	Severe	Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	n.p.	-	0.281			0.564						Moderate	Moderate	Casterton et al. (1996)
Triton X-100 (1%)	9002-93-1	liquid	surfactant	1%	n.p.	-	0.083			0.063						Mild	Mild	Casterton et al. (1996)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	n.p.	-	0.281			1.003						Severe	Severe	Casterton et al. (1996)
Tween 20	9005-64-5	liquid	surfactant	100%	n.p.	-	-0.006			0.005						Mild	Mild	Casterton et al. (1996)
Xylene	1330-20-7	liquid	n.p.	100%	n.p.	-	0.220			0.257						Moderate	Moderate	Casterton et al. (1996)
Amway all fabric bleach	-	n.p.	n.p.	100%	n.p.	-	0.400			1.435						Severe	Severe	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	n.p.	100%	n.p.	-	2.249			1.381						Severe	Severe	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	n.p.	100%	n.p.	-	0.683			0.477						Moderate	Moderate	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	n.p.	100%	n.p.	-	2.205			1.839						Severe	Severe	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	n.p.	100%	n.p.	-	0.290			0.493						Moderate	Moderate	Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	n.p.	100%	n.p.	-	0.204			0.311						Moderate	Moderate	Casterton et al. (1996)
Amway fabric softener	-	n.p.	n.p.	100%	n.p.	-	0.089			0.013						Mild	Mild	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	n.p.	100%	n.p.	-	0.039			0.326						Moderate	Moderate	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	n.p.	100%	n.p.	-	0.193			0.050						Mild	Mild	Casterton et al. (1996)
Amway prewash liquid	-	liquid	n.p.	100%	n.p.	-	0.142			0.079						Mild	Mild	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	n.p.	100%	n.p.	-	1.437			0.763						Severe	Severe	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	n.p.	100%	n.p.	-	0.138			0.028						Mild	Mild	Casterton et al. (1996)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Amway SA8 laundry liquid	-	liquid	n.p.	100%	n.p.	-	0.032			0.179						Moderate	Moderate	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	n.p.	100%	n.p.	-	0.415			0.285						Moderate	Moderate	Casterton et al. (1996)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	1							156			Severe	Severe	Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	2							138			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	3							232			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	4							156			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	5							132			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	6							191			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	7							190			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	8							166			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	9	94.1	6	18.9	1.948	6	0.455	123	6	14.4	Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	10							101			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	11							200			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	12							90			Severe		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	1							5			Mild	Mild	Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	2							4			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	3							10			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	4							3			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	5							5			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	6							28			Moderate		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	7							2			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	8							4			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	9	9.7	6	2.3	0.012	6	0.007	10	6	2.3	Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	10							6			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	11							2			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	1							7			Mild	Mild	Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	2							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	3							3			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	4							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	5							6			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	6							7			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	7							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	8							6			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	9	10.9	6	1.4	0.144	6	0.188	13	6	2.5	Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	10							11			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	11							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	12							11			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	1							-2			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	3							-3			Nonirritant		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	4							0			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	6							-1			Nonirritant		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	8							0			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	9	1.4	6	1.2	0.003	6	0.007	1	6	1.3	Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	10							0			Mild		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	1							128			Severe	Severe	Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	2							124			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	3							163			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	4							106			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	5							128			Severe		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	6							129			Severe	Severe	Gautheron et al. (1994)	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	7							142			Severe		Gautheron et al. (1994)	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	8							129			Severe		Gautheron et al. (1994)	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	9	84.6	6	3.3	5.42	6	0.949	166	6	14.5	Severe		Gautheron et al. (1994)	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	11							142			Severe		Gautheron et al. (1994)	
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	12							116			Severe		Gautheron et al. (1994)	
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	1							4			Mild		Mild	Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	2							1			Mild			Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	3							0			Mild			Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	4							1			Mild			Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	5							1			Mild			Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	6							3			Mild	Gautheron et al. (1994)		
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	7							1			Mild	Gautheron et al. (1994)		
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	8							-10			Nonirritant	Gautheron et al. (1994)		
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	9	3.1	6	2.3	0.029	6	0.014	4	6	2.2	Mild	Gautheron et al. (1994)		
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	10							-1			Nonirritant	Gautheron et al. (1994)		
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	11							1			Mild	Gautheron et al. (1994)		
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	12							6			Mild	Gautheron et al. (1994)		
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	1							0			Mild	Mild	Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	2							2			Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	4							1			Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	5							0			Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	6							0			Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	7							0			Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	8							0			Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	9	1.1	6	0.6	-0.002	6	0.008	1	6	0.7	Mild		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)	
BR11-35	9002-92-0	surfactant	n.p.	10%	n.p.	12							-2			Nonirritant		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	1							48			Moderate	Moderate	Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	2							44			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	3							64			Severe		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	4							35			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	5							35			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	6							30			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	7							80			Severe		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	8							32			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	9	34.2	6	3.1	0.495	6	0.199	42	6	5	Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	10							53			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	11							35			Moderate		Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	12							49			Moderate		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	1							92			Severe	Severe	Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	2							108			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	3							96			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	4							81			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	5							130			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	6							93			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	7							104			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	8							90			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	9	76.6	6	3.9	4.341	6	0.551	142	6	8.2	Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	11							118			Severe		Gautheron et al. (1994)	
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	12							108			Severe		Gautheron et al. (1994)	
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	1							96			Severe	Gautheron et al. (1994)		

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	2							72			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	3							106			Moderate		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	4							73			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	5							119			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	6							103			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	7							88			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	8							46			Moderate		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	9	13.9	6	2.6	5.718	6	0.511	100	6	8	Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	10							60			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	11							200			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	12							59			Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	1							53			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	2							41			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	3							105			Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	4							39			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	5							42			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	6							34			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	7							49			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	8							41			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	9	31.1	6	3.2	4.119	6	1.341	92	6	22	Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	11							36			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	12							56			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	1							104			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	2							134			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	3							82			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	4							118			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	5							110			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	6							66			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	7							88			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	8							193			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	9	75.2	6	14.2	0.416	6	0.116	82	6	13.7	Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	11							213			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	12							135			Severe		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	1							23			Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	2							23			Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	3							18			Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	4							28			Moderate		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	5							16			Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	6							31			Moderate		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	7							18			Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	8							71			Severe		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	9	19.3	6	4.8	-0.01	6	0.004	19	6	4.7	Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	10							20			Mild		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	11							34			Moderate		Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	12							14			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	2							3			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	3							1			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	4							3			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	5							1			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	6							5			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	7							3			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	8							1			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	9	0.7	6	1.8	0.097	6	0.176	2	6	2.6	Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	11							5			Mild		Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	12							8			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	1							10			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	2							10			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	3							14			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	4							11			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	5							11			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	6							14			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	7							10			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	8							10			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	9	6.3	6	1.7	0.204	6	0.056	9	6	1.4	Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	11							4			Mild		Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	12							22			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	1							-1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	2							0			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	3							-8			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	4							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	5							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	6							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	7							1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	8							-6			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	9	0.8	6	0.5	0.01	6	0.014	1	6	0.6	Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	10							-1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	11							3			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	12							1			Mild		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1							58			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2							67			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3							70			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	4							45			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	5							60			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	6							64			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	7							58			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	8							51			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	9	22.3	6	4.1	1.56	6	0.316	46	6	6.6	Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	11							104			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	12							45			Moderate		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	1							99			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	2							100			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	3							128			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	4							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	5							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	6							85			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	7							94			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	8							93			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	9	61.7	6	1.9	1.515	6	0.134	84	6	1.2	Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	10							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	11							101			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	12							86			Severe		Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	1							26			Moderate		Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	2							38			Moderate		Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	3							31			Moderate		Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	4							33			Moderate		Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	5							21			Moderate		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	6							29			Moderate	Moderate	Gautheron et al. (1994)	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	7							28			Moderate	Moderate	Gautheron et al. (1994)	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	8							38			Moderate	Moderate	Gautheron et al. (1994)	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	9	24	6	2.9	0.117	6	0.007	26	6	3.8	Moderate	Moderate	Gautheron et al. (1994)	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	10							no data			n.a.	Moderate	Gautheron et al. (1994)	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	11							38			Moderate	Moderate	Gautheron et al. (1994)	
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	12							42			Moderate	Moderate	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	1							73			Severe	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	2							63			Severe	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	3							61			Severe	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	4							65			Severe	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	5							33			Moderate	Moderate	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	6							34			Moderate	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	7							87			Severe	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	8							48			Moderate	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	9	20.6	6	2.5	1.97	6	0.197	50	6	4	Moderate	Moderate	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	10							39			Moderate	Moderate	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	11							68			Severe	Severe	Gautheron et al. (1994)	
Furan	110-00-9	liquid	n.p.	100%	n.p.	12							51			Moderate	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	1							63			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	2							81			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	3							90			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	4							62			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	5							108			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	6							66			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	7							90			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	8							57			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	9	85.2	6	5.6	0.154	6	0.041	88	6	5.3	Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	10							no data			n.a.	Severe	Severe	Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	11							75			Severe	Severe	Gautheron et al. (1994)	
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	12							63			Severe	Severe	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	3							1			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	4							1			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	6							-4			Nonirritant	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	8							4			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	9	-0.2	6	0.5	-0.005	6	0.005	0	6	0.5	Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	10							2			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	11							0			Mild	Mild	Gautheron et al. (1994)	
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	12							-1			Nonirritant	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	1							18			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	2							24			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	3							25			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	4							14			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	5							13			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	6							6			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	7							15			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	8							18			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	9	16.6	6	4.5	0.065	6	0.082	18	6	4.7	Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	10							4			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	11							23			Mild	Mild	Gautheron et al. (1994)	
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	12							21			Mild	Mild	Gautheron et al. (1994)	

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1							93			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2							40			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3							53			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	4							33			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	5							91			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	6							42			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	7							82			Severe	Severe	Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	8							76			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	9	18.3	6	3.6	3.438	6	0.562	70	6	6.9	Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	11							48			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	12							102			Severe		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	1							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	2							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	3							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	4							0			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	5							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	6							1			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	7							3			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	8							1			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	9	1.3	6	1.8	0.002	6	0.002	1	6	1.8	Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	10							-1			Nonirritant		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	12							6			Mild		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1							75			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2							73			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3							140			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	4							81			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	5							96			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	6							62			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	7							82			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	8							122			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	9	40.3	6	9.9	1.598	6	0.271	64	6	11.2	Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	10							81			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	11							114			Severe		Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	12							65			Severe		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	3							6			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	4							0			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	5							4			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	6							0			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	7							1			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	8							12			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	9	0.2	6	0.4	-0.001	6	0.003	0	6	0.4	Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	11							6			Mild		Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	12							-4			Nonirritant		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	1							53			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	2							50			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	3							48			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	4							28			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	5							45			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	6							35			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	7							48			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	8							43			Moderate		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	9	7.8	6	0.9	3.653	6	0.496	63	6	7.3	Severe		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	11							89			Severe		Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	12							48			Moderate		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	1							81			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	2							82			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	3							103			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	4							76			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	5							92			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	6							68			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	7							90			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	8							62			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	9	16.2	6	4.3	5.742	6	1.462	102	6	24.8	Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	11							76			Severe		Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	12							55			Moderate		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	1							3			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	2							6			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	3							3			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	4							3			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	7							7			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	8							3			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	9	0.5	6	0.5	0.016	6	0.004	1	6	0.5	Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	11							0			Mild		Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	12							6			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	2							-1			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	8							-8			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	9	-0.2	6	0.4	-0.004	6	0.002	0	6	0.4	Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	10							0			Mild		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	11							-4			Nonirritant		Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	n.p.	20%	n.p.	12							-3			Nonirritant		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	1							88			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	2							88			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	3							54			Moderate		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	4							71			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	5							81			Severe		Gautheron et al. (1994)

***In Vitro* Data for Substances Tested in the BCOP Assay: Sorted by Reference**

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	<i>In Vitro</i> Score ¹	n	SD - Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	Reference
Methanol	67-56-1	liquid	n.p.	100%	n.p.	6							108			Severe	Severe	Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	7							37			Moderate	Severe	Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	8							19			Mild	Severe	Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	9	73.7	6	6	1.698	6	0.56	99	6	12.8	Severe	Severe	Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	11							179			Severe	Severe	Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	12							102			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	1							61			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	2							69			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	3							66			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	4							47			Moderate	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	5							48			Moderate	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	6							62			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	7							65			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	8							62			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	9	45.1	6	7.1	0.8	6	0.137	57	6	8.9	Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	11							74			Severe	Severe	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	12							88			Severe	Severe	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	1							22			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	2							25			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	3							27			Moderate	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	4							19			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	5							21			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	6							23			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	7							16			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	8							16			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	9	11.2	6	2.7	0.546	6	0.244	19	6	3.1	Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	11							20			Mild	Mild	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	12							11			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	3							0			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	4							1			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	6							0			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	8							-4			Nonirritant	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	9	0.4	6	1.4	0.005	6	0.004	1	6	1.4	Mild	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	11							-3			Nonirritant	Mild	Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	12							-1			Nonirritant	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	1							11			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	2							8			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	3							9			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	4							4			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	5							6			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	6							7			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	7							6			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	8							6			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	9	16.5	6	1.7	0.008	6	0.018	17	6	1.9	Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	10							4			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	11							6			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	12							7			Mild	Mild	Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	1							65			Severe	Severe	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	2							33			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	3							42			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	4							49			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	5							66			Severe		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	6							48			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	7							37			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	8							25			Mild		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	9	27.7	6	5	2.212	6	0.377	61	6	6.9	Severe		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	11										Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	12							64			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	1							61			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	2							79			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	3							75			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	4							34			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	5							70			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	6							46			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	7							54			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	8							44			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	9	49.1	6	3.4	0.084	6	0.036	50	6	3.4	Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	10							67			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	11							62			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	12							76			Severe		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	1							8			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	2							13			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	3							11			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	4							1			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	5							2			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	6							5			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	7							7			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	8							0			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	9	1.4	6	1.9	0.015	6	0.011	2	6	1.9	Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	10							3			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	11							5			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	12							9			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	3							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	4							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	8							-6			Nonirritant		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	9	0.7	6	0.4	-0.008	6	0.008	1	6	0.4	Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	10							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	11							-3			Nonirritant		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	2							12			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	3							15			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	4							9			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	5							28			Moderate		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	6							6			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	7							6			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	8							16			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	9	11.1	6	1	0.143	6	0.052	13	6	1.6	Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	10							15			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	11							13			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	12							15			Mild		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	1							117			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	2							156			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	3							109			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	4							111			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	5							164			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	6							174			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	7							103			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	8							50			Moderate		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	9	134.9	6	9.7	0.287	6	0.216	139	6	10.2	Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	11							94			Severe		Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	12							19			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	2							7			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	3							14			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	4							4			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	5							6			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	6							9			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	7							6			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	8							11			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	9	5.2	6	1.7	0.066	6	0.059	6	6	1.5	Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	11							12			Mild		Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	12							5			Mild		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	1							102			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	2							123			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	3							186			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	4							79			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	5							102			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	6							77			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	7							124			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	8							132			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	9	44.4	6	3.3	4.015	6	0.849	105	6	15.7	Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	11							96			Severe		Gautheron et al. (1994)
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	12							115			Severe		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	1							17			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	2							29			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	3							8			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	4							46			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	5							52			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	6							24			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	7							15			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	8							18			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	9	57	6	5.4	0.063	6	0.04	58	6	5.8	Severe		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	11							3			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	12							72			Severe		Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	1							2			Mild		Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	2							2			Mild		Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	3							9			Mild		Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	4							5			Mild		Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	5							3			Mild		Gautheron et al. (1994)

***In Vitro* Data for Substances Tested in the BCOP Assay: Sorted by Reference**

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	<i>In Vitro</i> Score ¹	n	SD - Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	Reference
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	6							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	7							4			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	8							3			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	9	1.7	6	0.9	0.103	6	0.042	3	6	1.3	Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	10							9			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	11							11			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	12							4			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	1							5			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	3							2			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	4							6			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	6							4			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	7							2			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	8							19			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	9	2.6	6	1.4	-0.003	6	0.006	3	6	1.4	Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	11							18			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	12							6			Mild	Mild	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	1							146			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	2							175			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	3							169			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	4							152			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	5							140			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	6							120			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	7							129			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	8							173			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	9	85.8	6	9.2	4.373	6	1.028	151	6	20.7	Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	11							203			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	12							104			Severe	Severe	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	1							47			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	2							42			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	3							78			Severe	Severe	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	4							28			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	5							42			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	6							47			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	7							48			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	8							24			Mild	Mild	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	9	7.7	6	1.9	5.561	6	1.398	91	6	20	Severe	Severe	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	10							no data			n.a.	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	11							28			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	12							47			Moderate	Moderate	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	2							4			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	3							0			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	4							0			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	5							-1			Nonirritant	Nonirritant	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	6							1			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	8							3			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	9	2.6	6	0.9	0.025	6	0.011	3	6	1	Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	10							no data			n.a.	Moderate	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	11							5			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	12							6			Mild	Mild	Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	1							25			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	2							14			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	3							26			Moderate		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	4							11			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	5							27			Moderate		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	6							7			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	7							9			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	8							15			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	9	12.5	6	1.5	0.579	6	0.369	21	6	4.5	Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	10							10			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	11							7			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	12							21			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	1							-1			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	2							1			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	4							0			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	5							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	6							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	7							0			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	8							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	9	3	6	1.6	0.008	6	0.014	3	6	1.7	Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	12							0			Mild		Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	n.p.	10%	n.p.	-				0.847	3	0.199	20.8			Severe	Severe	Gettings et al. (1996)
Baby Shampoo No. 1 (HZP) 100%	-	n.p.	n.p.	10%	n.p.	-				0.261	3	0.05	4.0			Nonsevere	Nonsevere	Gettings et al. (1996)
Baby Shampoo No. 2 (HZF) 100%	-	n.p.	n.p.	10%	n.p.	-				0.425	3	0.082	8.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	n.p.	10%	n.p.	-				0.956	3	0.324	17.5			Severe	Severe	Gettings et al. (1996)
Cleansing Gel (HZQ) 100%	-	n.p.	n.p.	10%	n.p.	-				0.164	3	0.05	2.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	n.p.	10%	n.p.	-				0.02	3	0.016	0.2			Nonsevere	Nonsevere	Gettings et al. (1996)
Facial Cleansing Foam (HZR) 25%	-	n.p.	n.p.	10%	n.p.	-				0.239	3	0.02	4.1			Nonsevere	Nonsevere	Gettings et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	n.p.	10%	n.p.	-				0.004	3	0.004	1.8			Nonsevere	Nonsevere	Gettings et al. (1996)
Foam Bath (HZL) 100%	-	n.p.	n.p.	10%	n.p.	-				0.912	3	0.261	18.6			Severe	Severe	Gettings et al. (1996)
Gel Cleanser (HZE) 100%	-	n.p.	n.p.	10%	n.p.	-				0.194	3	0.048	3.1			Nonsevere	Nonsevere	Gettings et al. (1996)
Hand Soap (HZU) 25%	-	n.p.	n.p.	10%	n.p.	-				0.293	3	0.09	5.5			Nonsevere	Nonsevere	Gettings et al. (1996)
Liquid Soap No. 2 (HZW) 25%	-	n.p.	n.p.	10%	n.p.	-				0.352	3	0.1	5.6			Nonsevere	Nonsevere	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	n.p.	10%	n.p.	-				0.199	3	0.024	2.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	n.p.	10%	n.p.	-				0.05	3	0.025	0.1			Nonsevere	Nonsevere	Gettings et al. (1996)
Polishing Scrub (HZT) 100%	-	n.p.	n.p.	10%	n.p.	-				-0.001	3	0.001	3.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 1 (HZC) 25%	-	n.p.	n.p.	10%	n.p.	-				0.957	3	0.306	30.0			Severe	Severe	Gettings et al. (1996)
Shampoo No. 2 (HZX) 25%	-	n.p.	n.p.	10%	n.p.	-				0.705	3	0.289	14.0			Severe	Severe	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	n.p.	10%	n.p.	-				0.214	3	0.049	4.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 4 (HZV) 25%	-	n.p.	n.p.	10%	n.p.	-				0.268	3	0.045	8.4			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 5 (HZD) 25%	-	n.p.	n.p.	10%	n.p.	-				0.241	3	0.08	2.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 6 (HZN) 25%	-	n.p.	n.p.	10%	n.p.	-				0.267	3	0.076	4.5			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 7 (HZA) 100%	-	n.p.	n.p.	10%	n.p.	-				0.406	3	0.156	6.6			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 8 (HZG) 25%	-	n.p.	n.p.	10%	n.p.	-				0.197	3	0.058	2.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shower Gel (HZS) 100%	-	n.p.	n.p.	10%	n.p.	-				1.548	3	0.093	35.9			Severe	Severe	Gettings et al. (1996)
Skin Cleanser (HZI) 100%	-	n.p.	n.p.	10%	n.p.	-				0.769	3	0.036	15.8			Severe	Severe	Gettings et al. (1996)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	1 (1)	4.3	3	2.1	0.037	3	0.036	4.9	3	2.4	Mild		Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	1 (2)	5.0	3	1.2	0.059	3	0.031	5.9	3	1.4	Mild		Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	2 (1)	1.6	3	1.2	0.153	3	0.059	3.9	3	1.8	Mild		Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	2 (2)	2.0	3	0.6	0.107	3	0.044	3.6	3	1	Mild		Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	3 (1)	3.7	3	0.6	0.100	3	0.033	5.2	3	0.6	Mild		Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	3 (2)	4.3	3	0.6	0.158	3	0.07	6.7	3	1.5	Mild		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (1)	84.0	3	3.8	7.408	3	0.903	195.2	3	11.3	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (2)	85.6	3	3.2	3.305	3	0.225	135.2	3	5.2	Very severe		Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

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Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (3)	82.0	3	1.7	3.729	3	0.25	137.9	3	2.3	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (4)	85.0	3	5.2	4.766	3	1.132	156.5	3	18.6	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (5)	87.7	3	1.7	3.354	3	0.108	138.0	3	0.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (6)	91.7	3	7.0	5.67	3	1.096	176.8			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (7)	98.3	3	2.6	5.645	3	0.523	183.0			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (8)	87.7	3	2.9	5.848	3	0.581	175.4			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (1)	88.0	3	7.5	4.426	3	0.623	154.4	3	11.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (2)	94.6	3	10.4	4.148	3	0.662	156.9	3	18.6	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (3)	87.0	3	7.5	4.252	3	0.069	150.8	3	7.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (4)	93.0	3	3.0	4.278	3	1.058	157.2	3	18.0	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (5)	98.3	3	2.3	3.972	3	0.360	157.9	3	3.4	Very severe	Very Severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (6)	95.7	3	5.0	4.129	3	0.581	157.0			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (7)	98.0	3	5.1	4.144	3	0.232	160.2			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (1)	96.7	3	2.0	4.015	3	1.011	156.9	3	17.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (2)	92.6	3	11.8	4.719	3	1.547	163.4	3	16.2	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (3)	105.0	3	6.1	4.316	3	0.320	169.7	3	10.2	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (4)	95.3	3	4.0	4.497	3	1.007	162.8	3	11.4	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (5)	92.3	3	7.2	3.948	3	0.231	151.6	3	7.7	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (6)	93.7	3	4.9	4.624	3	1.708	163.1	3	22.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (7)	100.7	3	2.5	4.473	3	0.619	167.8	3	7.8	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (8)	96.7	3	2.0	9.016	3	1.011	156.9	3	17.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (9)	97.3	3	5.1	4.183	3	0.514	160.0	3	8.2	Very severe		Southee (1998)
Butyl cellulosolve	111-76-2	liquid	n.p.	100%	n.p.	1 (1)	39	3	7.8	4.625	3	0.471	108.3	3	12.9	Very severe		Southee (1998)
Butyl cellulosolve	111-76-2	liquid	n.p.	100%	n.p.	1 (2)	43	3	4.0	4.589	3	0.418	111.8	3	5.5	Very severe		Southee (1998)
Butyl cellulosolve	111-76-2	liquid	n.p.	100%	n.p.	2 (1)	29.6	3	1.5	4.213	3	0.78	92.8	3	13	Very severe	Very Severe	Southee (1998)
Butyl cellulosolve	111-76-2	liquid	n.p.	100%	n.p.	2 (2)	31.3	3	2.3	4.526	3	0.864	99.2	3	10.7	Very severe		Southee (1998)
Butyl cellulosolve	111-76-2	liquid	n.p.	100%	n.p.	3 (1)	37.7	3	1.0	3.813	3	0.933	94.9	3	13.8	Very severe		Southee (1998)
Butyl cellulosolve	111-76-2	liquid	n.p.	100%	n.p.	3 (2)	37.7	3	6.1	4.031	3	1.206	98.2	3	21.6	Very severe		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	1 (1)	53.7	3	4.6	0.012	3	0.012	53.9	3	4.9	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	1 (2)	47.7	3	3.5	0.002	3	0.02	47.7	3	3.4	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	2 (1)	46.3	3	3.2	0.05	3	0.021	47.1	3	3.1	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	2 (2)	46.4	3	2.9	0.058	3	0.014	47.2	3	2.9	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	3 (1)	42	3	4.5	0.013	3	0.016	42.2	3	4.3	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	95	3 (2)	41.3	3	4.0	0.035	3	0.006	41.8	3	3.9	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (1)	17.6	3	2.3	1.265	3	0.252	36.6	3	6.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (2)	16.4	3	5.5	1.415	3	0.389	37.6	3	10.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (3)	13.7	3	1.5	1.062	3	0.322	29.6	3	6.4	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (4)	12.7	3	1.0	1.933	3	0.397	41.7	3	5.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (5)	14.7	3	2.1	1.125	3	0.162	31.5	3	4.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (6)	12.7	3	14.9	1.995	3	0.035	42.6			Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (7)	18.7	3	1.5	2.445	3	0.733	55.4			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (1)	13.3	3	1.0	2.626	3	0.909	52.7	3	12.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (2)	17.0	3	2.3	2.504	3	0.703	54.5	3	8.3	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (3)	16.3	3	4.9	3.025	3	0.699	61.7	3	7.8	Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (4)	17.3	3	1.5	2.857	3	0.250	60.2	3	4.9	Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (5)	14.7	3	2.1	2.636	3	0.427	54.2	3	5.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (6)	17.6	3	0.6	3.718	3	0.798	73.4			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (7)	15.0	3	2.6	3.267	3	0.545	64.0			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (8)	13.0	3	0.6	2.561	3	0.867	51.4			Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (1)	16.6	3	2.1	2.027	3	1.026	47.0	3	14.3	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (2)	18.0	3	2.9	1.831	3	0.061	45.4	3	2.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (3)	19.3	3	2.6	1.673	3	0.071	44.4	3	3.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (4)	22.0	3	2.6	1.583	3	0.426	45.7	3	8.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (5)	18.6	3	1.5	2.395	3	0.380	54.6	3	4.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (6)	17.0	3	1.2	1.853	3	0.268	44.8	3	5.1	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (7)	19.3	3	3.8	1.527	3	0.344	42.2	3	8.8	Moderate		Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1 (1)	0.6	3	0.6	-0.005	3	0.002	0.6	3	0.6	Mild	Nonirritant	Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1 (2)	0.3	3	1.0	-0.003	3	0.002	0.3	3	1.0	Mild		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2 (1)	0.6	3	0.6	0.012	3	0.007	0.8	3	0.6	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2 (2)	0.7	3	0.6	0.008	3	0.009	0.8	3	0.7	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3 (1)	1.0	3	0.6	-0.003	3	0.005	1.0	3	0.6	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3 (2)	0.7	3	0.0	0.007	3	0.011	0.8	3	0.2	Nonirritant		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1 (1)	13.3	3	2.0	0.654	3	0.273	23.1	3	5.9	Mild	Moderate	Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1 (2)	9.7	3	4.2	0.499	3	0.109	17.2	3	5.8	Mild		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2 (1)	13.7	3	3.2	1.398	3	0.601	34.6	3	12.1	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2 (2)	13.0	3	4.4	1.743	3	0.871	39.1	3	16.4	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3 (1)	17.3	3	1.0	0.958	3	0.100	31.7	3	2.3	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3 (2)	17.7	3	2.1	0.818	3	0.607	29.9	3	11.2	Moderate		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (1)	91.3	3	2.1	3.379	3	0.106	142.0	3	3.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (2)	88.0	3	7.5	3.306	3	0.597	137.6	3	6.8	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (3)	73.7	3	10.1	2.565	3	1.063	112.2	3	24.7	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (4)	86.0	3	9.6	3.006	3	1.078	131.1	3	6.7	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (5)	97.0	3	15.5	3.241	3	0.233	145.6	3	12.0	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (6)	115.3	3	9.1	3.150	3	0.181	162.6	3		Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (7)	70.3	3	4.5	3.681	3	0.691	125.5	3		Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (1)	85.7	3	9.8	3.490	3	0.309	138.1	3	13.0	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (2)	88.0	3	13.0	3.471	3	0.381	140.1	3	11.9	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (3)	86.3	3	6.0	3.240	3	0.651	134.9	3	9.4	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (4)	92.3	3	7.9	4.324	3	1.048	157.2	3	12.5	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (5)	88.0	3	16.7	3.308	3	0.695	137.6	3	6.8	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (6)	97.3	3	12.9	3.709	3	0.866	152.9			Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (7)	100.0	3	9.1	3.316	3	0.183	148.7			Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (1)	83.0	3	14.8	3.774	3	0.828	139.6	3	26.0	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (2)	91.7	3	9.3	3.232	3	0.702	140.1	3	18.9	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (3)	80.4	3	3.1	2.907	3	0.642	124.0	3	6.9	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (4)	82.3	3	2.1	3.093	3	0.635	128.7	3	8.2	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (5)	76.6	3	8.3	3.118	3	0.464	123.4	3	14.8	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (6)	76.3	3	8.7	2.862	3	0.292	121.2	3	4.6	Very severe		Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (7)	77.3	3	2.0	3.602	3	0.413	131.3	3	8.2	Very severe	Southee (1998)	
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1 (1)	47.6	3	5.9	1.706	3	0.679	73.3	3	15.9	Severe	Severe	Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1 (2)	48	3	2.1	1.32	3	0.303	67.8	3	5.7	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2 (1)	61	3	2.9	3.183	3	0.86	108.7	3	11.9	Very severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2 (2)	62	3	6.7	2.648	3	1.074	101.7	3	21.1	Very severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3 (1)	55.7	3	5.0	0.972	3	0.479	70.2	3	3.5	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3 (2)	54.4	3	1.5	1.278	3	0.359	73.5	3	6.4	Severe		Southee (1998)
Parafluoraniine	371-40-4	liquid	water insoluble	100%	99	1 (1)	15.3	3	1.0	1.044	3	0.413	31	3	7.2	Moderate	Moderate	Southee (1998)
Parafluoraniine	371-40-4	liquid	water insoluble	100%	99	1 (2)	16.3	3	3.5	1.243	3	0.287	35	3	6.2	Moderate		Southee (1998)
Parafluoraniine	371-40-4	liquid	water insoluble	100%	99	2 (1)	13.3	3	2.1	1.663	3	0.372	38.3	3	7.5	Moderate		Southee (1998)
Parafluoraniine	371-40-4	liquid	water insoluble	100%	99	2 (2)	16.0	3	4.6	1.432	3	0.531	37.5	3	12.2	Moderate		Southee (1998)
Parafluoraniine	371-40-4	liquid	water insoluble	100%	99	3 (1)	11.0	3	1.0	0.738	3	0.154	22.1	3	2.7	Mild		Southee (1998)
Parafluoraniine	371-40-4	liquid	water insoluble	100%	99	3 (2)	15.4	3	1.2	0.7	3	0.151	28.9	3	3.4	Moderate		Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	1 (1)	10.7	3	2.6	0.034	3	0.044	11.2	3	3.2	Mild	Mild	Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	1 (2)	7.0	3	0.6	0.023	3	0.026	7.4	3	0.6	Mild		Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	2 (1)	5.0	3	1.7	0.013	3	0.012	5.2	3	1.9	Mild		Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	2 (2)	3.4	3	1.5	0.016	3	0.015	3.6	3	1.6	Mild		Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	3 (1)	7.3	3	4.4	0.028	3	0.014	7.7	3	4.2	Mild		Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	3 (2)	5.6	3	0.6	0.04	3	0.051	6.2	3	0.7	Mild		Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Reference

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference	
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	1 (1)	176.7	3	31.4	4.551	3	1.019	245.0	3	28.7	Very severe	Very Severe	Southee (1998)	
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	1 (2)	172.0	3	1.7	3.676	3	0.201	227.1	3	3.4	Very severe		Southee (1998)	
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	2 (1)	170.0	3	20.7	4.755	3	0.586	241.3	3	11.9	Very severe		Southee (1998)	
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	2 (2)	166.7	3	12.6	4.590	3	0.405	235.5	3	7.3	Very severe		Southee (1998)	
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	3 (1)	124.0	3	13.7	4.604	3	0.380	193.1	3	19.0	Very severe		Southee (1998)	
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	3 (2)	165.3	3	21.2	3.303	3	0.388	214.9	3	15.5	Very severe		Southee (1998)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	1 (1)	-0.8	3	0.0	0.408	3	0.024	5.4	3	0.4	Mild		Southee (1998)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	1 (2)	0.0	3	0.6	0.348	3	0.182	5.2	3	2.7	Mild		Southee (1998)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	2 (1)	0.7	3	1.0	1.012	3	0.461	15.9	3	7.6	Mild		Southee (1998)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	2 (2)	1.0	3	0.6	1.086	3	0.083	17.3	3	1.7	Mild		Southee (1998)	
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	3 (1)	0.7	3	0.6	0.518	3	0.11	8.7	3	1.4	Mild	Southee (1998)		
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	3 (2)	1.3	3	0.6	0.283	3	0.064	5.6	3	1.5	Mild	Southee (1998)		
Sodium oxalate	62-76-0	solid	water soluble	20%	99	1 (1)	8.4	3	1.2	0.128	3	0.16	10.3	3	1.4	Mild	Nonirritant	Southee (1998)	
Sodium oxalate	62-76-0	solid	water soluble	20%	99	1 (2)	3.4	3	0.6	0.071	3	0.03	4.4	3	1.0	Mild		Southee (1998)	
Sodium oxalate	62-76-0	solid	water soluble	20%	99	2 (1)	-1.0	3	1.7	0.05	3	0.054	-0.3	3	1.5	Nonirritant		Southee (1998)	
Sodium oxalate	62-76-0	solid	water soluble	20%	99	2 (2)	-1.0	3	2.1	0.055	3	0.012	-0.1	3	2.1	Nonirritant		Southee (1998)	
Sodium oxalate	62-76-0	solid	water soluble	20%	99	3 (1)	2.0	3	0.6	0.051	3	0.032	2.7	3	0.9	Nonirritant		Southee (1998)	
Sodium oxalate	62-76-0	solid	water soluble	20%	99	3 (2)	2.3	3	1.0	0.15	3	0.022	4.5	3	1.3	Mild		Southee (1998)	
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	1 (1)	3.3	3	1.0	0.023	3	0.004	3.7	3	1.1	Mild		Southee (1998)	
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	1 (2)	1.3	3	1.0	0.035	3	0.006	1.8	3	1.0	Mild		Southee (1998)	
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	2 (1)	1.4	3	0.6	0.298	3	0.123	5.8	3	2.4	Mild		Southee (1998)	
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	2 (2)	0.0	3	0.6	0.226	3	0.086	3.4	3	1.0	Mild		Southee (1998)	
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	3 (1)	2.7	3	1.0	0.023	3	0.009	3.0	3	1.1	Nonirritant	Southee (1998)		
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	3 (2)	1.4	3	0.6	0.038	3	0.013	1.9	3	0.6	Nonirritant	Southee (1998)		
Tween 20	9005-64-5	liquid	surfactant	100%	98	1 (1)	0.3	3	0.0	0.003	3	0.012	0.3	3	0.2	Mild	Nonirritant	Southee (1998)	
Tween 20	9005-64-5	liquid	surfactant	100%	98	1 (2)	0.0	3	1.5	0.004	3	0.01	0.0	3	1.6	Mild		Southee (1998)	
Tween 20	9005-64-5	liquid	surfactant	100%	98	2 (1)	0.4	3	0.6	0.001	3	0.002	0.4	3	0.6	Mild		Southee (1998)	
Tween 20	9005-64-5	liquid	surfactant	100%	98	2 (2)	0.4	3	0.6	0.003	3	0.008	0.4	3	0.5	Nonirritant		Southee (1998)	
Tween 20	9005-64-5	liquid	surfactant	100%	98	3 (1)	0.0	3	0.0	0.022	3	0.018	0.3	3	0.3	Nonirritant		Southee (1998)	
Tween 20	9005-64-5	liquid	surfactant	100%	98	3 (2)	0.0	3	1.0	0.001	3	0.022	0.0	3	1.3	Nonirritant		Southee (1998)	
1-1 (#1)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	83.6	-	-	Severe		Severe	Swanson and Harbell (2000)
1-2 (#2)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	12.4	-	-	Mild			Swanson and Harbell (2000)
1-3 (#3)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	29.6	-	-	Moderate			Swanson and Harbell (2000)
2-4 (#4)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	7.3	-	-	Mild			Swanson and Harbell (2000)
2-7 (#7)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	21.4	-	-	Moderate	Swanson and Harbell (2000)		
2-8 (#8)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	31.8	-	-	Moderate	Swanson and Harbell (2000)		
Benchmark-Group 1 (#12)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	60.1	-	-	Severe	Swanson and Harbell (2000)		
Benchmark-Group 2 (#13)	-	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	60.1	-	-	Severe	Swanson and Harbell (2000)		
Ethanol (#14)	64-17-5	liquid	n.p.	100%	n.p.	-	-	-	-	-	-	-	52.7	-	-	Moderate	Swanson and Harbell (2000)		
Toilet Bowl Cleaner (#1)	-	liquid	n.p.	100%	n.p.	-	8.700	5	-	0.323	5	-	13.5	5	-	Mild	Swanson et al. (1995)		
Toilet Bowl Cleaner (#4)	-	liquid	n.p.	100%	n.p.	-	10.5	5	-	0.303	5	-	15	5	-	Mild	Swanson et al. (1995)		
All Purpose Cleaner (#5)	-	liquid	n.p.	100%	n.p.	-	102.5	5	-	1.252	5	-	121.3	5	-	Severe	Swanson et al. (1995)		
Bathroom Cleaner (#6)	-	liquid	n.p.	100%	n.p.	-	64	5	-	0.95	5	-	78.3	5	-	Severe	Swanson et al. (1995)		
All Purpose Cleaner (#7)	-	liquid	n.p.	100%	n.p.	-	348.1	5	-	3.013	5	-	393.3	5	-	Severe	Swanson et al. (1995)		
Pot and Pan Cleaner (#8)	-	liquid	n.p.	100%	n.p.	-	-1.8	5	-	0.078	5	-	-0.6	5	-	Nonirritant	Swanson et al. (1995)		
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	n.p.	100%	n.p.	-	315.4	5	-	2.619	5	-	354.7	5	-	Severe	Swanson et al. (1995)		
Floor Cleaner (#10)	-	liquid	n.p.	100%	n.p.	-	45.2	5	-	1.675	5	-	70.3	5	-	Severe	Swanson et al. (1995)		
General Cleaner (#11)	-	liquid	n.p.	100%	n.p.	-	77.9	5	-	0.359	5	-	83.3	5	-	Severe	Swanson et al. (1995)		
General Cleaner (#12)	-	liquid	n.p.	100%	n.p.	-	95.5	5	-	1.197	5	-	113.5	5	-	Severe	Swanson et al. (1995)		
Cleaner/Degreaser (#13)	-	liquid	n.p.	100%	n.p.	-	314.3	5	-	2.623	5	-	353.6	5	-	Severe	Swanson et al. (1995)		
Floor Stripper (#14)	-	liquid	n.p.	100%	n.p.	-	122.5	5	-	2.318	5	-	157.3	5	-	Severe	Swanson et al. (1995)		
Heavy Duty Cleaner (#15)	-	liquid	n.p.	100%	n.p.	-	323.3	5	-	2.24	5	-	357.1	5	-	Severe	Swanson et al. (1995)		
Degreaser (#16)	-	liquid	n.p.	100%	n.p.	-	225.4	5	-	2.022	5	-	255.7	5	-	Severe	Swanson et al. (1995)		
Floor Stripper (#17)	-	liquid	n.p.	100%	n.p.	-	180.5	5	-	2.38	5	-	216.2	5	-	Severe	Swanson et al. (1995)		
Floor Stripper (#18)	-	liquid	n.p.	100%	n.p.	-	407.1	5	-	2.481	5	-	444.3	5	-	Severe	Swanson et al. (1995)		
Glass Cleaner (#19)	-	liquid	n.p.	100%	n.p.	-	98.3	5	-	2.499	5	-	135.8	5	-	Severe	Swanson et al. (1995)		

***In Vitro* Data for Substances Tested in the BCOP Assay: Sorted by Reference**

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₉₀	n	SD - OD ₂₉₀	<i>In Vitro</i> Score ¹	n	SD - Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	Reference
Metal Cleaner (#20)	-	liquid	n.p.	100%	n.p.	-	344.2	5		3.182	5		391.9	5		Severe	Severe	Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	n.p.	100%	n.p.	-	-2.1	5		0.119	5		-0.3	5		Nonirritant	Nonirritant	Swanson et al. (1995)
Meat Room Degreaser (#3)	-	liquid	n.p.	100%	n.p.	-	99.3	5		2.733	5		140.3	5		Severe	Severe	Swanson et al. (1995)

Abbreviations: CASRN=Chemical Abstract Services Registry Number; n=number of replicates; n.s.=not applicable; n.p.=not provided; OD=optical density; SD=standard deviation

¹*In Vitro* Score = mean opacity score + (15 x mean OD₂₉₀ value) represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each independent test result, according to the classification system used

³Consensus call represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls. When there was an even number of different irritancy classifications for a test substance, the more severe irritancy classification was used for the overall classification for that test substance.

*solubility uncertain

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Appendix C2

BCOP Data Sorted by Substance Name

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In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
1-1 (#1)	-	liquid	n.p.	100%	n.p.	-							83.6			Severe	Severe	Swanson and Harbell (2000)
1-2 (#2)	-	liquid	n.p.	100%	n.p.	-							12.4			Mild	Mild	Swanson and Harbell (2000)
1-3 (#3)	-	liquid	n.p.	100%	n.p.	-							29.6			Moderate	Moderate	Swanson and Harbell (2000)
2-4 (#4)	-	liquid	n.p.	100%	n.p.	-							7.3			Mild	Mild	Swanson and Harbell (2000)
2-7 (#7)	-	liquid	n.p.	100%	n.p.	-							21.4			Moderate	Moderate	Swanson and Harbell (2000)
2-8 (#8)	-	liquid	n.p.	100%	n.p.	-							31.8			Moderate	Moderate	Swanson and Harbell (2000)
Acetone	67-64-1	liquid	water soluble	100%	99	1	90.3			3.676			145.5			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	2	83.7			2.389			119.5			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	3	55.7			4.315			120.4			Very severe	Very Severe	Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	4	94.33			2.492			131.72			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	99	5	69.3			1.942			98.4			Very severe		Balls et al. (1995)
Acetone	67-64-1	liquid	water soluble	100%	n.p.	-	1.38			0.653						Severe	Severe	Casterton et al. (1996)
Alkyl phosphoric acid ester/amine salt	-	liquid	moderate	100%	n.p.	-	37.7			3.577			91.3			Severe	Severe	Bailey et al. (2004)
All Purpose Cleaner (#5)	-	liquid	n.p.	100%	n.p.	-	102.5	5		1.252	5		121.3	5		Severe	Severe	Swanson et al. (1995)
All Purpose Cleaner (#7)	-	liquid	n.p.	100%	n.p.	-	348.1	5		3.013	5		393.3	5		Severe	Severe	Swanson et al. (1995)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	1							156			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	2							138			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	3							232			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	4							156			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	5							132			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	6							191			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	7							190			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	8							166			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	9	94.1	6	18.9	1.948	6	0.455	123	6	14.4	Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	10							101			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	11							200			Severe		Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	n.p.	100%	n.p.	12							90			Severe		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	1							5			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	2							4			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	3							10			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	4							3			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	5							5			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	6							28			Moderate		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	7							2			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	8							4			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	9	9.7	6	2.3	0.012	6	0.007	10	6	2.3	Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	10							6			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	11							2			Mild		Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	2							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	3							3			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	4							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	5							6			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	6							7			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	7							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	8							6			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	9	10.9	6	1.4	0.144	6	0.188	13	6	2.5	Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	10							11			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	11							5			Mild		Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	n.p.	20%	n.p.	12							11			Mild		Gautheron et al. (1994)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	1	6.3			0.132			8.3			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	2	6			0.026			6.4			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	3	6			0.079			7.2			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	4	11.34			0.698			21.82			Mild		Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	water soluble	20%	>99.9	5	4.7			0.034			5.2			Mild		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	1 (1)	4.3	3	2.1	0.037	3	0.036	4.9	3	2.4	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	1 (2)	5.0	3	1.2	0.059	3	0.031	5.9	3	1.4	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	2 (1)	1.6	3	1.2	0.153	3	0.059	3.9	3	1.8	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	2 (2)	2.0	3	0.6	0.107	3	0.044	3.6	3	1	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	3 (1)	3.7	3	0.6	0.100	3	0.033	5.2	3	0.6	Mild	Mild	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	n.p.	100%	n.p.	3 (2)	4.3	3	0.6	0.158	3	0.07	6.7	3	1.5	Mild	Mild	Southee (1998)
Amway all fabric bleach	-	n.p.	n.p.	100%	n.p.	-	0.400			1.435						Severe	Severe	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	n.p.	100%	n.p.	-	2.249			1.381						Severe	Severe	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	n.p.	100%	n.p.	-	0.683			0.477						Moderate	Moderate	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	n.p.	100%	n.p.	-	2.205			1.839						Severe	Severe	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	n.p.	100%	n.p.	-	0.290			0.493						Moderate	Moderate	Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	n.p.	100%	n.p.	-	0.204			0.311						Moderate	Moderate	Casterton et al. (1996)
Amway fabric softener	-	n.p.	n.p.	100%	n.p.	-	0.089			0.013						Mild	Mild	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	n.p.	100%	n.p.	-	0.039			0.326						Moderate	Moderate	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	n.p.	100%	n.p.	-	0.193			0.050						Mild	Mild	Casterton et al. (1996)
Amway prewash liquid	-	liquid	n.p.	100%	n.p.	-	0.142			0.079						Mild	Mild	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	n.p.	100%	n.p.	-	1.437			0.763						Severe	Severe	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	n.p.	100%	n.p.	-	0.138			0.028						Mild	Mild	Casterton et al. (1996)
Amway SA8 laundry liquid	-	liquid	n.p.	100%	n.p.	-	0.032			0.179						Moderate	Moderate	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	n.p.	100%	n.p.	-	0.415			0.285						Moderate	Moderate	Casterton et al. (1996)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	1							-2			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	3							-3			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	4							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	6							-1			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	7							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	8							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	9	1.4	6	1.2	0.003	6	0.007	1	6	1.3	Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	10							0			Mild	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	11							-2			Nonirritant	Mild	Gautheron et al. (1994)
Anthracene	120-12-7	solid	n.p.	20%	n.p.	12							2			Mild	Mild	Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY)	-	n.p.	n.p.	100%	n.p.	-	0.092			0.182						Moderate	Moderate	Casterton et al. (1996)
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	n.p.	10%	n.p.	-				0.847	3	0.199	20.8			Severe	Severe	Gettings et al. (1996)
Aromatic hydrocarbon #1	-	liquid	negligible	100%	n.p.	-	2.7			0.000			2.7			Mild	Mild	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	negligible	100%	n.p.	-	4.3			0.017			4.6			Mild	Mild	Bailey et al. (2004)
Arvl phosphonates	-	liquid	moderate	100%	n.p.	-	20.3			1.399			41.3			Moderate	Moderate	Bailey et al. (2004)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	1	2			-0.011			1.8			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	2	1.7			-0.107			0.1			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	3	2.7			-0.003			2.6			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	4	0.33			0.03			0.788			Mild	Mild	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	water soluble	20%	100	5	0			0.082			1.2			Mild	Mild	Balls et al. (1995)
Baby Shampoo No. 1 (HZP)	-	n.p.	n.p.	100%	n.p.	-	-0.02			0.062						Mild	Mild	Casterton et al. (1996)
Baby Shampoo No. 1 (HZP) 100%	-	n.p.	n.p.	10%	n.p.	-				0.261	3	0.05	4.0			Nonsevere	Nonsevere	Gettings et al. (1996)
Baby Shampoo No. 2 (HZF)	-	n.p.	n.p.	100%	n.p.	-	0.067			0.265						Moderate	Moderate	Casterton et al. (1996)
Baby Shampoo No. 2 (HZF) 100%	-	n.p.	n.p.	10%	n.p.	-				0.425	3	0.082	8.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Bathroom Cleaner (#6)	-	liquid	n.p.	100%	n.p.	-	64	5		0.95	5		78.3	5		Severe	Severe	Swanson et al. (1995)
Benchmark-Group 1 (#12)	-	liquid	n.p.	100%	n.p.	-							60.1			Severe	Severe	Swanson and Harbell (2000)
Benchmark-Group 2 (#13)	-	liquid	n.p.	100%	n.p.	-							60.1			Severe	Severe	Swanson and Harbell (2000)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (1)	84.0	3	3.8	7.408	3	0.903	195.2	3	11.3	Very severe	Very severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (2)	85.6	3	3.2	3.305	3	0.225	135.2	3	5.2	Very severe	Very severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (3)	82.0	3	1.7	3.729	3	0.25	137.9	3	2.3	Very severe	Very severe	Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (4)	85.0	3	5.2	4.766	3	1.132	156.5	3	18.6	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (5)	87.7	3	1.7	3.354	3	0.108	138.0	3	0.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (6)	91.7	3	7.0	5.67	3	1.096	176.8			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (7)	98.3	3	2.6	5.645	3	0.523	183.0			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	1 (8)	87.7	3	2.9	5.848	3	0.581	175.4			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (1)	88.0	3	7.5	4.426	3	0.623	154.4	3	11.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (2)	94.6	3	10.4	4.148	3	0.662	156.9	3	18.6	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (3)	87.0	3	7.5	4.252	3	0.069	150.8	3	7.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (4)	93.0	3	3.0	4.278	3	1.058	157.2	3	18.0	Very severe	Very Severe	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (5)	98.3	3	2.3	3.972	3	0.360	157.9	3	3.4	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (6)	95.7	3	5.0	4.129	3	0.581	157.0			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	2 (7)	98.0	3	5.1	4.144	3	0.232	160.2			Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (1)	96.7	3	2.0	4.015	3	1.011	156.9	3	17.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (2)	92.6	3	11.8	4.719	3	1.547	163.4	3	16.2	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (3)	105.0	3	6.1	4.316	3	0.320	169.7	3	10.2	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (4)	95.3	3	4.0	4.497	3	1.007	162.8	3	11.4	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (5)	92.3	3	7.2	3.948	3	0.231	151.6	3	7.7	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (6)	93.7	3	4.9	4.624	3	1.708	163.1	3	22.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (7)	100.7	3	2.5	4.473	3	0.619	167.8	3	7.8	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (8)	96.7	3	2.0	9.016	3	1.011	156.9	3	17.1	Very severe		Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	surfactant	10%	n.p.	3 (9)	97.3	3	5.1	4.183	3	0.514	160.0	3	8.2	Very severe		Southee (1998)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	1	59			3.588			112.8			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	2	37			3.566			90.5			Very severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	3	34.3			4.336			99.4			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	4	22			2.699			62.49			Severe		Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	surfactant	1%	98	5	38			2.706			78.6			Severe		Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	surfactant	1%	n.p.	-	0.970			0.764						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	1	75.3			4.456			142.2			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	2	79.3			5.223			157.7			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	3	61.7			4.142			123.8			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	4	63			4.967			137.5			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	98	5	74.7			3.096			121.1			Very severe		Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	surfactant	10%	n.p.	-	1.612			1.180						Severe	Severe	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	1	126.6			3.264			126.6			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	2	163.7			6.599			163.7			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	3	110.7			3.891			110.7			Very severe	Very Severe	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	4	130.41			4.338			130.41			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	98	5	111.1			3.117			111.1			Very severe		Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	surfactant	5%	n.p.	-	1.332			0.776						Severe	Severe	Casterton et al. (1996)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	1							128			Severe	Severe	Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	2							124			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	3							163			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	4							106			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	5							128			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	6							129			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	7							142			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	8							129			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	9	84.6	6	3.3	5.42	6	0.949	166	6	14.5	Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	11							142			Severe		Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	n.p.	10%	n.p.	12							116			Severe		Gautheron et al. (1994)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	1	169.7			0.218			173			Very severe	Very Severe	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	2	286.7			0.134			288.7			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	3	90			0.073			91.1			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	4	147			0.191			149.86			Very severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	water insoluble	20%	-	5	141.3			0.266			145.3			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	1							4			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	3							0			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	5							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	6							3			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	7							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	8							-10			Nonirritant		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	9	3.1	6	2.3	0.029	6	0.014	4	6	2.2	Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	10							-1			Nonirritant		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	11							1			Mild		Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	n.p.	20%	n.p.	12							6			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	1							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	2							2			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	4							1			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	5							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	6							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	7							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	8							0			Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	9	1.1	6	0.6	-0.002	6	0.008	1	6	0.7	Mild		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
BRU-35	9002-92-0	surfactant	n.p.	10%	n.p.	12							-2			Nonirritant		Gautheron et al. (1994)
4-Bromophenotole	-	n.p.	n.p.	100%	n.p.	-	0.079			0.018						Mild	Mild	Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	n.p.	100%	n.p.	-	0.007			0.103						Moderate	Moderate	Casterton et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	n.p.	10%	n.p.	-				0.956	3	0.324	17.5			Severe	Severe	Gettings et al. (1996)
n-Butanol	71-36-3	liquid	n.p.	100%	n.p.	-	0.414			0.671						Severe	Severe	Casterton et al. (1996)
2-Butoxyethanol	111-76-2	liquid	n.p.	100%	n.p.	-	0.394			1.160						Severe	Severe	Casterton et al. (1996)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	1	9			2.7			49.5			Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	2	7.7			1.989			37.5			Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	3	5.7			2.546			43.9			Moderate	Moderate	Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	4	5			1.257			23.86			Mild		Balls et al. (1995)
Butyl acetate	123-86-4	liquid	water insoluble*	100%	n.p.	5	2.3			1.051			18.1			Mild		Balls et al. (1995)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	1 (1)	39	3	7.8	4.625	3	0.471	108.3	3	12.9	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	1 (2)	43	3	4.0	4.589	3	0.418	111.8	3	5.5	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	2 (1)	29.6	3	1.5	4.213	3	0.78	92.8	3	13	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	2 (2)	31.3	3	2.3	4.526	3	0.864	99.2	3	10.7	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	3 (1)	37.7	3	1.0	3.813	3	0.933	94.9	3	13.8	Very severe		Southee (1998)
Butyl cellulolve	111-76-2	liquid	n.p.	100%	n.p.	3 (2)	37.7	3	6.1	4.031	3	1.206	98.2	3	21.6	Very severe		Southee (1998)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	1							48			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	2							44			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	3							64			Severe		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	4							35			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	5							35			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	6							30			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	7							80			Severe		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	8							32			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	9	34.2	6	3.1	0.495	6	0.199	42	6	5	Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	10							53			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	11							35			Moderate		Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	water soluble	100%	n.p.	12							49			Moderate		Gautheron et al. (1994)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	1	37.3			3.553			90.6			Very severe		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	2	22.7			0.682			32.9			Moderate		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	3	22			0.63			31.5			Moderate		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	4	48.67			2.192			81.55			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference	
gamma-Butyrolactone	96-48-0	liquid	water soluble	100%	>99	5	31.7			2.357			67.1			Severe		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	1	28		-0.008			27.8			Moderate		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	2	26.3		0.055			27.2			Moderate		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	3	34.7		0.007			34.8			Moderate	Moderate	Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	4	102		0.061			102.918			Very severe		Balls et al. (1995)	
Captan 90 concentrate	133-06-2	solid	water soluble	20%	20%	90	5	26.3		0.004			26.4			Moderate		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	1	97.3		0.02			97.6			Very severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	2	96.3		0.116			98.1			Very severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	3	57.3		0.012			57.5			Severe	Severe	Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	4	64		0.022			64.33			Severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	5	72		0.128			73.9			Severe		Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	100%	n.p.	-	0.331			0.002						Mild	Mild	Casterton et al. (1996)	
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	1 (1)	53.7	3	4.6	0.012	3	0.012	53.9	3	4.9	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	1 (2)	47.7	3	3.5	0.002	3	0.02	47.7	3	3.4	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	2 (1)	46.3	3	3.2	0.05	3	0.021	47.1	3	3.1	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	2 (2)	46.4	3	2.9	0.058	3	0.014	47.2	3	2.9	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	3 (1)	42	3	4.5	0.013	3	0.016	42.2	3	4.3	Moderate		Southee (1998)
4-Carboxybenzaldehyde	619-66-9	solid	water insoluble*	20%	20%	95	3 (2)	41.3	3	4.0	0.035	3	0.006	41.8	3	3.9	Moderate		Southee (1998)
Carboxylic acid amides	-	solid	moderate	100%	n.p.	-	10.7			1.125			27.5			Moderate	Moderate	Bailey et al. (2004)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	1	6.7		0.293			11			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	2	1.7		0.163			4.1			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	3	3		0.606			12.1			Mild	Mild	Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	4	3.33		0.066			4.33			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0.10%	n.p.	98	5	6.3		0.543			14.5			Mild		Balls et al. (1995)	
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	surfactant	0%	n.p.	-	0.082			0.089						Mild	Mild	Casterton et al. (1996)	
Cetylpyridinium bromide (1%)	140-72-7	liquid	surfactant	1%	n.p.	-	0.425			0.364						Moderate	Moderate	Casterton et al. (1996)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	1	22.7		1.389			43.5			Moderate		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	2	27.7		4.128			89.6			Very severe		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	3	24.7		3.759			81			Very severe	Very Severe	Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	4	17		3.97			71.22			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	98	5	23		3.58			76.7			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (10%)	140-72-7	liquid	surfactant	10%	n.p.	-	0.855			0.705						Severe	Severe	Casterton et al. (1996)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	1	31.7		2.705			72.2			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	2	38.3		3.195			86.3			Very severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	3	18.3		3.015			63.6			Severe	Severe	Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	4	25.33		2.892			68.72			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	98	5	34		2.097			65.4			Severe		Balls et al. (1995)	
Cetylpyridinium bromide (6%)	140-72-7	liquid	surfactant	6%	n.p.	-	0.908			0.775						Severe	Severe	Casterton et al. (1996)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	1	141			0.399			147			Very severe		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	2	124			-0.071			122.9			Very severe		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	3	96.3			0.062			97.3			Very severe	Very Severe	Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	4	97.66			0.277			101.78			Very severe		Balls et al. (1995)	
Chlorhexidine	55-56-1	solid	water insoluble*	20%	n.p.	5	98.7			0.189			101.5			Very severe		Balls et al. (1995)	
2-Chloro-2,4,4-trimethylpentane	-	liquid	negligible	100%	n.p.	-	4.0			0.004			4.1			Mild	Mild	Bailey et al. (2004)	
Clarified slurry oil	-	liquid	negligible	100%	n.p.	-	2.3			0.000			2.3			Mild	Mild	Bailey et al. (2004)	
Cleaner/Degreaser (#13)	-	liquid	n.p.	100%	n.p.	-	314.3	5		2.623	5		353.6	5		Severe	Severe	Swanson et al. (1995)	
Cleansing Gel (HZQ)	-	n.p.	n.p.	100%	n.p.	-	0.034			0.073						Mild	Mild	Casterton et al. (1996)	
Cleansing Gel (HZQ) 100%	-	n.p.	n.p.	10%	n.p.	-				0.164	3	0.05	2.3			Nonsevere	Nonsevere	Gettings et al. (1996)	
Cutting fluid (conc.) #1	-	liquid	emulsifies	100%	n.p.	-	3.3			0.001			3.5			Mild	Mild	Bailey et al. (2004)	
Cutting fluid (conc.) #2	-	liquid	emulsifies	100%	n.p.	-	4.3			0.038			4.9			Mild	Mild	Bailey et al. (2004)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	1	18.3			4.442			85			Very severe		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	2	7.3			2.838			49.9			Moderate		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	3	12			3.87			70.1			Severe	Moderate	Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	4	11.66			2.71			52.24			Moderate		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	5	7			2.392			43.2			Moderate		Balls et al. (1995)	
Cyclohexanol	108-93-0	liquid	water soluble	100%	n.p.	-	0.312			0.647						Severe	Severe	Casterton et al. (1996)	

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	1							92			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	2							108			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	3							96			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	4							81			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	5							130			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	6							93			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	7							104			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	8							90			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	9	76.6	6	3.9	4.341	6	0.551	142	6	8.2	Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	11							118			Severe		Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	n.p.	100%	n.p.	12							108			Severe		Gautheron et al. (1994)
Degreaser (#16)	-	liquid	n.p.	100%	n.p.	-	225.4	5		2.022	5		255.7	5		Severe	Severe	Swanson et al. (1995)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	1							96			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	2							72			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	3							106			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	4							73			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	5							119			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	6							103			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	7							88			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	8							46			Moderate		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	9	13.9	6	2.6	5.718	6	0.511	100	6	8	Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	10							60			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	11							200			Severe		Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	n.p.	10%	n.p.	12							59			Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	1							53			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	2							41			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	3							105			Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	4							39			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	5							42			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	6							34			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	7							49			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	8							41			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	9	31.1	6	3.2	4.119	6	1.341	92	6	22	Severe		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	11							36			Moderate		Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	n.p.	100%	n.p.	12							56			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	1							104			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	2							134			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	3							82			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	4							118			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	5							110			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	6							66			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	7							88			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	8							193			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	9	75.2	6	14.2	0.416	6	0.116	82	6	13.7	Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	11							213			Severe		Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	n.p.	20%	n.p.	12							135			Severe		Gautheron et al. (1994)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	1	304.3			-0.017			304.1			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	2	389.3			0.117			391.1			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	3	418			-0.002			418			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	4	467			-0.016			467.09			Very severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	water insoluble*	20%	99	5	304			0.234			307.5			Very severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	1	9			0.058			9.9			Mild		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	2	10.3			0.059			11.2			Mild		Balls et al. (1995)

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2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	3	9.7			0.078			10.8			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	4	14.33			0.007			14.43			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	99	5	5.4			0.012			5.6			Mild	Mild	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	water insoluble*	100%	n.p.	-	0.124			0.106						Mild	Mild	Casteron et al. (1996)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	1							23			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	2							23			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	3							18			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	4							28			Moderate	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	5							16			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	6							31			Moderate	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	7							18			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	8							71			Severe	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	9	19.3	6	4.8	-0.01	6	0.004	19	6	4.7	Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	10							20			Mild	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	11							34			Moderate	Mild	Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	n.p.	20%	n.p.	12							14			Mild	Mild	Gautheron et al. (1994)
2,4-Difluoronitrobenzene	446-35-5	liquid	n.p.	100%	n.p.	-	0.049			0.008						Mild	Mild	Casteron et al. (1996)
1,3-Diisopropylbenzene	99-62-7	liquid	n.p.	100%	n.p.	-	0.029			0.000						Mild	Mild	Casteron et al. (1996)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	1							0			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	2							3			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	3							1			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	4							3			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	5							1			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	6							5			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	7							3			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	8							1			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	9	0.7	6	1.8	0.097	6	0.176	2	6	2.6	Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	11							5			Mild	Mild	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	n.p.	20%	n.p.	12							8			Mild	Mild	Gautheron et al. (1994)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	1	65			2.583			103.8			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	2	58.3			3.78			115			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	3	62.7			4.601			131.7			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	4	84			3.803			130.26			Very severe	Very Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	96	5	37			2.783			78.8			Severe	Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	water insoluble	100%	n.p.	-	1.30			1.11						Severe	Severe	Casteron et al. (1996)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	1	12			0.415			18.2			Mild	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	2	10.7			0.979			25.3			Moderate	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	3	6.7			0.925			20.5			Mild	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	4	21.33			0.68			31.533			Moderate	Mild	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	water insoluble	20%	99.5	5	4.7			0.245			8.3			Mild	Mild	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	1							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	2							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	3							14			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	4							11			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	5							11			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	6							14			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	7							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	8							10			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	9	6.3	6	1.7	0.204	6	0.056	9	6	1.4	Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	11							4			Mild	Mild	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	n.p.	100%	n.p.	12							22			Mild	Mild	Gautheron et al. (1994)
Dodecane	112-40-3	liquid	n.p.	100%	n.p.	-	0.086			0.006						Mild	Mild	Casteron et al. (1996)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	1							-1			Mild	Mild	Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	2							0			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	3							-8			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	4							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	5							2			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	7							1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	8							-6			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	9	0.8	6	0.5	0.01	6	0.014	1	6	0.6	Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	10							-1			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	11							3			Mild		Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	n.p.	20%	n.p.	12							1			Mild		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1	31			2.893			74.4			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2	21.3			2.123			53.2			Moderate		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3	16.3			3.134			63.3			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	4	36			4.134			98.01			Very severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	5	30			2.277			64.2			Severe		Balls et al. (1995)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1							58			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2							67			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3							70			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	4							45			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	5							60			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	6							64			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	7							58			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	8							51			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	9	22.3	6	4.1	1.56	6	0.316	46	6	6.6	Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	11							104			Severe		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	12							45			Moderate		Gautheron et al. (1994)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (1)	17.6	3	2.3	1.265	3	0.252	36.6	3	6.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (2)	16.4	3	5.5	1.415	3	0.389	37.6	3	10.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (3)	13.7	3	1.5	1.062	3	0.322	29.6	3	6.4	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (4)	12.7	3	1.0	1.933	3	0.397	41.7	3	5.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (5)	14.7	3	2.1	1.125	3	0.162	31.5	3	4.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (6)	12.7	3	14.9	1.995	3	0.035	42.6			Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	1 (7)	18.7	3	1.5	2.445	3	0.733	55.4			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (1)	13.3	3	1.0	2.626	3	0.909	52.7	3	12.8	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (2)	17.0	3	2.3	2.504	3	0.703	54.5	3	8.3	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (3)	16.3	3	4.9	3.025	3	0.699	61.7	3	7.8	Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (4)	17.3	3	1.5	2.857	3	0.250	60.2	3	4.9	Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (5)	14.7	3	2.1	2.636	3	0.427	54.2	3	5.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (6)	17.6	3	0.6	3.718	3	0.798	73.4			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (7)	15.0	3	2.6	3.267	3	0.545	64.0			Severe		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	2 (8)	13.0	3	0.6	2.561	3	0.867	51.4			Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (1)	16.6	3	2.1	2.027	3	1.026	47.0	3	14.3	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (2)	18.0	3	2.9	1.831	3	0.061	45.4	3	2.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (3)	19.3	3	2.6	1.673	3	0.071	44.4	3	3.0	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (4)	22.0	3	2.6	1.583	3	0.426	45.7	3	8.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (5)	18.6	3	1.5	2.395	3	0.380	54.6	3	4.5	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (6)	17.0	3	1.2	1.853	3	0.268	44.8	3	5.1	Moderate		Southee (1998)
Ethanol	64-17-5	liquid	water soluble	100%	n.p.	3 (7)	19.3	3	3.8	1.527	3	0.344	42.2	3	8.8	Moderate		Southee (1998)
Ethanol (#14)	64-17-5	liquid	n.p.	100%	n.p.	-							52.7			Moderate	Moderate	Swanson and Harbell (2000)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	1							99			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	2							100			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	3							128			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	4							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	5							75			Severe		Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	6							85			Severe		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	7							94			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	8							93			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	9	61.7	6	1.9	1.515	6	0.134	84	6	1.2	Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	10							75			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	11							101			Severe	Severe	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	n.p.	100%	n.p.	12							86			Severe	Severe	Gautheron et al. (1994)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	8.7			0.737			19.7			Mild	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	5.7			1.513			28.4			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	3	9		2.543			47.1			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	4	13.33		2.065			44.31			Moderate	Moderate	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	water soluble	100%	n.p.	99	5	11		0.64			20.6			Mild	Moderate	Balls et al. (1995)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	1							26			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	2							38			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	3							31			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	4							33			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	5							21			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	6							29			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	7							28			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	8							38			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	9	24	6	2.9	0.117	6	0.007	26	6	3.8	Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	10							no data			n.a.	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	11							38			Moderate	Moderate	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	n.p.	100%	n.p.	12							42			Moderate	Moderate	Gautheron et al. (1994)
2-Ethylhexanol	104-76-7	liquid	water soluble	100%	n.p.	-	0.321			0.352						Moderate	Moderate	Casteron et al. (1996)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	1	8.3			3.58			62			Severe	Severe	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	2	9			1.279			28.2			Moderate	Nonsevere	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	3	4.3			1.761			30.7			Moderate	Nonsevere	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	4	7			3.347			58.71			Severe	Severe	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	water soluble	100%	n.p.	5	7			0.837			19.6			Mild	Severe	Balls et al. (1995)
Ethylhexyl acid phosphate ester	-	liquid	moderate	100%	n.p.	-	117.3			0.880			130.5			Severe	Severe	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	negligible	100%	n.p.	-	5.7			0.207			8.8			Mild	Mild	Bailey et al. (2004)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	1	26.7			0.052			27.5			Moderate	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	2	14.3			-0.014			14.1			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	3	5.7			-0.012			5.5			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	4	5.33			0.014			5.543			Mild	Mild	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	water soluble*	100%	n.p.	5	18.7			0.061			19.6			Mild	Mild	Balls et al. (1995)
3-Ethyltoluene	620-14-4	liquid	n.p.	100%	n.p.	-	0.029			0.009						Mild	Mild	Casteron et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	1	10.3			1.136			27.4			Moderate	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	2	5			1.916			33.7			Moderate	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	3	1.3			0.609			10.5			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	4	5.33			0.22			8.633			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	5	3.6			0.357			9			Mild	Mild	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	water insoluble*	100%	n.p.	-	0.330			0.257						Moderate	Moderate	Casteron et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	n.p.	100%	n.p.	-	0.034			0.068						Mild	Mild	Casteron et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	n.p.	10%	n.p.	-				0.02	3	0.016	0.2			Nonsevere	Nonsevere	Gettings et al. (1996)
Facial Cleaning Foam (HZR) 25%	-	n.p.	n.p.	10%	n.p.	-				0.239	3	0.02	4.1			Nonsevere	Nonsevere	Gettings et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	n.p.	100%	n.p.	-	0.067			0.001						Mild	Mild	Casteron et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	n.p.	10%	n.p.	-				0.004	3	0.004	1.8			Nonsevere	Nonsevere	Gettings et al. (1996)
Floor Cleaner (#10)	-	liquid	n.p.	100%	n.p.	-	45.2	5		1.675	5		70.3	5		Severe	Severe	Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	n.p.	100%	n.p.	-	-2.1	5		0.119	5		-0.3	5		Nonirritant	Nonirritant	Swanson et al. (1995)
Floor Stripper (#14)	-	liquid	n.p.	100%	n.p.	-	122.5	5		2.318	5		157.3	5		Severe	Severe	Swanson et al. (1995)
Floor Stripper (#17)	-	liquid	n.p.	100%	n.p.	-	180.5	5		2.38	5		216.2	5		Severe	Severe	Swanson et al. (1995)
Floor Stripper (#18)	-	liquid	n.p.	100%	n.p.	-	407.1	5		2.481	5		444.3	5		Severe	Severe	Swanson et al. (1995)
Foam Bath (HZL)	-	n.p.	n.p.	100%	n.p.	-	0.094			0.238						Moderate	Moderate	Casteron et al. (1996)
Foam Bath (HZL) 100%	-	n.p.	n.p.	10%	n.p.	-				0.912	3	0.261	18.6			Severe	Severe	Gettings et al. (1996)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	1	2.6			2.859			45.5			Moderate	Severe	Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	2	4.3			9.837			151.9			Very severe		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	3	6.3			3.904			64.9			Severe	Nonsevere	Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	4	13			0.668			23.023			Mild		Balls et al. (1995)
Fomesafen	72128-02-0	solid	water soluble	20%	97.5	5	5.7			0.834			18.2			Mild		Balls et al. (1995)
Furan	110-00-9	liquid	n.p.	100%	n.p.	1							73			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	2							63			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	3							61			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	4							65			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	5							33			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	6							34			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	7							87			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	8							48			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	9	20.6	6	2.5	1.97	6	0.197	50	6	4	Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	10							39			Moderate		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	11							68			Severe		Gautheron et al. (1994)
Furan	110-00-9	liquid	n.p.	100%	n.p.	12							51			Moderate		Gautheron et al. (1994)
Gel Cleanser (HZE)	-	n.p.	n.p.	100%	n.p.	-	0.009			0.124						Mild	Mild	Casterton et al. (1996)
Gel Cleanser (HZE) 100%	-	n.p.	n.p.	10%	n.p.	-				0.194	3	0.048	3.1			Nonsevere	Nonsevere	Gettings et al. (1996)
General Cleaner (#11)	-	liquid	n.p.	100%	n.p.	-	77.9	5		0.359	5		83.3	5		Severe	Severe	Swanson et al. (1995)
General Cleaner (#12)	-	liquid	n.p.	100%	n.p.	-	95.5	5		1.197	5		113.5	5		Severe	Severe	Swanson et al. (1995)
Glass Cleaner (#19)	-	liquid	n.p.	100%	n.p.	-	98.3	5		2.499	5		135.8	5		Severe	Severe	Swanson et al. (1995)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	1							63			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	2							81			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	3							90			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	4							62			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	5							108			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	6							66			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	7							90			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	8							57			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	9	85.2	6	5.6	0.154	6	0.041	88	6	5.3	Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	11							75			Severe		Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	n.p.	20%	n.p.	12							63			Severe		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	1							2			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	3							1			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	6							-4			Nonirritant		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	8							4			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	9	-0.2	6	0.5	-0.005	6	0.005	0	6	0.5	Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	10							2			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	11							0			Mild		Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	n.p.	20%	n.p.	12							-1			Nonirritant		Gautheron et al. (1994)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1	-2			-0.001			-2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2	-0.7			0.029			-0.2			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3	0			0.018			0.3			Mild	Mild	Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	4	3			0.005			3.08			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	5	0			0.01			0.1			Mild		Balls et al. (1995)
Glycerol	56-81-5	liquid	water soluble	100%	n.p.	-	-0.020			0.013						Mild	Mild	Casterton et al. (1996)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1 (1)	0.6	3	0.6	-0.005	3	0.002	0.6	3	0.6	Mild		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	1 (2)	0.3	3	1.0	-0.003	3	0.002	0.3	3	1.0	Mild		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2 (1)	0.6	3	0.6	0.012	3	0.007	0.8	3	0.6	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	2 (2)	0.7	3	0.6	0.008	3	0.009	0.8	3	0.7	Nonirritant		Southee (1998)
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3 (1)	1.0	3	0.6	-0.003	3	0.005	1.0	3	0.6	Nonirritant		Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Glycerol	56-81-5	liquid	water soluble	100%	>99.5	3 (2)	0.7	3	0.0	0.007	3	0.011	0.8	3	0.2	Nonirritant		Southee (1998)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	1							18			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	2							24			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	3							25			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	4							14			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	5							13			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	6							6			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	7							15			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	8							18			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	9	16.6	6	4.5	0.065	6	0.082	18	6	4.7	Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	10							4			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	11							23			Mild		Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	n.p.	100%	n.p.	12							21			Mild		Gautheron et al. (1994)
Hand Soap (HZU) 25%	-	n.p.	n.p.	10%	n.p.	-				0.293	3	0.09	5.5			Nonsevere	Nonsevere	Gettings et al. (1996)
Heavy Duty Cleaner (#15)	-	liquid	n.p.	100%	n.p.	-	323.3	5		2.24	5		357.1	5		Severe	Severe	Swanson et al. (1995)
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	n.p.	100%	n.p.	-	315.4	5		2.619	5		354.7	5		Severe	Severe	Swanson et al. (1995)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1							93			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2							40			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3							53			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	4							33			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	5							91			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	6							42			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	7							82			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	8							76			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	9	18.3	6	3.6	3.438	6	0.562	70	6	6.9	Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	11							48			Moderate		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	12							102			Severe		Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1 (1)	13.3	3	2.0	0.654	3	0.273	23.1	3	5.9	Mild		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	1 (2)	9.7	3	4.2	0.499	3	0.109	17.2	3	5.8	Mild		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2 (1)	13.7	3	3.2	1.398	3	0.601	34.6	3	12.1	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	2 (2)	13.0	3	4.4	1.743	3	0.871	39.1	3	16.4	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3 (1)	17.3	3	1.0	0.958	3	0.100	31.7	3	2.3	Moderate		Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	n.p.	10%	n.p.	3 (2)	17.7	3	2.1	0.818	3	0.607	29.9	3	11.2	Moderate		Southee (1998)
1,5-Hexadiene	592-42-7	liquid	n.p.	100%	n.p.	-	0.164			0.085						Mild	Mild	Casterton et al. (1996)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	1							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	2							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	3							2			Mild		Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	4							0			Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Hexane	110-54-3	liquid	n.p.	100%	n.p.	5							2			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	6							1			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	7							3			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	8							1			Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	9	1.3	6	1.8	0.002	6	0.002	1	6	1.8	Mild	Mild	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	10							-1			Nonirritant	Nonirritant	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	11							-2			Nonirritant	Nonirritant	Gautheron et al. (1994)
Hexane	110-54-3	liquid	n.p.	100%	n.p.	12							6			Mild	Mild	Gautheron et al. (1994)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	1	17.7			3.591			71.5			Severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	2	16			4.509			83.6			Very severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	3	7			3.746			63.2			Severe	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	4	15.33			2.191			48.19			Moderate	Severe/Very Severe	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	water insoluble*	100%	98	5	10.7			2.145			42.9			Moderate	Severe/Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	1	68.3			2.232			116.8			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	2	93			2.724			133.9			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	3	62.3			2.741			103.4			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	4	97.34			1.424			118.7			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	99	5	54.3			2.431			90.8			Very severe	Very Severe	Balls et al. (1995)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1							75			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2							73			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3							140			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	4							81			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	5							96			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	6							62			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	7							82			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	8							122			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	9	40.3	6	9.9	1.598	6	0.271	64	6	11.2	Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	10							81			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	11							114			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	12							65			Severe	Severe	Gautheron et al. (1994)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (1)	91.3	3	2.1	3.379	3	0.106	142.0	3	3.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (2)	88.0	3	7.5	3.306	3	0.597	137.6	3	6.8	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (3)	73.7	3	10.1	2.565	3	1.063	112.2	3	24.7	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (4)	86.0	3	9.6	3.006	3	1.078	131.1	3	6.7	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (5)	97.0	3	15.5	3.241	3	0.233	145.6	3	12.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (6)	115.3	3	9.1	3.150	3	0.181	162.6	3		Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	1 (7)	70.3	3	4.5	3.681	3	0.691	125.5	3		Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (1)	85.7	3	9.8	3.490	3	0.309	138.1	3	13.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (2)	88.0	3	13.0	3.471	3	0.381	140.1	3	11.9	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (3)	86.3	3	6.0	3.240	3	0.651	134.9	3	9.4	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (4)	92.3	3	7.9	4.324	3	1.048	157.2	3	12.5	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (5)	88.0	3	16.7	3.308	3	0.695	137.6	3	6.8	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (6)	97.3	3	12.9	3.709	3	0.866	152.9			Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	2 (7)	100.0	3	9.1	3.316	3	0.183	148.7			Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (1)	83.0	3	14.8	3.774	3	0.828	139.6	3	26.0	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (2)	91.7	3	9.3	3.232	3	0.702	140.1	3	18.9	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (3)	80.4	3	3.1	2.907	3	0.642	124.0	3	6.9	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (4)	82.3	3	2.1	3.093	3	0.635	128.7	3	8.2	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (5)	76.6	3	8.3	3.118	3	0.464	123.4	3	14.8	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (6)	76.3	3	8.7	2.862	3	0.292	121.2	3	4.6	Very severe	Very Severe	Southee (1998)
Imidazole	288-32-4	solid	water soluble	20%	n.p.	3 (7)	77.3	3	2.0	3.602	3	0.413	131.3	3	8.2	Very severe	Very Severe	Southee (1998)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	1							0			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	3							6			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	4							0			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	5							4			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	6							0			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	7							1			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	8							12			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	9	0.2	6	0.4	-0.001	6	0.003	0	6	0.4	Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	11							6			Mild	Mild	Gautheron et al. (1994)
Iminodibenzyl	494-19-9	solid	n.p.	20%	n.p.	12							-4			Nonirritant	Mild	Gautheron et al. (1994)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	1	17			2.494			54.4			Moderate	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	2	20			3.598			74			Severe	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	3	19			3.248			67.7			Severe	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	4	26			1.052			41.78			Moderate	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	99.9	5	21.4			1.39			42.2			Moderate	Moderate	Balls et al. (1995)
Isobutanol	78-83-1	liquid	water insoluble*	100%	n.p.	-	0.453			0.688						Severe	Severe	Casterton et al. (1996)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	1	11.7			1.868			39.7			Moderate	Moderate	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	2	23.3			2.409			59.5			Severe	Moderate	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	3	16			3.755			72.3			Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	4	30.66			3.189			78.5			Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	99.9	5	18.3			1.4			39.3			Moderate	Moderate	Balls et al. (1995)
Isopropanol	67-63-0	liquid	water soluble	100%	n.p.	-	0.593			0.526						Moderate	Moderate	Casterton et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	1							53			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	2							50			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	3							48			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	4							28			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	5							45			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	6							35			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	7							48			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	8							43			Moderate	Moderate	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	9	7.8	6	0.9	3.653	6	0.496	63	6	7.3	Severe	Severe	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	11							89			Severe	Severe	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	n.p.	10%	n.p.	12							48			Moderate	Moderate	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	1							81			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	2							82			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	3							103			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	4							76			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	5							92			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	6							68			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	7							90			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	8							62			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	9	16.2	6	4.3	5.742	6	1.462	102	6	24.8	Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	10							no data			n.a.	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	11							76			Severe	Severe	Gautheron et al. (1994)
Laurylsulfobetaine	14933-08-5	surfactant	n.p.	10%	n.p.	12							55			Moderate	Moderate	Gautheron et al. (1994)
Liquid Soap No. 2 (HZW) 25%	-	n.p.	n.p.	10%	n.p.	-				0.352	3	0.1	5.6			Nonsevere	Nonsevere	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	n.p.	10%	n.p.	-				0.199	3	0.024	2.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	1							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	2							6			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	3							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	4							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	6							1			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	7							7			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	8							3			Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	9	0.5	6	0.5	0.016	6	0.004	1	6	0.5	Mild	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	10							no data			n.a.	Mild	Gautheron et al. (1994)
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	11							0			Mild	Mild	Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Magnesium carbonate	56378-72-4	solid	n.p.	20%	n.p.	12							6			Mild		Gautheron et al. (1994)
Maneb	12427-38-2	solid	water soluble	20%	90	1	67.6			-0.045			67			Severe		Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	2	17			-0.008			16.9			Mild		Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	3	21			-0.002			21			Mild	Nonsevere	Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	4	56.33			0.495			63.76			Severe		Balls et al. (1995)
Maneb	12427-38-2	solid	water soluble	20%	90	5	33.3			0.029			33.8			Moderate		Balls et al. (1995)
Meat Room Degreaser (#3)	-	liquid	n.p.	100%	n.p.	-	99.3	5		2.733	5		140.3	5		Severe	Severe	Swanson et al. (1995)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	2							-1			Nonirritant		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	4							1			Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	8							-8			Nonirritant		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	9	-0.2	6	0.4	-0.004	6	0.002	0	6	0.4	Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	10							0			Mild		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	11							-4			Nonirritant		Gautheron et al. (1994)
2-Mercaptopurimidine	1450-85-7	solid	n.p.	20%	n.p.	12							-3			Nonirritant		Gautheron et al. (1994)
Metal Cleaner (#20)	-	liquid	n.p.	100%	n.p.	-	344.2	5		3.182	5		391.9	5		Severe	Severe	Swanson et al. (1995)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	1							88			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	2							88			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	3							54			Moderate		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	4							71			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	5							81			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	6							108			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	7							37			Moderate		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	8							19			Mild		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	9	73.7	6	6	1.698	6	0.56	99	6	12.8	Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	11							179			Severe		Gautheron et al. (1994)
Methanol	67-56-1	liquid	n.p.	100%	n.p.	12							102			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	1							61			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	2							69			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	3							66			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	4							47			Moderate		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	5							48			Moderate		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	6							62			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	7							65			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	8							62			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	9	45.1	6	7.1	0.8	6	0.137	57	6	8.9	Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	11							74			Severe		Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	n.p.	100%	n.p.	12							88			Severe		Gautheron et al. (1994)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	1	51.6			1.301			71.2			Severe		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	2	42			0.299			46.5			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	3	38.3			0.887			51.6			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	4	43.1			0.72			53.9			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	98	5	45.3			0.384			51.1			Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	liquid	water soluble	100%	n.p.	-	1.07			0.236						Moderate	Moderate	Casterton et al. (1996)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	1	16.3			0.002			16.3			Mild		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	2	6.7			-0.052			5.9			Mild		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	3	10.3			-0.015			10.1			Mild	Mild	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	4	17.33			0.013			17.53			Mild		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	water soluble*	100%	99	5	11			-0.003			11			Mild		Balls et al. (1995)
Methyl cyclopentadiene dimer	-	liquid	negligible	100%	n.p.	-	0.7			0.001			0.7			Mild	Mild	Bailey et al. (2004)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	1	1.3			0.169			3.8			Mild		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	2	2.3			0.152			4.6			Mild		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	3	0.3			0.071			1.4			Mild	Mild	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	4	1			0.047			1.71			Mild		Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	water insoluble*	100%	>99	5	0.3			0.161			2.7			Mild		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1	68			1.665			93			Very severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2	51.3			1.069			67.4			Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3	34			1.212			52.2			Moderate		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	4	58			1.38			78.71			Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	5	51.7			0.607			60.8			Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	n.p.	-	1.110			0.395						Moderate	Moderate	Casterton et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1 (1)	47.6	3	5.9	1.706	3	0.679	73.3	3	15.9	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	1 (2)	48	3	2.1	1.32	3	0.303	67.8	3	5.7	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2 (1)	61	3	2.9	3.183	3	0.86	108.7	3	11.9	Very severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	2 (2)	62	3	6.7	2.648	3	1.074	101.7	3	21.1	Very severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3 (1)	55.7	3	5.0	0.972	3	0.479	70.2	3	3.5	Severe		Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	water soluble	100%	99	3 (2)	54.4	3	1.5	1.278	3	0.359	73.5	3	6.4	Severe		Southee (1998)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	1	4.7			0.273			8.8			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	2	8.7			0.759			20.1			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	3	5.7			0.307			10.3			Mild	Mild	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	4	8			0.35			13.25			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	98	5	5.7			0.305			10.3			Mild		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	water insoluble*	100%	n.p.	-	0.413			0.172						Moderate	Moderate	Casterton et al. (1996)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	1							22			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	2							25			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	3							27			Moderate		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	4							19			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	5							21			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	6							23			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	7							16			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	8							16			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	9	11.2	6	2.7	0.546	6	0.244	19	6	3.1	Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	11							20			Mild		Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	n.p.	100%	n.p.	12							11			Mild		Gautheron et al. (1994)
1-Methylpropyl benzene	135-98-8	liquid	n.p.	100%	n.p.	-	0.041			0.005						Mild	Mild	Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	n.p.	100%	n.p.	-	-0.007			0.01						Mild	Mild	Casterton et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	n.p.	10%	n.p.	-				0.05	3	0.025	0.1			Nonsevere	Nonsevere	Gettings et al. (1996)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	1							2			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	2							1			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	3							0			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	4							1			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	5							0			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	6							0			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	7							1			Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	8							-4			Nonirritant		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	9	0.4	6	1.4	0.005	6	0.004	1	6	1.4	Mild		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	11							-3			Nonirritant		Gautheron et al. (1994)
MYRJ-45	-	surfactant	n.p.	10%	n.p.	12							-1			Nonirritant		Gautheron et al. (1994)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	1	119.4			0.095			120.8			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	2	65.7			0.045			66.3			Severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	3	41			0.065			42			Moderate		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	4	86.67			0.137			88.73			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	water insoluble*	20%	96	5	70			0.168			72.5			Severe		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	1	73.3			4.177			136			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	2	83			4.124			144.9			Very severe	Very Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	3	73			5.864			161			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	4	108			3.55			161.2			Very severe		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	water soluble*	20%	95	5	94.7			3.222			143			Very severe		Balls et al. (1995)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	1							11			Mild	Mild	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	2							8			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	3							9			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	4							4			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	5							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	6							7			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	7							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	8							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	9	16.5	6	1.7	0.008	6	0.018	17	6	1.9	Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	10							4			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	11							6			Mild		Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	n.p.	100%	n.p.	12							7			Mild		Gautheron et al. (1994)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	1	11			2.159			43.4			Moderate	Moderate	Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	2	13			4.392			78.9			Severe		Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	3	10			1.984			39.8			Moderate		Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	4	6			0.569			14.54			Mild		Balls et al. (1995)
n-Octanol	111-87-5	liquid	water insoluble*	100%	>99	5	6			1.464			28			Moderate		Balls et al. (1995)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	1							65			Severe		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	2							33			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	3							42			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	4							49			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	5							66			Severe		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	6							48			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	7							37			Moderate		Gautheron et al. (1994)
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	8							25			Mild	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	9	27.7	6	5	2.212	6	0.377	61	6	6.9	Severe	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	10							no data			n.a.	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	11							31			Moderate	Gautheron et al. (1994)	
Octanol	111-87-5	liquid	water insoluble*	100%	n.p.	12							64			Severe	Gautheron et al. (1994)	
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1	17.3			0.809			29.5			Moderate	Moderate	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2	11.3			1.006			26.4			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3	18.7			1.474			40.8			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	4	18			0.8996			31.82			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	5	13.3			0.679			23.5			Moderate		Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	n.p.	-	0.413			0.106						Moderate		Casterton et al. (1996)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1 (1)	15.3	3	1.0	1.044	3	0.413	31	3	7.2	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	1 (2)	16.3	3	3.5	1.243	3	0.287	35	3	6.2	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2 (1)	13.3	3	2.1	1.663	3	0.372	38.3	3	7.5	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	2 (2)	16.0	3	4.6	1.432	3	0.531	37.5	3	12.2	Moderate		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3 (1)	11.0	3	1.0	0.738	3	0.154	22.1	3	2.7	Mild		Southee (1998)
Parafluoraniiline	371-40-4	liquid	water insoluble	100%	99	3 (2)	15.4	3	1.2	0.7	3	0.151	28.9	3	3.4	Moderate		Southee (1998)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	1							61			Severe	Severe	Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	2							79			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	3							75			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	4							34			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	5							70			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	6							46			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	7							54			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	8							44			Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	9	49.1	6	3.4	0.084	6	0.036	50	6	3.4	Moderate		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	10							67			Severe		Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	11							62			Severe		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
2,4-Pentanedione	123-54-6	liquid	n.p.	100%	n.p.	12							76			Severe		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	1							8			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	2							13			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	3							11			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	4							1			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	5							2			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	6							5			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	7							7			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	8							0			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	9	1.4	6	1.9	0.015	6	0.011	2	6	1.9	Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	10							3			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	11							5			Mild		Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	n.p.	100%	n.p.	12							9			Mild		Gautheron et al. (1994)
Petroleum wax	-	solid	negligible	100%	n.p.	-	0.3			-0.001			0.3			Mild	Mild	Bailey et al. (2004)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	1							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	2							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	3							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	4							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	5							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	6							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	7							0			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	8							-6			Nonirritant		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	9	0.7	6	0.4	-0.008	6	0.008	1	6	0.4	Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	10							1			Mild		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	11							-3			Nonirritant		Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	n.p.	20%	n.p.	12							2			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	2							12			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	3							15			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	4							9			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	5							28			Moderate		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	6							6			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	7							6			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	8							16			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	9	11.1	6	1	0.143	6	0.052	13	6	1.6	Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	10							15			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	11							13			Mild		Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	n.p.	20%	n.p.	12							15			Mild		Gautheron et al. (1994)
Polishing Scrub (HZT)	-	n.p.	n.p.	100%	n.p.	-	0.027			0.015						Mild	Mild	Casterton et al. (1996)
Polishing Scrub (HZT) 100%	-	n.p.	n.p.	10%	n.p.	-				-0.001	3	0.001	3.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Polyalkenylsuccinate ester/amine salt	-	liquid	moderate	100%	n.p.	-	2.3			0.000			2.3			Mild	Mild	Bailey et al. (2004)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	1	0.3			0.019			0.6			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	2	2			0.036			2.5			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	3	-1.7			0.021			-1.3			Nonirritant	Mild	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	4	1			0.005			1.08			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	5	2.7			0.01			2.8			Mild		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	surfactant	100%	n.p.	-	-0.015			0.008						Mild	Mild	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	surfactant	100%	n.p.	-	-0.013			0.008						Mild	Mild	Casterton et al. (1996)
Pot and Pan Cleaner (#8)	-	liquid	n.p.	100%	n.p.	-	-1.8	5		0.078	5		-0.6	5		Nonirritant	Nonirritant	Swanson et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	1	8.7			0.499			16.2			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	2	11			0.793			22.9			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	3	8.3			0.248			12			Mild	Mild	Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	4	7			0.692			17.38			Mild		Balls et al. (1995)
Potassium cyanate	590-28-3	solid	water soluble	20%	97	5	3			0.234			6.5			Mild		Balls et al. (1995)
Process oil	-	liquid	negligible	100%	n.p.	-	2.7			0.004			2.7			Mild	Mild	Bailey et al. (2004)
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	1	120.7			-0.022			120.3			Very severe		Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	2	87.7			-0.234			84.2			Very severe	Very Severe	Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	3	125			0.044			125.7			Very severe		Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	4	121.33			0.051			123.09			Very severe		Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	98	5	153.7			0.011			153.8			Very severe		Balls et al. (1995)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	1							117			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	2							156			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	3							109			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	4							111			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	5							164			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	6							174			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	7							103			Severe		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	8							50			Moderate		Gautheron et al. (1994)	
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	9	134.9	6	9.7	0.287	6	0.216	139	6	10.2	Severe	Gautheron et al. (1994)		
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	10							no data			n.a.	Gautheron et al. (1994)		
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	11							94			Severe	Gautheron et al. (1994)		
Promethazine hydrochloride	58-33-3	solid	water soluble*	20%	n.p.	12							19			Mild	Gautheron et al. (1994)		
Propylene glycol	57-55-6	liquid	n.p.	100%	n.p.	-	0.076			0.024						Mild	Mild	Casterton et al. (1996)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	1							7			Mild		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	2							7			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	3							14			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	4							4			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	5							6			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	6							9			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	7							6			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	8							11			Mild	Gautheron et al. (1994)		
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	9	5.2	6	1.7	0.066	6	0.059	6	6	1.5	Mild	Mild	Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	11							12			Mild		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	n.p.	12							5			Mild		Gautheron et al. (1994)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	1 (1)	10.7	3	2.6	0.034	3	0.044	11.2	3	3.2	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	1 (2)	7.0	3	0.6	0.023	3	0.026	7.4	3	0.6	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	2 (1)	5.0	3	1.7	0.013	3	0.012	5.2	3	1.9	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	2 (2)	3.4	3	1.5	0.016	3	0.015	3.6	3	1.6	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	3 (1)	7.3	3	4.4	0.028	3	0.014	7.7	3	4.2	Mild		Southee (1998)	
Propyl-4-hydroxybenzoate	94-13-3	solid	n.p.	20%	100	3 (2)	5.6	3	0.6	0.04	3	0.051	6.2	3	0.7	Mild		Southee (1998)	
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	1	73.7			4.468			140.7			Very severe		Very Severe	Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	2	83.7			4.117			145.4			Very severe			Balls et al. (1995)
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	3	61			4.763			132.4			Very severe	Balls et al. (1995)		
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	4	87.33			7.445			199.02			Very severe	Balls et al. (1995)		
Pyridine	110-86-1	liquid	water soluble	100%	>99.9	5	74.7			3.204			122.7			Very severe	Balls et al. (1995)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	1							102			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	2							123			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	3							186			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	4							79			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	5							102			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	6							77			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	7							124			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	8							132			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	9	44.4	6	3.3	4.015	6	0.849	105	6	15.7	Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	10							no data			n.a.	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	11							96			Severe	Gautheron et al. (1994)		
Pyridine	110-86-1	liquid	water soluble	100%	n.p.	12							115			Severe	Gautheron et al. (1994)		
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	1	1			-0.047			0.3			Mild	Mild	Balls et al. (1995)	
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	2	0.3			0.002			0.4			Mild		Balls et al. (1995)	
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	3	1.7			0.028			2.1			Mild		Balls et al. (1995)	
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	4	2.34			-0.033			1.85			Mild		Balls et al. (1995)	

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	5	2			0.07			3.1			Mild		Balls et al. (1995)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	1							17			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	2							29			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	3							8			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	4							46			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	5							52			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	6							24			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	7							15			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	8							18			Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	9	57	6	5.4	0.063	6	0.04	58	6	5.8	Moderate		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	11							3			Mild		Gautheron et al. (1994)
Quinacrine	69-05-6	solid	water soluble*	20%	n.p.	12							72			Severe		Gautheron et al. (1994)
Shampoo No. 1 (HZC) 25%	-	n.p.	n.p.	10%	n.p.	-				0.957	3	0.306	30.0			Severe	Severe	Gettings et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	n.p.	100%	n.p.	-	0.087			0.184						Moderate	Moderate	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	n.p.	10%	n.p.	-				0.705	3	0.289	14.0			Severe	Severe	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	n.p.	10%	n.p.	-				0.214	3	0.049	4.3			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 4 (HZV) 25%	-	n.p.	n.p.	10%	n.p.	-				0.268	3	0.045	8.4			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 5 (HZD) 25%	-	n.p.	n.p.	10%	n.p.	-				0.241	3	0.08	2.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 6 (HZN) 25%	-	n.p.	n.p.	10%	n.p.	-				0.267	3	0.076	4.5			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 7 (HZA)	-	n.p.	n.p.	100%	n.p.	-	0.113			0.205						Moderate	Moderate	Casterton et al. (1996)
Shampoo No. 7 (HZA) 100%	-	n.p.	n.p.	10%	n.p.	-				0.406	3	0.156	6.6			Nonsevere	Nonsevere	Gettings et al. (1996)
Shampoo No. 8 (HZG) 25%	-	n.p.	n.p.	10%	n.p.	-				0.197	3	0.058	2.7			Nonsevere	Nonsevere	Gettings et al. (1996)
Shower Gel (HZS)	-	n.p.	n.p.	100%	n.p.	-	0.189			0.303						Moderate	Moderate	Casterton et al. (1996)
Shower Gel (HZS) 100%	-	n.p.	n.p.	10%	n.p.	-				1.548	3	0.093	35.9			Severe	Severe	Gettings et al. (1996)
Skin Cleanser (HZI)	-	n.p.	n.p.	100%	n.p.	-	0.127			0.261						Moderate	Moderate	Casterton et al. (1996)
Skin Cleanser (HZI) 100%	-	n.p.	n.p.	10%	n.p.	-				0.769	3	0.036	15.8			Severe	Severe	Gettings et al. (1996)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	1	100.3			4.471			167.4			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	2	80.7			3.504			133.2			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	3	88.7			3.856			146.5			Very severe	Very Severe	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	4	116.66			3.628			171.08			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	reagent grade	5	88			2.888			132.3			Very severe		Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	water soluble	1%	n.p.	-	1.69			1.28						Severe	Severe	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	1	232.3			3.53			285.2			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	2	173.3			3.382			224.1			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	3	197			3.849			254.7			Very severe	Very Severe	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	4	283			4.329			348.27			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	reagent grade	5	197.3			3.321			247.2			Very severe		Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	-	1.97			1.23						Severe	Severe	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	1 (1)	176.7	3	31.4	4.551	3	1.019	245.0	3	28.7	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	1 (2)	172.0	3	1.7	3.676	3	0.201	227.1	3	3.4	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	2 (1)	170.0	3	20.7	4.755	3	0.586	241.3	3	11.9	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	2 (2)	166.7	3	12.6	4.590	3	0.405	235.5	3	7.3	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	3 (1)	124.0	3	13.7	4.604	3	0.380	193.1	3	19.0	Very severe		Southee (1998)
Sodium hydroxide (10%)	1310-73-2	liquid	water soluble	10%	n.p.	3 (2)	165.3	3	21.2	3.303	3	0.388	214.9	3	15.5	Very severe		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	1	4			2.884			47.3			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	2	6			5.801			93			Very severe		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	3	3.3			3.988			63.2			Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	4	1.66			3.862			59.61			Severe		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	98	5	7.7			3.042			53.3			Moderate		Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	15%	n.p.	-	0.163			0.424						Moderate	Moderate	Casterton et al. (1996)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	1 (1)	-0.8	3	0.0	0.408	3	0.024	5.4	3	0.4	Mild		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	1 (2)	0.0	3	0.6	0.348	3	0.182	5.2	3	2.7	Mild		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	2 (1)	0.7	3	1.0	1.012	3	0.461	15.9	3	7.6	Mild		Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	2 (2)	1.0	3	0.6	1.086	3	0.083	17.3	3	1.7	Mild	Mild	Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	3 (1)	0.7	3	0.6	0.518	3	0.11	8.7	3	1.4	Mild		Southee (1998)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Sodium lauryl sulfate (15%)	151-21-3	liquid	surfactant	10%	98	3 (2)	1.3	3	0.6	0.283	3	0.064	5.6	3	1.5	Mild	Moderate	Southee (1998)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	1	12.3			1.29			31.7			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	2	3.3			1.892			31.7			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	3	0.3			1.801			27.3			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	4	6			1.348			26.22			Moderate	Moderate	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	98	5	0			0.82			12.3			Mild	Mild	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	surfactant	3%	n.p.	-	0.040			0.113						Mild	Mild	Casterton et al. (1996)
Sodium lauryl sulfate (30 %)	151-21-3	liquid	surfactant	30%	n.p.	-	0.095			0.312						Moderate	Moderate	Casterton et al. (1996)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	1	1.3			0.054			2.1			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	2	6.7			0.059			7.6			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	3	3			0.187			5.8			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	4	43			0.556			49.59			Moderate	Moderate	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	>99	5	4			0.081			4.9			Mild	Mild	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	2							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	3							9			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	4							5			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	5							3			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	6							2			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	7							4			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	8							3			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	9	1.7	6	0.9	0.103	6	0.042	3	6	1.3	Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	10							9			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	11							11			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	n.p.	12							4			Mild	Mild	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	1 (1)	8.4	3	1.2	0.128	3	0.16	10.3	3	1.4	Mild	Mild	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	1 (2)	3.4	3	0.6	0.071	3	0.03	4.4	3	1.0	Mild	Mild	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	2 (1)	-1.0	3	1.7	0.05	3	0.054	-0.3	3	1.5	Nonirritant	Nonirritant	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	2 (2)	-1.0	3	2.1	0.055	3	0.012	-0.1	3	2.1	Nonirritant	Nonirritant	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	3 (1)	2.0	3	0.6	0.051	3	0.032	2.7	3	0.9	Nonirritant	Nonirritant	Southee (1998)
Sodium oxalate	62-76-0	solid	water soluble	20%	99	3 (2)	2.3	3	1.0	0.15	3	0.022	4.5	3	1.3	Mild	Mild	Southee (1998)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	1	10			8.908			143.6			Very severe	Very severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	2	13.7			6.982			118.4			Very severe	Very severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	3	10			5.749			96.2			Very severe	Very severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	4	11			3.568			64.531			Severe	Severe	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	water soluble	20%	98.6	5	9.7			3.547			62.9			Severe	Severe	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	1	24			-0.023			23.6			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	2	8.3			-0.027			7.9			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	3	14.3			-0.008			14.2			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	4	21.33			-0.045			20.65			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	water insoluble*	20%	97	5	6			0.19			8.9			Mild	Mild	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	1							5			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	2							1			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	3							2			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	4							6			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	5							0			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	6							4			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	7							2			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	8							19			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	9	2.6	6	1.4	-0.003	6	0.006	3	6	1.4	Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	10							no data			n.a.	n.a.	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	11							18			Mild	Mild	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	n.p.	20%	n.p.	12							6			Mild	Mild	Gautheron et al. (1994)
Thiadiazole alkyl derivative	-	liquid	negligible	100%	n.p.	-	7.3			0.237			10.9			Moderate	Moderate	Bailey et al. (2004)
Thiourea	62-56-6	solid	water soluble	20%	>99	1	88			4.095			149.4			Very severe	Very severe	Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	2	106.3			2.19			139.2			Very severe	Very severe	Balls et al. (1995)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Thiourea	62-56-6	solid	water soluble	20%	>99	3	82			3.572			135.6			Very severe	Very Severe	Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	4	81.01			3.76			137.44			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	water soluble	20%	>99	5	74			1.671			99.1			Very severe		Balls et al. (1995)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	1							146			Severe	Severe	Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	2							175			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	3							169			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	4							152			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	5							140			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	6							120			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	7							129			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	8							173			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	9	85.8	6	9.2	4.373	6	1.028	151	6	20.7	Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	11							203			Severe		Gautheron et al. (1994)
Thiourea	62-56-6	solid	n.p.	20%	n.p.	12							104			Severe		Gautheron et al. (1994)
Toilet Bowl Cleaner (#1)	-	liquid	n.p.	100%	n.p.	-	8.700	5		0.323	5		13.5	5		Mild	Mild	Swanson et al. (1995)
Toilet Bowl Cleaner (#4)	-	liquid	n.p.	100%	n.p.	-	10.5	5		0.303	5		15	5		Mild		Swanson et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	1	9.3			2.26			43.3			Moderate	Moderate	Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	2	6			1.813			33.2			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	3	5.3			2.122			37.2			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	4	2			2.427			38.41			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	99	5	4			1.473			26.1			Moderate		Balls et al. (1995)
Toluene	108-88-3	liquid	water insoluble*	100%	n.p.	-	0.420			0.805						Severe		Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	1	79.3			0.173			81.9			Very severe	Severe/Very Severe	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	2	49			0.053			49.8			Moderate		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	3	73.7			0.111			75.3			Severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	4	92.33			0.042			92.97			Very severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	reagent grade	5	78.4			0.067			79.3			Severe		Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	water soluble	3%	n.p.	-	0.029			0.011						Mild		Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	1	228			2.93			272			Very severe	Very Severe	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	2	154.7			4.687			225			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	3	245.3			3.44			296.9			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	4	277			3.072			323.08			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	reagent grade	5	157			3.115			203.7			Very severe		Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	water soluble	30%	n.p.	-	1.43			0.031						Severe		Casterton et al. (1996)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	1							47			Moderate	Moderate	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	2							42			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	3							78			Severe		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	4							28			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	5							42			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	6							47			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	7							48			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	8							24			Mild		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	9	7.7	6	1.9	5.561	6	1.398	91	6	20	Severe		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	11							28			Moderate		Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	n.p.	100%	n.p.	12							47			Moderate		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	1							2			Mild	Mild	Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	2							4			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	3							0			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	4							0			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	5							-1			Nonirritant		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	6							1			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	7							1			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	8							3			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	9	2.6	6	0.9	0.025	6	0.011	3	6	1	Mild		Gautheron et al. (1994)

In Vitro Data for Substances Tested in the BCOP Assay: Sorted by Substance Name

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₂₀₀	n	SD - OD ₂₀₀	In Vitro Score ¹	n	SD - Score	In Vitro Classification ²	Consensus Classification ³	Reference
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	11							5			Mild		Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	n.p.	100%	n.p.	12							6			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	1							25			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	2							14			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	3							26			Moderate		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	4							11			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	5							27			Moderate		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	6							7			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	7							9			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	8							15			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	9	12.5	6	1.5	0.579	6	0.369	21	6	4.5	Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	10							10			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	11							7			Mild		Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	n.p.	100%	n.p.	12							21			Mild		Gautheron et al. (1994)
Triton X-100 (1%)	9002-93-1	liquid	surfactant	1%	n.p.	-	0.083			0.063						Mild		Casterton et al. (1996)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	1	6			5.312			85.7			Very severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	2	6.7			4.624			76			Severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	3	6			5.337			86.1			Very severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	4	3.33			3.617			57.58			Severe		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	98	5	7.7			2.567			46.2			Moderate		Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	surfactant	10%	n.p.	-	0.281			1.003						Severe		Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	1	5.3			4.6			74.3			Severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	2	8.3			6.553			106.6			Very severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	3	3.7			5.099			80.2			Very severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	4	5			4.79			76.79			Very severe		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	98	5	7.7			3.06			53.6			Moderate		Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	5%	n.p.	-	0.281			0.564						Moderate		Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	1 (1)	3.3	3	1.0	0.023	3	0.004	3.7	3	1.1	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	1 (2)	1.3	3	1.0	0.035	3	0.006	1.8	3	1.0	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	2 (1)	1.4	3	0.6	0.298	3	0.123	5.8	3	2.4	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	2 (2)	0.0	3	0.6	0.226	3	0.086	3.4	3	1.0	Mild		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	3 (1)	2.7	3	1.0	0.023	3	0.009	3.0	3	1.1	Nonirritant		Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	surfactant	10%	98	3 (2)	1.4	3	0.6	0.038	3	0.013	1.9	3	0.6	Nonirritant		Southee (1998)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	1							-1			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	2							1			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	3							-1			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	4							0			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	5							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	6							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	7							0			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	8							2			Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	9	3	6	1.6	0.008	6	0.014	3	6	1.7	Mild		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	10							no data			n.a.		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	11							-2			Nonirritant		Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	n.p.	10%	n.p.	12							0			Mild		Gautheron et al. (1994)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	1	-0.7			0.006			-0.6			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	2	-0.3			-0.052			-1.1			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	3	-2			0.026			-1.6			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	4	2.67			0.0003			2.711			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	n.p.	98	5	0.1			0.026			0.4			Mild		Balls et al. (1995)
Tween 20	9005-64-5	liquid	surfactant	100%	98	1 (1)	0.3	3	0.0	0.003	3	0.012	0.3	3	0.2	Mild		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	1 (2)	0.0	3	1.5	0.004	3	0.01	0.0	3	1.6	Mild		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	2 (1)	0.4	3	0.6	0.001	3	0.002	0.4	3	0.6	Mild		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	2 (2)	0.4	3	0.6	0.003	3	0.008	0.4	3	0.5	Nonirritant		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	98	3 (1)	0.0	3	0.0	0.022	3	0.018	0.3	3	0.3	Nonirritant		Southee (1998)

***In Vitro* Data for Substances Tested in the BCOP Assay: Sorted by Substance Name**

Substance	CASRN	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	Mean Opacity	n	SD - Opacity	Mean OD ₆₉₀	n	SD - OD ₆₉₀	<i>In Vitro</i> Score ¹	n	SD - Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	Reference
Tween 20	9005-64-5	liquid	surfactant	100%	98	3 (2)	0.0	3	1.0	0.001	3	0.022	0.0	3	1.3	Nonirritant		Southee (1998)
Tween 20	9005-64-5	liquid	surfactant	100%	n.p.	-	-0.006			0.005						Mild	Mild	Casterton et al. (1996)
Xylene	1330-20-7	liquid	n.p.	100%	n.p.	-	0.220			0.257						Moderate	Moderate	Casterton et al. (1996)

Abbreviations: CASRN=Chemical Abstract Services Registry Number; n=number of replicates; n.s.=not applicable; n.p.=not provided; OD=optical density; SD=standard deviation

¹*In Vitro* Score = mean opacity score + (15 x mean OD₆₉₀ value) represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each independent test result, according to the classification system used

³Consensus call represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls. When there was an even number of different irritancy classifications for a test substance, the more severe irritancy classification was used for the overall classification for that test substance.

*solubility uncertain

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Appendix D

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications

D1	BCOP Data Sorted by Reference	D-3
D2	BCOP Data Sorted by Substance Name	D-29

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Appendix D1

BCOP Data Sorted by Reference

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Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Alkyl phosphoric acid ester/amine salt	-	liquid	100%	n.p.	-	91.3	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
Aromatic hydrocarbon #1	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	100%	n.p.	-	4.6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aryl phosphonates	-	liquid	100%	n.p.	-	41.3	Moderate	Moderate	Category 2B		SCNM	SCNM	Bailey et al. (2004)
Carboxylic acid amides	-	solid	100%	n.p.	-	27.5	Moderate	Moderate	Category 1	4	Category I	R41	Bailey et al. (2004)
2-Chloro-2,4,4-trimethylpentane	-	liquid	100%	n.p.	-	4.1	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Clarified slurry oil	-	liquid	100%	n.p.	-	2.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Cutting fluid (conc.) #1	-	liquid	100%	n.p.	-	3.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Cutting fluid (conc.) #2	-	liquid	100%	n.p.	-	4.9	Mild	Mild	Nonirritant		Category III	Nonirritant	Bailey et al. (2004)
Ethylhexyl acid phosphate ester	-	liquid	100%	n.p.	-	130.5	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	100%	n.p.	-	8.8	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Methyl cyclopentadiene dimer	-	liquid	100%	n.p.	-	0.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Petroleum wax	-	solid	100%	n.p.	-	0.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Polyalkenylsuccinate ester/amine salt	-	liquid	100%	n.p.	-	2.3	Mild	Mild	SCNM		Category III	SCNM	Bailey et al. (2004)
Process oil	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Thiadiazole alkyl derivative	-	liquid	100%	n.p.	-	10.9	Moderate	Moderate	SCNM		Category III	SCNM	Bailey et al. (2004)
Acetone	67-64-1	liquid	100%	99	1	145.5	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	2	119.5	Very severe						Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	3	120.4	Very severe						Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	4	131.72	Very severe						Balls et al. (1995)
Acetone	67-64-1	liquid	100%	99	5	98.4	Very severe						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	1	8.3	Mild	Mild	Category 2B		Category III	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	2	6.4	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	3	7.2	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	4	21.82	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	5	5.2	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	1	1.8	Mild	Mild	SCNM ¹¹		SCNM	SCNM	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	2	0.1	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	3	2.6	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	4	0.788	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	5	1.2	Mild						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	1	142.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	2	157.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	3	123.8	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	4	137.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	5	121.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	1	126.6	Very severe	Very Severe	Category 1	2	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	2	163.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	3	110.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	4	130.41	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	5	111.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	1	112.8	Very severe	Very Severe	Category 1	1	Category II	R41	Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	2	90.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	3	99.4	Very severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	4	62.49	Severe						Balls et al. (1995)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	5	78.6	Severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	1	173	Very severe	Very Severe	Category 1	2	SCNM	R41	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	2	288.7	Very severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	3	91.1	Very severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	4	149.86	Very severe						Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	5	145.3	Very severe						Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	1	49.5	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	2	37.5	Moderate						Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	3	43.9	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Butyl acetate	123-86-4	liquid	100%	99	4	23.86	Mild						Balls et al. (1995)
Butyl acetate	123-86-4	liquid	100%	99	5	18.1	Mild						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	1	90.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	2	32.9	Moderate						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	3	31.5	Moderate						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	4	81.55	Very severe						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	5	67.1	Severe						Balls et al. (1995)
gamma-Butyrolactone	96-48-0	liquid	100%	>99	5	67.1	Severe						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	1	27.8	Moderate	Moderate	Category 1	4	Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	2	27.2	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	3	34.8	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	4	102.918	Very severe						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	5	26.4	Moderate						Balls et al. (1995)
Captan 90 concentrate	133-06-2	solid	20%	90	5	26.4	Moderate						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1	97.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2	98.1	Very severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3	57.5	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	4	64.33	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	5	73.9	Severe						Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	5	73.9	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	1	72.2	Severe	Severe	Category 1	2	SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	2	86.3	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	3	63.6	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	4	68.72	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	5	65.4	Severe						Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	5	65.4	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	1	43.5	Moderate	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	2	89.6	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	3	81	Very severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	4	71.22	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	5	76.7	Severe						Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	5	76.7	Severe						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	1	11	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	2	4.1	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	3	12.1	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	4	4.33	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	5	14.5	Mild						Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	5	14.5	Mild						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p. ¹²	1	147	Very severe	Very Severe	Category 1	4	SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	2	122.9	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	3	97.3	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	4	101.78	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	5	101.5	Very severe						Balls et al. (1995)
Chlorhexidine	55-56-1	solid	20%	n.p.	5	101.5	Very severe						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	1	85	Very severe	Moderate	Category 1	2	Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	2	49.9	Moderate						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	3	70.1	Severe						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	4	52.24	Moderate						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	5	43.2	Moderate						Balls et al. (1995)
Cyclohexanol	108-93-0	liquid	100%	97	5	43.2	Moderate						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	1	304.1	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	2	391.1	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	3	418	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	4	467.09	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	5	307.5	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	5	307.5	Very severe						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	1	9.9	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	2	11.2	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	3	10.8	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	4	14.43	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	5	5.6	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	5	5.6	Mild						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	1	103.8	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	2	115	Very severe						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	3	131.7	Very severe	Very Severe	SCNM		Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	4	130.26	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	5	78.8	Severe	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	1	18.2	Mild						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	2	25.3	Moderate	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	3	20.5	Mild						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	4	31.533	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	5	8.3	Mild						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	1	74.4	Severe	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	2	53.2	Moderate						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	3	63.3	Severe	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	4	98.01	Very severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	5	64.2	Severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	1	19.7	Mild						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	2	28.4	Moderate	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	3	47.1	Moderate						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	4	44.31	Moderate	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	5	20.6	Mild						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	1	62	Severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	2	28.2	Moderate						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	3	30.7	Moderate	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	4	58.71	Severe						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	5	19.6	Mild	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	1	27.5	Moderate						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	2	14.1	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	3	5.5	Mild						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	4	5.543	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	5	19.6	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	1	27.4	Moderate	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	2	33.7	Moderate						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	3	10.5	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	4	8.633	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	5	9	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	1	45.5	Moderate						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	2	151.9	Very severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	3	64.9	Severe						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	4	23.023	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	5	18.2	Mild						Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	1	-2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	2	-0.2	Mild						Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	3	0.3	Mild	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	4	3.08	Mild						Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	5	0.1	Mild	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	1	71.5	Severe						Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	2	83.6	Very severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	3	63.2	Severe						Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	4	48.19	Moderate	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
n-Hexanol	111-27-3	liquid	100%	98	5	42.9	Moderate						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	1	116.8	Very severe	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	2	133.9	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	3	103.4	Very severe	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	4	118.7	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	5	90.8	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	1	54.4	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Isobutanol	78-83-1	liquid	100%	99.9	2	74	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	3	67.7	Severe						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	4	41.78	Moderate						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	5	42.2	Moderate						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	1	39.7	Moderate	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	2	59.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	3	72.3	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	4	78.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	5	39.3	Moderate						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	1	67	Severe	Nonsevere	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	2	16.9	Mild						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	3	21	Mild						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	4	63.76	Severe						Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	5	33.8	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	1	71.2	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	2	46.5	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	3	51.6	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	4	53.9	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	5	51.1	Moderate						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	1	16.3	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	2	5.9	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	3	10.1	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	4	17.53	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	5	11	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	1	3.8	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	2	4.6	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	3	1.4	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	4	1.71	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	5	2.7	Mild						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1	93	Very severe	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2	67.4	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3	52.2	Moderate						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	4	78.71	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	5	60.8	Severe						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	1	8.8	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	2	20.1	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	3	10.3	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	4	13.25	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	5	10.3	Mild						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	1	120.8	Very severe	Very Severe	Category 1	NC	Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	2	66.3	Severe						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	3	42	Moderate						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	4	88.73	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	5	72.5	Severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	1	136	Very severe	Very Severe	Category 1	1	Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	2	144.9	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	3	161	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	4	161.2	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	5	143	Very severe						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	1	43.4	Moderate	Moderate	Category 2B		Category II	R36	Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	2	78.9	Severe						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	3	39.8	Moderate						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	4	14.54	Mild						Balls et al. (1995)
n-Octanol	111-87-5	liquid	100%	>99	5	28	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Parafluoraniiline	371-40-4	liquid	100%	99	1	29.5	Moderate	Moderate	SCNM		SCNM	SCNM	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	2	26.4	Moderate						Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	3	40.8	Moderate						Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	4	31.82	Moderate						Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	5	23.5	Moderate						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	1	0.6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	2	2.5	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	3	-1.3	Nonirritant						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	4	1.08	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	5	2.8	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	1	16.2	Mild	Mild	SCNM		SCNM	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	2	22.9	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	3	12	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	4	17.38	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	5	6.5	Mild						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	1	120.3	Very severe	Very Severe	Category 1	3	Category I	R41	Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	2	84.2	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	3	125.7	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	4	123.09	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	5	153.8	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	1	140.7	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	2	145.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	3	132.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	4	199.02	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	5	122.7	Very severe						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	1	0.3	Mild	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	2	0.4	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	3	2.1	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	4	1.85	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	5	3.1	Mild						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	1	285.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	2	224.1	Very severe						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	3	254.7	Very severe						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	4	348.27	Very severe						Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	5	247.2	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	1	167.4	Very severe	Very Severe	Category 2B		Category III	R36	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	2	133.2	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	3	146.5	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	4	171.08	Very severe						Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	5	132.3	Very severe						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	1	31.7	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	2	31.7	Moderate						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	3	27.3	Moderate						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	4	26.22	Moderate						Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	5	12.3	Mild						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	1	47.3	Moderate	Severe	Category 1	NC	Category I	R36	Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	2	93	Very severe						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	3	63.2	Severe						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	4	59.61	Severe						Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	5	53.3	Moderate						Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	1	2.1	Mild	Mild	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	2	7.6	Mild						Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	3	5.8	Mild						Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	>99	4	49.59	Moderate						Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Sodium oxalate	62-76-0	solid	20%	>99	5	4.9	Mild	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	1	143.6	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	2	118.4	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	3	96.2	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	4	64.531	Severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	5	62.9	Severe	Balls et al. (1995)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	1	23.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	2	7.9	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	3	14.2	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	4	20.65	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	5	8.9	Mild						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	1	149.4	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	2	139.2	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	3	135.6	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	4	137.44	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	5	99.1	Very severe						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	1	43.3	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	2	33.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	3	37.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	4	38.41	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	5	26.1	Moderate						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	1	272	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	2	225	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	3	296.9	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	4	323.08	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	5	203.7	Very severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	1	81.9	Very severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	2	49.8	Moderate						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	3	75.3	Severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	4	92.97	Very severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	5	79.3	Severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	1	74.3	Severe	Very Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	2	106.6	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	3	80.2	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	4	76.79	Very severe						Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	5	53.6	Moderate						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	1	85.7	Very severe	Severe/Very Severe	Category 1	NC	Category II	R41	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	2	76	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	3	86.1	Very severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	4	57.58	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	5	46.2	Moderate						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	1	-0.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	2	-1.1	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	3	-1.6	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	4	2.711	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	5	0.4	Mild						Balls et al. (1995)
Anti-Dandruff Shampoo (HZY)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Baby Shampoo No. 1 (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Baby Shampoo No. 2 (HZF)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Cleansing Gel (HZQ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Foam Bath (HZL)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Gel Cleanser (HZE)	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	SCNM	Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polishing Scrub (HZT)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Shampoo No. 7 (HZA)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Shower Gel (HZS)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Skin Cleanser (HZI)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Acetone	67-64-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A		Category II	R36	Casterton et al. (1996)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	n.p.	-	-	Severe	Severe	Category 1	1	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)
4-Bromophenotole	-	n.p.	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
n-Butanol	71-36-3	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)
2-Butoxyethanol	111-76-2	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)
4-Carboxybenzaldehyde	619-66-9	solid	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	R36	Casterton et al. (1996)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Cetylpyridinium bromide (1%)	140-72-7	liquid	1%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	n.p.	-	-	Severe	Severe	Category 1	2	SCNM	R41	Casterton et al. (1996)
Cyclohexanol	108-93-0	liquid	100%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	SCNM	Casterton et al. (1996)
2,4-Difluoronitrobenzene	446-35-5	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
1,3-Diisopropylbenzene	99-62-7	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	n.p.	-	-	Severe	Severe	SCNM		Category I	SCNM	Casterton et al. (1996)
Dodecane	112-40-3	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
2-Ethylhexanol	104-76-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category II	R36	Casterton et al. (1996)
3-Ethyltoluene	620-14-4	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Glycerol	56-81-5	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
1,5-Hexadiene	592-42-7	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Isobutanol	78-83-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A		Category II	R36	Casterton et al. (1996)
Isopropanol	67-63-0	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	SCNM	Casterton et al. (1996)
Methyl acetate	79-20-9	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category II	R36	Casterton et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	R36	Casterton et al. (1996)
Methyl isobutyl ketone	108-10-1	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
1-Methylpropyl benzene	135-98-8	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Paraffluoriline	371-40-4	liquid	100%	n.p.	-	-	Moderate	Moderate	SCNM		SCNM	SCNM	Casterton et al. (1996)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Propylene glycol	57-55-6	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Sodium hydroxide (1%)	1310-73-2	liquid	1%	n.p.	-	-	Severe	Severe	Category 2B		Category III	R36	Casterton et al. (1996)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	n.p.	-	-	Moderate	Moderate	Category 1	NC	Category I	R36	Casterton et al. (1996)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Sodium lauryl sulfate (30 %)	151-21-3	liquid	30%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Toluene	108-88-3	liquid	100%	n.p.	-	-	Severe	Severe	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	5%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	Nonirritant	Casterton et al. (1996)
Triton X-100 (1%)	9002-93-1	liquid	1%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Triton X-100 (10%)	9002-93-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 1	NC	Category II	R41	Casterton et al. (1996)
Tween 20	9005-64-5	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Xylene	1330-20-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category II	Nonirritant	Casterton et al. (1996)
Amway all fabric bleach	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	SCNM	R41	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	100%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway fabric softener	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R36	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		SCNM	Nonirritant	Casterton et al. (1996)
Amway prewash liquid	-	liquid	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	SCNM	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	Nonirritant	Casterton et al. (1996)
Amway SA8 laundry liquid	-	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Allyl alcohol	107-18-6	liquid	100%	n.p.	1	156	Severe	Severe	Category 2A		Category III	R36	Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	2	138	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	3	232	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	4	156	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	5	132	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	6	191	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	7	190	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	8	166	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	9	123	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	10	101	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	11	200	Severe						Gautheron et al. (1994)
Allyl alcohol	107-18-6	liquid	100%	n.p.	12	90	Severe						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	1	5	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	2	4	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	3	10	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	5	5	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	6	28	Moderate						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	7	2	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	8	4	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	9	10	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	10	6	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	11	2	Mild						Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	12	2	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	1	7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	2	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	4	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	5	6	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	6	7	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	7	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	8	6	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
2-Aminophenol	95-55-6	solid	20%	n.p.	10	11	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	11	5	Mild						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	12	11	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	1	-2	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	3	-3	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	6	-1	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	8	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	10	0	Mild	Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	11	-2	Nonirritant	Gautheron et al. (1994)					
Anthracene	120-12-7	solid	20%	n.p.	12	2	Mild	Gautheron et al. (1994)					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	1	128	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	2	124	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	3	163	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	4	106	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	5	128	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	6	129	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	7	142	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	8	129	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	9	166	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	10	no data	n.a. ¹³						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	11	142	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	12	116	Severe						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	1	4	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	3	0	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	5	1	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	6	3	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	8	-10	Nonirritant						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	9	4	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	11	1	Mild						Gautheron et al. (1994)
Betaine monohydrate	590-47-6	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	1	0	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	2	2	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	4	1	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	5	0	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	6	0	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	7	0	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	8	0	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	9	1	Mild						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	12	-2	Nonirritant						Gautheron et al. (1994)
Butyrolactone	96-48-0	liquid	100%	n.p.	1	48	Moderate					Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	100%	n.p.	2	44	Moderate					Gautheron et al. (1994)	
Butyrolactone	96-48-0	liquid	100%	n.p.	3	64	Severe					Gautheron et al. (1994)	

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Butyrolactone	96-48-0	liquid	100%	n.p.	4	35	Moderate	Moderate	Category 2A		Category II	R36	Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	5	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	6	30	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	7	80	Severe						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	8	32	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	9	42	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	10	53	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	11	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	12	49	Moderate						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	1	92	Severe						Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	100%	n.p.	2	108	Severe											Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	100%	n.p.	3	96	Severe											Gautheron et al. (1994)
Cyclohexanone	108-94-1	liquid	100%	n.p.	4	81	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	5	130	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	6	93	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	7	104	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	8	90	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	9	142	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	11	118	Severe	Gautheron et al. (1994)										
Cyclohexanone	108-94-1	liquid	100%	n.p.	12	108	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	1	96	Severe	Severe	Category 2A		Category II	R36	Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	2	72	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	3	106	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	4	73	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	5	119	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	6	103	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	7	88	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	8	46	Moderate						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	9	100	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	10	60	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	11	200	Severe						Gautheron et al. (1994)					
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	12	59	Severe						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	1	53	Moderate	Moderate	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	2	41	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	3	105	Severe						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	4	39	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	5	42	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	7	49	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	8	41	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	9	92	Severe						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	11	36	Moderate						Gautheron et al. (1994)					
Diacetone alcohol	123-42-2	liquid	100%	n.p.	12	56	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	1	104	Severe	Severe	Category 1	2	Category I	R41	Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	2	134	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	3	82	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	4	118	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	5	110	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	6	66	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	7	88	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	8	193	Severe						Gautheron et al. (1994)					
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	9	82	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	11	213	Severe						Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	12	135	Severe						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	1	23	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	2	23	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	3	18	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	4	28	Moderate						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	5	16	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	6	31	Moderate						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	7	18	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	8	71	Severe						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	9	19	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	10	20	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	11	34	Moderate						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	12	14	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	1	0	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	2	3	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	5	1	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	6	5	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	7	3	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	8	1	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	9	2	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	11	5	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	12	8	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	1	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	2	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	3	14	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	5	11	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	6	14	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	7	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	8	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	9	9	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	11	4	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	12	22	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	1	-1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	2	0	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	3	-8	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	4	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	5	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	6	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	8	-6	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	10	-1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	11	3	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	12	1	Mild						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	1	58	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	2	67	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	3	70	Severe						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Ethanol	64-17-5	liquid	100%	n.p.	4	45	Moderate	Severe	SCNM		Category II	Nonirritant	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	5	60	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	6	64	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	7	58	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	8	51	Moderate						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	9	46	Moderate						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	11	104	Severe						Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	12	45	Moderate						Gautheron et al. (1994)					
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	1	99	Severe						Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	2	100	Severe											Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	3	128	Severe											Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	4	75	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	5	75	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	6	85	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	7	94	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	8	93	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	9	84	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	10	75	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	11	101	Severe	Gautheron et al. (1994)										
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	12	86	Severe	Gautheron et al. (1994)										
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	1	26	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	2	38	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	3	31	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	4	33	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	5	21	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	6	29	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	7	28	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	8	38	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	9	26	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	11	38	Moderate						Gautheron et al. (1994)					
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	12	42	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	1	73	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	2	63	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	3	61	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	4	65	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	5	33	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	7	87	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	8	48	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	10	39	Moderate						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	11	68	Severe						Gautheron et al. (1994)					
Furan	110-00-9	liquid	100%	n.p.	12	51	Moderate						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	1	63	Severe	Severe	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	2	81	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	3	90	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	4	62	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	5	108	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	6	66	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	7	90	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	8	57	Severe						Gautheron et al. (1994)					
Gluconolactone	90-80-2	solid	20%	n.p.	9	88	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Gluconolactone	90-80-2	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	11	75	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	12	63	Severe						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	1	2	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	6	-4	Nonirritant	Mild	SCNM		SCNM	SCNM	Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	8	4	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	10	2	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	12	-1	Nonirritant						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	1	18	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	2	24	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	3	25	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	4	14	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	5	13	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	6	6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	7	15	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	8	18	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	9	18	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	11	23	Mild						Gautheron et al. (1994)
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1	93	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2	40	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3	53	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	4	33	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	5	91	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	6	42	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	7	82	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	8	76	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	9	70	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	11	48	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	12	102	Severe						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	1	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	2	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	3	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	4	0	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Hexane	110-54-3	liquid	100%	n.p.	5	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	7	3	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	8	1	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)					
Hexane	110-54-3	liquid	100%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Imidazole	288-32-4	solid	20%	n.p.	1	75	Severe						Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	2	73	Severe											Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	3	140	Severe											Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	4	81	Severe											Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	5	96	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	6	62	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	7	82	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	8	122	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	9	64	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	10	81	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	11	114	Severe	Gautheron et al. (1994)										
Imidazole	288-32-4	solid	20%	n.p.	12	65	Severe	Gautheron et al. (1994)										
Iminodibenzyl	494-19-9	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	3	6	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	5	4	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	6	0	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	8	12	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	11	6	Mild						Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	12	-4	Nonirritant						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	1	53	Moderate	Moderate	Category 2B		Category III	Nonirritant	Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	2	50	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	3	48	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	4	28	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	5	45	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	6	35	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	7	48	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	8	43	Moderate						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	9	63	Severe						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	11	89	Severe						Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	12	48	Moderate						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	1	81	Severe	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	2	82	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	3	103	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	4	76	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	5	92	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	6	68	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	7	90	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	8	62	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	9	102	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	11	76	Severe	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	12	55	Moderate						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	1	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	2	6	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	7	7	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	1	0	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	2	-1	Nonirritant											Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	3	-1	Nonirritant											Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	4	1	Mild											Gautheron et al. (1994)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	5	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	6	1	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	7	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	8	-8	Nonirritant	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	9	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	10	0	Mild	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	11	-4	Nonirritant	Gautheron et al. (1994)										
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	12	-3	Nonirritant	Gautheron et al. (1994)										
Methanol	67-56-1	liquid	100%	n.p.	1	88	Severe	Severe	Nonirritant		Category II	Nonirritant	Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	2	88	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	3	54	Moderate						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	4	71	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	5	81	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	6	108	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	7	37	Moderate						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	8	19	Mild						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	9	99	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	11	179	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	12	102	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	1	61	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	2	69	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	3	66	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	4	47	Moderate						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	5	48	Moderate						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	6	62	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	7	65	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	8	62	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	9	57	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	11	74	Severe						Gautheron et al. (1994)					
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	12	88	Severe						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	1	22	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	2	25	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	3	27	Moderate						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	4	19	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	5	21	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	6	23	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	7	16	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	8	16	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	9	19	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	11	20	Mild						Gautheron et al. (1994)					
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	12	11	Mild						Gautheron et al. (1994)					
MYRJ-45	-	surfactant	10%	n.p.	1	2	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	2	1	Mild											Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	3	0	Mild											Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	4	1	Mild											Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	5	0	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	6	0	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	7	1	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	8	-4	Nonirritant	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	9	1	Mild	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	11	-3	Nonirritant	Gautheron et al. (1994)										
MYRJ-45	-	surfactant	10%	n.p.	12	-1	Nonirritant	Gautheron et al. (1994)										
1-Nitropropane	108-03-2	liquid	100%	n.p.	1	11	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	2	8	Mild											Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	3	9	Mild											Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	4	4	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	5	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	7	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	8	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	9	17	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	11	6	Mild						Gautheron et al. (1994)					
1-Nitropropane	108-03-2	liquid	100%	n.p.	12	7	Mild						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	1	65	Severe						Moderate	Category 2B		Category III	R36	Gautheron et al. (1994)
Octanol	111-87-5	liquid	100%	n.p.	2	33	Moderate											Gautheron et al. (1994)
Octanol	111-87-5	liquid	100%	n.p.	3	42	Moderate											Gautheron et al. (1994)
Octanol	111-87-5	liquid	100%	n.p.	4	49	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	5	66	Severe	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	6	48	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	7	37	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	8	25	Mild	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	9	61	Severe	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	11	31	Moderate	Gautheron et al. (1994)										
Octanol	111-87-5	liquid	100%	n.p.	12	64	Severe	Gautheron et al. (1994)										
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	1	61	Severe	Severe	Nonirritant		Category III	Nonirritant						Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	2	79	Severe											Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	3	75	Severe											Gautheron et al. (1994)
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	4	34	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	5	70	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	6	46	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	7	54	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	8	44	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	10	67	Severe						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	11	62	Severe	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	12	76	Severe						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	1	8	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	2	13	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	3	11	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	4	1	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	5	2	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	6	5	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	7	7	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	8	0	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	9	2	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	10	3	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	11	5	Mild						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	12	9	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	1	0	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	2	1	Mild											Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	3	1	Mild											Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	4	0	Mild											Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	5	0	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	6	1	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	7	0	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	8	-6	Nonirritant	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	9	1	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	10	1	Mild	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	11	-3	Nonirritant	Gautheron et al. (1994)										
Phenylbutazone	50-33-9	solid	20%	n.p.	12	2	Mild	Gautheron et al. (1994)										
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	1	7	Mild	Mild	Nonirritant		Category III	Nonirritant						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	2	12	Mild											Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	3	15	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	4	9	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	5	28	Moderate						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	6	6	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	8	16	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	10	15	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	11	13	Mild						Gautheron et al. (1994)					
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	12	15	Mild						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	1	117	Severe	Severe	Category 1	3	Category I	R41	Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	2	156	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	3	109	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	4	111	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	5	164	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	6	174	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	7	103	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	8	50	Moderate						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	9	139	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	11	94	Severe						Gautheron et al. (1994)					
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	12	19	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	1	7	Mild											Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	2	7	Mild											Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	3	14	Mild	Gautheron et al. (1994)										
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	4	4	Mild	Gautheron et al. (1994)										

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	5	6	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	6	9	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	8	11	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	9	6	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	11	12	Mild						Gautheron et al. (1994)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	12	5	Mild						Gautheron et al. (1994)					
Pyridine	110-86-1	liquid	100%	n.p.	1	102	Severe						Severe	Category 1	4	Category II	R41	Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	2	123	Severe											Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	3	186	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	4	79	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	5	102	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	6	77	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	7	124	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	8	132	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	9	105	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	11	96	Severe	Gautheron et al. (1994)										
Pyridine	110-86-1	liquid	100%	n.p.	12	115	Severe	Gautheron et al. (1994)										
Quinacrine	69-05-6	solid	20%	n.p.	1	17	Mild	Moderate	Category 1	1	Category I	R41						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	2	29	Moderate											Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	3	8	Mild											Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	4	46	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	5	52	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	6	24	Mild						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	7	15	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	8	18	Moderate						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	9	58	Severe						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	11	3	Mild						Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	12	72	Severe						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	1	2	Mild						Mild	Category 1	4	Category I	R41	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	2	2	Mild											Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	3	9	Mild											Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	4	5	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	5	3	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	6	2	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	7	4	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	8	3	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	9	3	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	10	9	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	11	11	Mild	Gautheron et al. (1994)										
Sodium oxalate	62-76-0	solid	20%	n.p.	12	4	Mild	Gautheron et al. (1994)										
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	1	5	Mild	Mild	Nonirritant		Category II	Nonirritant						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	2	1	Mild											Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	3	2	Mild											Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	4	6	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	6	4	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	7	2	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	8	19	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	9	3	Mild						Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	11	18	Mild	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	1	146	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	2	175	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	3	169	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	4	152	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	5	140	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	6	120	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	7	129	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	8	173	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	9	151	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	11	203	Severe						Gautheron et al. (1994)					
Thiourea	62-56-6	solid	20%	n.p.	12	104	Severe						Gautheron et al. (1994)					
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	1	47	Moderate						Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	2	42	Moderate											Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	3	78	Severe	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	4	28	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	5	42	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	6	47	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	7	48	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	8	24	Mild	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	9	91	Severe	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	11	28	Moderate	Gautheron et al. (1994)										
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	12	47	Moderate	Gautheron et al. (1994)										
Triethanolamine	102-71-6	liquid	100%	n.p.	1	2	Mild	Mild			Category IV	Nonirritant	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	2	4	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	3	0	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	5	-1	Nonirritant						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	7	1	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	9	3	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	11	5	Mild						Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	12	6	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	1	25	Mild	Mild			Category III	Nonirritant	Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	2	14	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	3	26	Moderate						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	5	27	Moderate						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	7	9	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	8	15	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	9	21	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	10	10	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	11	7	Mild						Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	1	-1	Nonirritant						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)					
Triton X-155	9010-44-0	surfactant	10%	n.p.	4	0	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Triton X-155	9010-44-0	surfactant	10%	n.p.	5	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	6	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	7	0	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	8	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	9	3	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	12	0	Mild						Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	10%	n.p.	-	20.8	Severe	Severe	Category I	1	Category I	R41	Gettings et al. (1996)
Babv Shampoo No. 1 (HZP) 100%	-	n.p.	10%	n.p.	-	4.0	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Babv Shampoo No. 2 (HZF) 100%	-	n.p.	10%	n.p.	-	8.3	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	10%	n.p.	-	17.5	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Cleansing Gel (HZQ) 100%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	10%	n.p.	-	0.2	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Facial Cleansing Foam (HZR) 25%	-	n.p.	10%	n.p.	-	4.1	Nonsevere	Nonsevere	SCNM		Category I	SCNM	Gettings et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	10%	n.p.	-	1.8	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Foam Bath (HZL) 100%	-	n.p.	10%	n.p.	-	18.6	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Gel Cleanser (HZE) 100%	-	n.p.	10%	n.p.	-	3.1	Nonsevere	Nonsevere	SCNM		Category I	SCNM	Gettings et al. (1996)
Hand Soap (HZU) 25%	-	n.p.	10%	n.p.	-	5.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Liquid Soap No. 2 (HZW) 25%	-	n.p.	10%	n.p.	-	5.6	Nonsevere	Nonsevere	Category 2B		Category III	Nonirritant	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	10%	n.p.	-	0.1	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Polishing Scrub (HZZ) 100%	-	n.p.	10%	n.p.	-	3.7	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Shampoo No. 1 (HZC) 25%	-	n.p.	10%	n.p.	-	30.0	Severe	Severe	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 2 (HZZ)	-	n.p.	10%	n.p.	-	14.0	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	10%	n.p.	-	4.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 4 (HZV) 25%	-	n.p.	10%	n.p.	-	8.4	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 5 (HZD) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 6 (HZN) 25%	-	n.p.	10%	n.p.	-	4.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 7 (HZA) 100%	-	n.p.	10%	n.p.	-	6.6	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)
Shampoo No. 8 (HZG) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shower Gel (HZS) 100%	-	n.p.	10%	n.p.	-	35.9	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Skin Cleanser (HZI) 100%	-	n.p.	10%	n.p.	-	15.8	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (1)	4.9	Mild	Mild	Category 2B		Category III	R36	Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (2)	5.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (1)	3.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (2)	3.6	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (1)	5.2	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (2)	6.7	Mild						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (1)	195.2	Very severe	Very Severe	Category 1	4	SCNM	R41	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (2)	135.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (3)	137.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (4)	156.5	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (5)	138.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (6)	176.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (7)	183.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (8)	175.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (1)	154.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (2)	156.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (3)	150.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (4)	157.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (5)	157.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (6)	157.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (7)	160.2	Very severe						Southee (1998)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (1)	156.9	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (2)	163.4	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (3)	169.7	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (4)	162.8	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (5)	151.6	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (6)	163.1	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (7)	167.8	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (8)	156.9	Very severe						Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (9)	160.0	Very severe						Southee (1998)					
Butyl cellulose	111-76-2	liquid	100%	n.p.	1 (1)	108.3	Very severe						Very Severe	Category 1	1	Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	liquid	100%	n.p.	1 (2)	111.8	Very severe	Southee (1998)										
Butyl cellulose	111-76-2	liquid	100%	n.p.	2 (1)	92.8	Very severe	Southee (1998)										
Butyl cellulose	111-76-2	liquid	100%	n.p.	2 (2)	99.2	Very severe	Southee (1998)										
Butyl cellulose	111-76-2	liquid	100%	n.p.	3 (1)	94.9	Very severe	Moderate	Category 2A		Category II	R36	Southee (1998)					
Butyl cellulose	111-76-2	liquid	100%	n.p.	3 (2)	98.2	Very severe						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (1)	53.9	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (2)	47.7	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (1)	47.1	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (2)	47.2	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (1)	42.2	Moderate						Southee (1998)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (2)	41.8	Moderate						Southee (1998)					
Ethanol	64-17-5	liquid	100%	n.p.	1 (1)	36.6	Moderate						Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (2)	37.6	Moderate											Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (3)	29.6	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (4)	41.7	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (5)	31.5	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (6)	42.6	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	1 (7)	55.4	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (1)	52.7	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (2)	54.5	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (3)	61.7	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (4)	60.2	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (5)	54.2	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (6)	73.4	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (7)	64.0	Severe	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	2 (8)	51.4	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (1)	47.0	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (2)	45.4	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (3)	44.4	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (4)	45.7	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (5)	54.6	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (6)	44.8	Moderate	Southee (1998)										
Ethanol	64-17-5	liquid	100%	n.p.	3 (7)	42.2	Moderate	Southee (1998)										
Glycerol	56-81-5	liquid	100%	>99.5	1 (1)	0.6	Mild	Nonirritant	Nonirritant		Category IV	Nonirritant						Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	1 (2)	0.3	Mild											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	2 (1)	0.8	Nonirritant											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	2 (2)	0.8	Nonirritant											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	3 (1)	1.0	Nonirritant											Southee (1998)
Glycerol	56-81-5	liquid	100%	>99.5	3 (2)	0.8	Nonirritant											Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (1)	23.1	Mild						Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (2)	17.2	Mild						Southee (1998)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (1)	34.6	Moderate	Moderate	Category 1	4	Category I	R41	Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (2)	39.1	Moderate						Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (1)	31.7	Moderate						Southee (1998)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (2)	29.9	Moderate						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (1)	142.0	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (2)	137.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (3)	112.2	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (4)	131.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (5)	145.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (6)	162.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	1 (7)	125.5	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (1)	138.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (2)	140.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (3)	134.9	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (4)	157.2	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (5)	137.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (6)	152.9	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	2 (7)	148.7	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (1)	139.6	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (2)	140.1	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (3)	124.0	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (4)	128.7	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (5)	123.4	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (6)	121.2	Very severe						Southee (1998)					
Imidazole	288-32-4	solid	20%	n.p.	3 (7)	131.3	Very severe	Southee (1998)										
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (1)	73.3	Severe	Severe	Category 2B		Category III	R36	Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (2)	67.8	Severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (1)	108.7	Very severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (2)	101.7	Very severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (1)	70.2	Severe						Southee (1998)					
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (2)	73.5	Severe						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	1 (1)	31	Moderate	Moderate	SCNM		SCNM	SCNM	Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	1 (2)	35	Moderate						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	2 (1)	38.3	Moderate						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	2 (2)	37.5	Moderate						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	3 (1)	22.1	Mild						Southee (1998)					
Paraffluoraniline	371-40-4	liquid	100%	99	3 (2)	28.9	Moderate						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (1)	11.2	Mild	Mild	Nonirritant		Category III	Nonirritant	Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (2)	7.4	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (1)	5.2	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (2)	3.6	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (1)	7.7	Mild						Southee (1998)					
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (2)	6.2	Mild						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (1)	245.0	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (2)	227.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (1)	241.3	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (2)	235.5	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (1)	193.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (2)	214.9	Very severe						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (1)	5.4	Mild											Southee (1998)
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (2)	5.2	Mild											Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (1)	15.9	Mild	Mild	Category 1	NC	Category I	SCNM	Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (2)	17.3	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (1)	8.7	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (2)	5.6	Mild						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	1 (1)	10.3	Mild	Nonirritant	Category 1	4	Category I	R41	Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	1 (2)	4.4	Mild						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	2 (1)	-0.3	Nonirritant						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	2 (2)	-0.1	Nonirritant						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	3 (1)	2.7	Nonirritant						Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	3 (2)	4.5	Mild						Southee (1998)					
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (1)	3.7	Mild						Mild	Category 2B		Category III	R36	Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (2)	1.8	Mild											Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (1)	5.8	Mild	Southee (1998)										
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (2)	3.4	Mild	Southee (1998)										
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (1)	3.0	Nonirritant	Southee (1998)										
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (2)	1.9	Nonirritant	Southee (1998)										
Tween 20	9005-64-5	liquid	100%	98	1 (1)	0.3	Mild	Nonirritant	Nonirritant		Category III	Nonirritant	Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	1 (2)	0.0	Mild						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	2 (1)	0.4	Mild						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	2 (2)	0.4	Nonirritant						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	3 (1)	0.3	Nonirritant						Southee (1998)					
Tween 20	9005-64-5	liquid	100%	98	3 (2)	0.0	Nonirritant						Southee (1998)					
1-1 (#1)	-	liquid	100%	n.p.	-	83.6	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)					
1-2 (#2)	-	liquid	100%	n.p.	-	12.4	Mild	Mild	Category 2A		Category II	R36	Swanson and Harbell (2000)					
1-3 (#3)	-	liquid	100%	n.p.	-	29.6	Moderate	Moderate	Category 2A		Category II	R36	Swanson and Harbell (2000)					
2-4 (#4)	-	liquid	100%	n.p.	-	7.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-7 (#7)	-	liquid	100%	n.p.	-	21.4	Moderate	Moderate	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-8 (#8)	-	liquid	100%	n.p.	-	31.8	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Swanson and Harbell (2000)					
Benchmark-Group 1 (#12)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)					
Benchmark-Group 2 (#13)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 1	1	Category I	R41	Swanson and Harbell (2000)					
Ethanol (#14)	64-17-5	liquid	100%	n.p.	-	52.7	Moderate	Moderate	Category 2A		Category I	R36	Swanson and Harbell (2000)					
Toilet Bowl Cleaner (#1)	-	liquid	100%	n.p.	-	13.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson et al. (1995)					
Toilet Bowl Cleaner (#4)	-	liquid	100%	n.p.	-	15	Mild	Mild	Nonirritant		SCNM	Nonirritant	Swanson et al. (1995)					
All Purpose Cleaner (#5)	-	liquid	100%	n.p.	-	121.3	Severe	Severe					Swanson et al. (1995)					
Bathroom Cleaner (#6)	-	liquid	100%	n.p.	-	78.3	Severe	Severe	SCNM		Category III	Nonirritant	Swanson et al. (1995)					
All Purpose Cleaner (#7)	-	liquid	100%	n.p.	-	393.3	Severe	Severe					Swanson et al. (1995)					
Pot and Pan Cleaner (#8)	-	liquid	100%	n.p.	-	-0.6	Nonirritant	Nonirritant					Swanson et al. (1995)					
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	100%	n.p.	-	354.7	Severe	Severe					Swanson et al. (1995)					
Floor Cleaner (#10)	-	liquid	100%	n.p.	-	70.3	Severe	Severe					Swanson et al. (1995)					
General Cleaner (#11)	-	liquid	100%	n.p.	-	83.3	Severe	Severe					Swanson et al. (1995)					
General Cleaner (#12)	-	liquid	100%	n.p.	-	113.5	Severe	Severe					Swanson et al. (1995)					
Cleaner/Degreaser (#13)	-	liquid	100%	n.p.	-	353.6	Severe	Severe					Swanson et al. (1995)					
Floor Stripper (#14)	-	liquid	100%	n.p.	-	157.3	Severe	Severe					Swanson et al. (1995)					
Heavy Duty Cleaner (#15)	-	liquid	100%	n.p.	-	357.1	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)					
Degreaser (#16)	-	liquid	100%	n.p.	-	255.7	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)					
Floor Stripper (#17)	-	liquid	100%	n.p.	-	216.2	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)					
Floor Stripper (#18)	-	liquid	100%	n.p.	-	444.3	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Reference

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Glass Cleaner (#19)	-	liquid	100%	n.p.	-	135.8	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Metal Cleaner (#20)	-	liquid	100%	n.p.	-	391.9	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	100%	n.p.	-	-0.3	Nonirritant	Nonirritant					Swanson et al. (1995)
Meat Room Degreaser (#3)	-	liquid	100%	n.p.	-	140.3	Severe	Severe					Swanson et al. (1995)

¹CASRN=Chemical Abstract Services Registry Number

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

³Consensus classification represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls

⁴GHS=Globally Harmonized System (UN [2003])

⁵Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye

⁶NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are both severe and persistent; and 4: corneal opacity score equal to 4 at any time; NC: not classified because none of the above criteria were met

⁷EPA=U.S. Environmental Protection Agency (EPA [1996]).

⁸Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr

⁹EU=European Union (EU [2001]).

¹⁰Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

¹¹SCNM=Study Criteria Not Met

¹²n.p.=Not provided

¹³n.a.=Not applicable

Appendix D2

BCOP Data Sorted by Substance Name

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Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
1-1 (#1)	-	liquid	100%	n.p.	-	83.6	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)					
1-2 (#2)	-	liquid	100%	n.p.	-	12.4	Mild	Mild	Category 2A		Category II	R36	Swanson and Harbell (2000)					
1-3 (#3)	-	liquid	100%	n.p.	-	29.6	Moderate	Moderate	Category 2A		Category II	R36	Swanson and Harbell (2000)					
2-4 (#4)	-	liquid	100%	n.p.	-	7.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-7 (#7)	-	liquid	100%	n.p.	-	21.4	Moderate	Moderate	Nonirritant		Category IV	Nonirritant	Swanson and Harbell (2000)					
2-8 (#8)	-	liquid	100%	n.p.	-	31.8	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Swanson and Harbell (2000)					
Acetone	67-64-1	liquid	100%	99	1	145.5	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	2	119.5	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	3	120.4	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	4	131.72	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	99	5	98.4	Very severe						Balls et al. (1995)					
Acetone	67-64-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A		Category II	R36	Casterton et al. (1996)					
Alkyl phosphoric acid ester/amine salt	-	liquid	100%	n.p.	-	91.3	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)					
All Purpose Cleaner (#5)	-	liquid	100%	n.p.	-	121.3	Severe	Severe					Swanson et al. (1995)					
All Purpose Cleaner (#7)	-	liquid	100%	n.p.	-	393.3	Severe	Severe					Swanson et al. (1995)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	1	156	Severe	Severe	Category 2A		Category III	R36	Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	2	138	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	3	232	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	4	156	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	5	132	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	6	191	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	7	190	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	8	166	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	9	123	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	10	101	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	11	200	Severe						Gautheron et al. (1994)					
Allyl alcohol	107-18-6	liquid	100%	n.p.	12	90	Severe						Gautheron et al. (1994)					
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	1	5	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	2	4	Mild											Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	3	10	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	4	3	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	5	5	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	6	28	Moderate	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	7	2	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	8	4	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	9	10	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	10	6	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	11	2	Mild	Gautheron et al. (1994)										
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	12	2	Mild	Gautheron et al. (1994)										
2-Aminophenol	95-55-6	solid	20%	n.p.	1	7	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
2-Aminophenol	95-55-6	solid	20%	n.p.	2	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	4	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	5	6	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	6	7	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	7	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	8	6	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	10	11	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	11	5	Mild						Gautheron et al. (1994)					
2-Aminophenol	95-55-6	solid	20%	n.p.	12	11	Mild						Gautheron et al. (1994)					
Ammonium nitrate	6484-52-2	solid	20%	>99.9	1	8.3	Mild											Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	2	6.4	Mild	Balls et al. (1995)										
Ammonium nitrate	6484-52-2	solid	20%	>99.9	3	7.2	Mild	Balls et al. (1995)										

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Ammonium nitrate	6484-52-2	solid	20%	>99.9	4	21.82	Mild	Mild	Category 2B		Category III	R36	Balls et al. (1995)
Ammonium nitrate	6484-52-2	solid	20%	>99.9	5	5.2	Mild						Balls et al. (1995)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (1)	4.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	1 (2)	5.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (1)	3.9	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	2 (2)	3.6	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (1)	5.2	Mild						Southee (1998)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	3 (2)	6.7	Mild						Southee (1998)
Amway all fabric bleach	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound for soft water	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway automatic dishwashing compound, standard formula	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway concrete floor cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	SCNM	R41	Casterton et al. (1996)
Amway Dish Drops dishwashing liquid	-	n.p.	100%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)
Amway dry chlorine bleach	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway fabric softener	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Amway Kool Wash delicate fabric detergent	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R36	Casterton et al. (1996)
Amway LOC all purpose cleaner	-	n.p.	100%	n.p.	-	-	Mild	Mild	SCNM		SCNM	Nonirritant	Casterton et al. (1996)
Amway prewash liquid	-	liquid	100%	n.p.	-	-	Mild	Mild	SCNM		Category I	Nonirritant	Casterton et al. (1996)
Amway Pursue disinfectant cleaner	-	n.p.	100%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Amway Redu dye stain remover	-	n.p.	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	Nonirritant	Casterton et al. (1996)
Amway SA8 laundry liquid	-	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Amway SA8 limited phos laundry powder	-	solid	100%	n.p.	-	-	Moderate	Moderate	Category 1	4	Category I	R41	Casterton et al. (1996)
Anthracene	120-12-7	solid	20%	n.p.	1	-2	Nonirritant	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	3	-3	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	6	-1	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	8	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	10	0	Mild						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Anthracene	120-12-7	solid	20%	n.p.	12	2	Mild						Gautheron et al. (1994)
Anti-Dandruff Shampoo (HZY)	-	n.p.	100%	n.p.	-	-	Moderate						Moderate
Anti-Dandruff Shampoo (HZY) 100%	-	n.p.	10%	n.p.	-	20.8	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Aromatic hydrocarbon #1	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	100%	n.p.	-	4.6	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Aryl phosphonates	-	liquid	100%	n.p.	-	41.3	Moderate	Moderate	Category 2B		SCNM	SCNM	Bailey et al. (2004)
L-Aspartic acid	70-47-3	solid	20%	100	1	1.8	Mild	Mild	SCNM ¹¹		SCNM	SCNM	Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	2	0.1	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	3	2.6	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	4	0.788	Mild						Balls et al. (1995)
L-Aspartic acid	70-47-3	solid	20%	100	5	1.2	Mild						Balls et al. (1995)
Baby Shampoo No. 1 (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Baby Shampoo No. 1 (HZZ) 100%	-	n.p.	10%	n.p.	-	4.0	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Baby Shampoo No. 2 (HZF)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Baby Shampoo No. 2 (HZF) 100%	-	n.p.	10%	n.p.	-	8.3	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)
Bathroom Cleaner (#6)	-	liquid	100%	n.p.	-	78.3	Severe	Severe	SCNM		Category III	Nonirritant	Swanson et al. (1995)
Benchmark-Group 1 (#12)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)
Benchmark-Group 2 (#13)	-	liquid	100%	n.p.	-	60.1	Severe	Severe	Category 1	1	Category I	R41	Swanson and Harbell (2000)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (1)	195.2	Very severe	Very Severe	Category 1	4	SCNM	R41	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (2)	135.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (3)	137.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (4)	156.5	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (5)	138.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (6)	176.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (7)	183.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	1 (8)	175.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (1)	154.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (2)	156.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (3)	150.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (4)	157.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (5)	157.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (6)	157.0	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	2 (7)	160.2	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (1)	156.9	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (2)	163.4	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (3)	169.7	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (4)	162.8	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (5)	151.6	Very severe						Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (6)	163.1	Very severe	Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (7)	167.8	Very severe	Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (8)	156.9	Very severe	Southee (1998)					
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	3 (9)	160.0	Very severe	Southee (1998)					
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	1	112.8	Very severe	Very Severe	Category 1	1	Category II	R41	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	2	90.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	3	99.4	Very severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	4	62.49	Severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	98	5	78.6	Severe						Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	liquid	1%	n.p.	-	-	Severe	Severe	Category 1	1	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	1	142.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	2	157.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	3	123.8	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	4	137.5	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	5	121.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	1	126.6	Very severe	Very Severe	Category 1	2	Category I	R41	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	2	163.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	3	110.7	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	4	130.41	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	5	111.1	Very severe						Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	1	128	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	2	124	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	3	163	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	4	106	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	5	128	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	6	129	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	7	142	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	8	129	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	9	166	Severe						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	10	no data	n.a. ¹³						Gautheron et al. (1994)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	11	142	Severe						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	12	116	Severe						Gautheron et al. (1994)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	1	173	Very severe	Very Severe	Category 1	2	SCNM	R41	Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	2	288.7	Very severe						Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	3	91.1	Very severe						Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	4	149.86	Very severe						Balls et al. (1995)					
Benzoyl-L-tartaric acid	2743-38-6	solid	20%	-	5	145.3	Very severe						Balls et al. (1995)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	1	4	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	3	0	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	5	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	6	3	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	8	-10	Nonirritant						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	9	4	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	11	1	Mild						Gautheron et al. (1994)					
Betaine monohydrate	590-47-6	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
BRIJ-35	9002-92-0	surfactant	10%	n.p.	1	0	Mild						Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	2	2	Mild											Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	3	-1	Nonirritant											Gautheron et al. (1994)
BRIJ-35	9002-92-0	surfactant	10%	n.p.	4	1	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	5	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	6	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	7	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	8	0	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	9	1	Mild	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	10	no data	n.a.	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	11	-2	Nonirritant	Gautheron et al. (1994)										
BRIJ-35	9002-92-0	surfactant	10%	n.p.	12	-2	Nonirritant	Gautheron et al. (1994)										
4-Bromophenetole	-	n.p.	100%	n.p.	-	-	Mild	Mild										Casterton et al. (1996)
Bubble Bath (HZK)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41						Casterton et al. (1996)
Bubble Bath (HZK) 100%	-	n.p.	100%	n.p.	-	17.5	Severe	Severe	Category 1	1	Category I	R41						Gettings et al. (1996)
n-Butanol	71-36-3	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)					
2-Butoxyethanol	111-76-2	liquid	100%	n.p.	-	-	Severe	Severe					Casterton et al. (1996)					
Butyl acetate	123-86-4	liquid	100%	99	1	49.5	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	2	37.5	Moderate						Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	3	43.9	Moderate						Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	4	23.86	Mild						Balls et al. (1995)					
Butyl acetate	123-86-4	liquid	100%	99	5	18.1	Mild						Balls et al. (1995)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	1 (1)	108.3	Very severe	Very Severe	Category 1	1	Category II	R41	Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	1 (2)	111.8	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	2 (1)	92.8	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	2 (2)	99.2	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	3 (1)	94.9	Very severe						Southee (1998)					
Butyl cellulosolve	111-76-2	liquid	100%	n.p.	3 (2)	98.2	Very severe	Southee (1998)										
Butyrolactone	96-48-0	liquid	100%	n.p.	1	48	Moderate	Moderate	Category 2A		Category II	R36	Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	2	44	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	3	64	Severe						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	4	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	5	35	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	6	30	Moderate						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	7	80	Severe						Gautheron et al. (1994)					
Butyrolactone	96-48-0	liquid	100%	n.p.	8	32	Moderate						Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference				
Butyrolactone	96-48-0	liquid	100%	n.p.	9	42	Moderate						Gautheron et al. (1994)				
Butyrolactone	96-48-0	liquid	100%	n.p.	10	53	Moderate						Gautheron et al. (1994)				
Butyrolactone	96-48-0	liquid	100%	n.p.	11	35	Moderate						Gautheron et al. (1994)				
Butyrolactone	96-48-0	liquid	100%	n.p.	12	49	Moderate						Gautheron et al. (1994)				
gamma-Butyrolactone	96-48-0	liquid	100%	>99	1	90.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)				
gamma-Butyrolactone	96-48-0	liquid	100%	>99	2	32.9	Moderate						Balls et al. (1995)				
gamma-Butyrolactone	96-48-0	liquid	100%	>99	3	31.5	Moderate						Balls et al. (1995)				
gamma-Butyrolactone	96-48-0	liquid	100%	>99	4	81.55	Very severe						Balls et al. (1995)				
gamma-Butyrolactone	96-48-0	liquid	100%	>99	5	67.1	Severe						Balls et al. (1995)				
Captan 90 concentrate	133-06-2	solid	20%	90	1	27.8	Moderate	Moderate	Category 1	4	Category I	R41	Balls et al. (1995)				
Captan 90 concentrate	133-06-2	solid	20%	90	2	27.2	Moderate						Balls et al. (1995)				
Captan 90 concentrate	133-06-2	solid	20%	90	3	34.8	Moderate						Balls et al. (1995)				
Captan 90 concentrate	133-06-2	solid	20%	90	4	102.918	Very severe						Balls et al. (1995)				
Captan 90 concentrate	133-06-2	solid	20%	90	5	26.4	Moderate					Balls et al. (1995)					
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1	97.6	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2	98.1	Very severe						Balls et al. (1995)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3	57.5	Severe						Balls et al. (1995)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	4	64.33	Severe						Balls et al. (1995)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	5	73.9	Severe						Balls et al. (1995)				
4-Carboxybenzaldehyde	619-66-9	solid	100%	n.p.	-	-	Mild	Mild	Category 2A		Category II	R36	Casterton et al. (1996)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (1)	53.9	Moderate	Moderate	Category 2A		Category II	R36	Southee (1998)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	1 (2)	47.7	Moderate						Southee (1998)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (1)	47.1	Moderate						Southee (1998)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	2 (2)	47.2	Moderate						Southee (1998)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (1)	42.2	Moderate						Southee (1998)				
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	3 (2)	41.8	Moderate					Southee (1998)					
Carboxylic acid amides	-	solid	100%	n.p.	-	27.5	Moderate	Moderate	Category 1	4	Category I	R41	Bailey et al. (2004)				
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	1	11	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)				
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	2	4.1	Mild						Balls et al. (1995)				
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	3	12.1	Mild						Balls et al. (1995)				
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	4	4.33	Mild						Balls et al. (1995)				
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	5	14.5	Mild						Balls et al. (1995)				
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0%	n.p.	-	-	Mild										Casterton et al. (1996)
Cetylpyridinium bromide (1%)	140-72-7	liquid	1%	n.p.	-	-	Moderate						Moderate				
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	1	43.5	Moderate	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)				
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	2	89.6	Very severe						Balls et al. (1995)				
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	3	81	Very severe						Balls et al. (1995)				
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	4	71.22	Severe						Balls et al. (1995)				
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	5	76.7	Severe						Balls et al. (1995)				
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)				
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	1	72.2	Severe	Severe	Category 1	2	SCNM	R41	Balls et al. (1995)				
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	2	86.3	Very severe						Balls et al. (1995)				
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	3	63.6	Severe						Balls et al. (1995)				
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	4	68.72	Severe						Balls et al. (1995)				
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	5	65.4	Severe						Balls et al. (1995)				
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	n.p.	-	-	Severe	Severe	Category 1	2	SCNM	R41	Casterton et al. (1996)				
Chlorhexidine	55-56-1	solid	20%	n.p. ¹²	1	147	Very severe	Very Severe	Category 1	4	SCNM	SCNM	Balls et al. (1995)				
Chlorhexidine	55-56-1	solid	20%	n.p.	2	122.9	Very severe						Balls et al. (1995)				
Chlorhexidine	55-56-1	solid	20%	n.p.	3	97.3	Very severe						Balls et al. (1995)				
Chlorhexidine	55-56-1	solid	20%	n.p.	4	101.78	Very severe						Balls et al. (1995)				
Chlorhexidine	55-56-1	solid	20%	n.p.	5	101.5	Very severe						Balls et al. (1995)				
2-Chloro-2,4,4-trimethylpentane	-	liquid	100%	n.p.	-	4.1	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)				
Clarified slurry oil	-	liquid	100%	n.p.	-	2.3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)				
Cleaner/Degreaser (#13)	-	liquid	100%	n.p.	-	353.6	Severe	Severe					Swanson et al. (1995)				

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Cleansing Gel (HZQ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)					
Cleansing Gel (HZQ) 100%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Cutting fluid (conc.) #1	-	liquid	100%	n.p.	-	3.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)					
Cutting fluid (conc.) #2	-	liquid	100%	n.p.	-	4.9	Mild	Mild	Nonirritant		Category III	Nonirritant	Bailey et al. (2004)					
Cyclohexanol	108-93-0	liquid	100%	n.p.	1	85	Very severe	Moderate	Category 1	2	Category I	R41	Balls et al. (1995)					
Cyclohexanol	108-93-0	liquid	100%	n.p.	2	49.9	Moderate						Balls et al. (1995)					
Cyclohexanol	108-93-0	liquid	100%	n.p.	3	70.1	Severe						Balls et al. (1995)					
Cyclohexanol	108-93-0	liquid	100%	n.p.	4	52.24	Moderate						Balls et al. (1995)					
Cyclohexanol	108-93-0	liquid	100%	n.p.	5	43.2	Moderate						Balls et al. (1995)					
Cyclohexanol	108-93-0	liquid	100%	n.p.	-	-	Severe	Severe	Category 1	2	Category I	R41	Casterton et al. (1996)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	1	92	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	2	108	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	3	96	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	4	81	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	5	130	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	6	93	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	7	104	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	8	90	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	9	142	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	11	118	Severe						Gautheron et al. (1994)					
Cyclohexanone	108-94-1	liquid	100%	n.p.	12	108	Severe						Gautheron et al. (1994)					
Degreaser (#16)	-	liquid	100%	n.p.	-	255.7	Severe						Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	1	96	Severe						Severe	Category 2A		Category II	R36	Gautheron et al. (1994)
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	2	72	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	3	106	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	4	73	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	5	119	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	6	103	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	7	88	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	8	46	Moderate	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	9	100	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	10	60	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	11	200	Severe	Gautheron et al. (1994)										
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	12	59	Severe	Gautheron et al. (1994)										
Diacetone alcohol	123-42-2	liquid	100%	n.p.	1	53	Moderate	Moderate	SCNM		SCNM	Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	2	41	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	3	105	Severe					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	4	39	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	5	42	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	6	34	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	7	49	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	8	41	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	9	92	Severe					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	10	no data	n.a.					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	11	36	Moderate					Gautheron et al. (1994)						
Diacetone alcohol	123-42-2	liquid	100%	n.p.	12	56	Severe					Gautheron et al. (1994)						
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	1	104	Severe					Severe	Category 1	2	Category I	R41	Gautheron et al. (1994)	
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	2	134	Severe	Gautheron et al. (1994)										
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	3	82	Severe	Gautheron et al. (1994)										
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	4	118	Severe	Gautheron et al. (1994)										
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	5	110	Severe	Gautheron et al. (1994)										
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	6	66	Severe	Gautheron et al. (1994)										
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	7	88	Severe	Gautheron et al. (1994)										

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	8	193	Severe						Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	9	82	Severe						Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	11	213	Severe						Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	12	135	Severe						Gautheron et al. (1994)
Dibenzyl phosphate	1623-08-1	solid	20%	99	1	304.1	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	2	391.1	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	3	418	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	4	467.09	Very severe						Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	solid	20%	99	5	307.5	Very severe					Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	1	9.9	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	2	11.2	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	3	10.8	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	4	14.43	Mild						Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	5	5.6	Mild					Balls et al. (1995)	
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	n.p.	-	-	Mild						Balls et al. (1995)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	1	23	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	2	23	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	3	18	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	4	28	Moderate						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	5	16	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	6	31	Moderate						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	7	18	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	8	71	Severe						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	9	19	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	10	20	Mild						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	11	34	Moderate						Gautheron et al. (1994)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	12	14	Mild						Gautheron et al. (1994)
2,4-Difluoronitrobenzene	446-35-5	liquid	100%	n.p.	-	-	Mild	Mild				Casterton et al. (1996)	
1,3-Diisopropylbenzene	99-62-7	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	2	3	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	5	1	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	6	5	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	7	3	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	8	1	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	9	2	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	11	5	Mild						Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	12	8	Mild						Gautheron et al. (1994)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	1	103.8	Very severe	Very Severe			Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	2	115	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	3	131.7	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	4	130.26	Very severe						Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	5	78.8	Severe					Balls et al. (1995)	
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	n.p.	-	-	Severe	Severe	SCNM		Category I	SCNM	Casterton et al. (1996)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	1	18.2	Mild	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	2	25.3	Moderate						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	3	20.5	Mild						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	4	31.533	Moderate						Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	5	8.3	Mild						Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	1	10	Mild						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	2	10	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	3	14	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	5	11	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	6	14	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	7	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	8	10	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	9	9	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	11	4	Mild						Gautheron et al. (1994)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	12	22	Mild						Gautheron et al. (1994)
Dodecane	112-40-3	liquid	100%	n.p.	-	-	Mild						Mild
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	1	-1	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	2	0	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	3	-8	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	4	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	5	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	6	2	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	8	-6	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	10	-1	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	11	3	Mild						Gautheron et al. (1994)
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	12	1	Mild						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	1	74.4	Severe	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	2	53.2	Moderate						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	3	63.3	Severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	4	98.01	Very severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	5	64.2	Severe						Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	1	58	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	2	67	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	3	70	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	4	45	Moderate						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	5	60	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	6	64	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	7	58	Severe						Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	8	51	Moderate	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	9	46	Moderate	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	11	104	Severe	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	12	45	Moderate	Gautheron et al. (1994)					
Ethanol	64-17-5	liquid	100%	n.p.	1 (1)	36.6	Moderate	Moderate	Category 2A		Category III	Nonirritant	Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	1 (2)	37.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (3)	29.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (4)	41.7	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (5)	31.5	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (6)	42.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	1 (7)	55.4	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (1)	52.7	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (2)	54.5	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (3)	61.7	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (4)	60.2	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (5)	54.2	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (6)	73.4	Severe						Southee (1998)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Ethanol	64-17-5	liquid	100%	n.p.	2 (7)	64.0	Severe						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	2 (8)	51.4	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (1)	47.0	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (2)	45.4	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (3)	44.4	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (4)	45.7	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (5)	54.6	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (6)	44.8	Moderate						Southee (1998)
Ethanol	64-17-5	liquid	100%	n.p.	3 (7)	42.2	Moderate						Southee (1998)
Ethanol (#14)	64-17-5	liquid	100%	n.p.	-	52.7	Moderate	Moderate	Category 2A		Category I	R36	Swanson and Harbell (2000)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	1	99	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	2	100	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	3	128	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	4	75	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	5	75	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	6	85	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	7	94	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	8	93	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	9	84	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	10	75	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	11	101	Severe						Gautheron et al. (1994)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	12	86	Severe						Gautheron et al. (1994)
Ethyl acetate	141-78-6	liquid	100%	99	1	19.7	Mild						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	2	28.4	Moderate						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	3	47.1	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	4	44.31	Moderate						Balls et al. (1995)
Ethyl acetate	141-78-6	liquid	100%	99	5	20.6	Mild						Balls et al. (1995)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	1	26	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	2	38	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	3	31	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	4	33	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	5	21	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	6	29	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	7	28	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	8	38	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	9	26	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	11	38	Moderate						Gautheron et al. (1994)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	12	42	Moderate						Gautheron et al. (1994)
2-Ethylhexanol	104-76-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Category 2A		Category II	R36	Casterton et al. (1996)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	1	62	Severe						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	2	28.2	Moderate						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	3	30.7	Moderate	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	4	58.71	Severe						Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	5	19.6	Mild						Balls et al. (1995)
Ethylhexyl acid phosphate ester	-	liquid	100%	n.p.	-	130.5	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	liquid	100%	n.p.	-	8.8	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	1	27.5	Moderate						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	2	14.1	Mild						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	3	5.5	Mild	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	4	5.543	Mild						Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	5	19.6	Mild						Balls et al. (1995)
3-Ethyltoluene	620-14-4	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	1	27.4	Moderate						Balls et al. (1995)

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Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	2	33.7	Moderate	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	3	10.5	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	4	8.633	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	5	9	Mild						Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Eye Make-Up Remover (HZH)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Eye Make-Up Remover (HZH) 100%	-	n.p.	10%	n.p.	-	0.2	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Facial Cleansing Foam (HZR) 25%	-	n.p.	10%	n.p.	-	4.1	Nonsevere	Nonsevere	Nonsevere	SCNM	Category I	SCNM	Gettings et al. (1996)
Facial Cleanser (HZZ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Facial Cleanser (HZZ) 100%	-	n.p.	10%	n.p.	-	1.8	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Floor Cleaner (#10)	-	liquid	100%	n.p.	-	70.3	Severe	Severe					Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	100%	n.p.	-	-0.3	Nonirritant	Nonirritant					Swanson et al. (1995)
Floor Stripper (#14)	-	liquid	100%	n.p.	-	157.3	Severe	Severe					Swanson et al. (1995)
Floor Stripper (#17)	-	liquid	100%	n.p.	-	216.2	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)
Floor Stripper (#18)	-	liquid	100%	n.p.	-	444.3	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Foam Bath (HZZ)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Foam Bath (HZZ) 100%	-	n.p.	10%	n.p.	-	18.6	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Fomesafen	72128-02-0	solid	20%	97.5	1	45.5	Moderate	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	2	151.9	Very severe						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	3	64.9	Severe						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	4	23.023	Mild						Balls et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	5	18.2	Mild						Balls et al. (1995)
Furan	110-00-9	liquid	100%	n.p.	1	73	Severe	Severe	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	2	63	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	3	61	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	4	65	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	5	33	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	6	34	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	7	87	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	8	48	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	10	39	Moderate						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	11	68	Severe						Gautheron et al. (1994)
Furan	110-00-9	liquid	100%	n.p.	12	51	Moderate						Gautheron et al. (1994)
Gel Cleanser (HZE)	-	n.p.	100%	n.p.	-	-	Mild						Mild
Gel Cleanser (HZE) 100%	-	n.p.	10%	n.p.	-	3.1	Nonsevere	Nonsevere	SCNM		Category I	SCNM	Gettings et al. (1996)
General Cleaner (#11)	-	liquid	100%	n.p.	-	83.3	Severe	Severe					Swanson et al. (1995)
General Cleaner (#12)	-	liquid	100%	n.p.	-	113.5	Severe	Severe					Swanson et al. (1995)
Glass Cleaner (#19)	-	liquid	100%	n.p.	-	135.8	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Gluconolactone	90-80-2	solid	20%	n.p.	1	63	Severe	Severe	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	2	81	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	3	90	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	4	62	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	5	108	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	6	66	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	7	90	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	8	57	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	9	88	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	11	75	Severe						Gautheron et al. (1994)
Gluconolactone	90-80-2	solid	20%	n.p.	12	63	Severe						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	1	2	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	4	1	Mild	Mild	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	6	-4	Nonirritant						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	7	1	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	8	4	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	10	2	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)					
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	12	-1	Nonirritant						Gautheron et al. (1994)					
Glycerol	56-81-5	liquid	100%	>99.5	1	-2	Mild						Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	2	-0.2	Mild											Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	3	0.3	Mild											Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	4	3.08	Mild	Balls et al. (1995)										
Glycerol	56-81-5	liquid	100%	>99.5	5	0.1	Mild	Balls et al. (1995)										
Glycerol	56-81-5	liquid	100%	n.p.	-	-	Mild	Casterton et al. (1996)										
Glycerol	56-81-5	liquid	100%	>99.5	1 (1)	0.6	Mild	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	1 (2)	0.3	Mild						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	2 (1)	0.8	Nonirritant						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	2 (2)	0.8	Nonirritant						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	3 (1)	1.0	Nonirritant						Southee (1998)					
Glycerol	56-81-5	liquid	100%	>99.5	3 (2)	0.8	Nonirritant						Southee (1998)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	1	18	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	2	24	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	3	25	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	4	14	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	5	13	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	6	6	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	7	15	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	8	18	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	9	18	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	11	23	Mild						Gautheron et al. (1994)					
3-Glycidoxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)					
Hand Soap (HZU) 25%	-	n.p.	10%	n.p.	-	5.5	Nonsevere						Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Heavy Duty Cleaner (#15)	-	liquid	100%	n.p.	-	357.1	Severe						Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	100%	n.p.	-	354.7	Severe	Severe	Category 1				Swanson et al. (1995)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1	93	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2	40	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3	53	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	4	33	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	5	91	Severe						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	6	42	Moderate						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	7	82	Severe						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	8	76	Severe						Gautheron et al. (1994)					
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	9	70	Severe						Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	11	48	Moderate						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	12	102	Severe						Gautheron et al. (1994)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (1)	23.1	Mild	Moderate	Category 1	4	Category I	R41	Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	1 (2)	17.2	Mild						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (1)	34.6	Moderate						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	2 (2)	39.1	Moderate						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (1)	31.7	Moderate						Southee (1998)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	3 (2)	29.9	Moderate						Southee (1998)
1,5-Hexadiene	592-42-7	liquid	100%	n.p.	-	-	Mild						Mild
Hexane	110-54-3	liquid	100%	n.p.	1	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	2	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	3	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	4	0	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	5	2	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	6	1	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	7	3	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	8	1	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	9	1	Mild						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	10	-1	Nonirritant						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Hexane	110-54-3	liquid	100%	n.p.	12	6	Mild						Gautheron et al. (1994)
n-Hexanol	111-27-3	liquid	100%	98	1	71.5	Severe						Severe/Very Severe
n-Hexanol	111-27-3	liquid	100%	98	2	83.6	Very severe	Balls et al. (1995)					
n-Hexanol	111-27-3	liquid	100%	98	3	63.2	Severe	Balls et al. (1995)					
n-Hexanol	111-27-3	liquid	100%	98	4	48.19	Moderate	Balls et al. (1995)					
n-Hexanol	111-27-3	liquid	100%	98	5	42.9	Moderate	Balls et al. (1995)					
Imidazole	288-32-4	solid	20%	99	1	116.8	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	2	133.9	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	3	103.4	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	4	118.7	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	99	5	90.8	Very severe						Balls et al. (1995)
Imidazole	288-32-4	solid	20%	n.p.	1	75	Severe	Severe	Category 1	4	Category I	R41	Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	2	73	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	3	140	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	4	81	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	5	96	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	6	62	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	7	82	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	8	122	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	9	64	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	10	81	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	11	114	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	12	65	Severe						Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	1 (1)	142.0	Very severe						
Imidazole	288-32-4	solid	20%	n.p.	1 (2)	137.6	Very severe						Southee (1998)

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Imidazole	288-32-4	solid	20%	n.p.	1 (3)	112.2	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (4)	131.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (5)	145.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (6)	162.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	1 (7)	125.5	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (1)	138.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (2)	140.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (3)	134.9	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (4)	157.2	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (5)	137.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (6)	152.9	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	2 (7)	148.7	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (1)	139.6	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (2)	140.1	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (3)	124.0	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (4)	128.7	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (5)	123.4	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (6)	121.2	Very severe						Southee (1998)
Imidazole	288-32-4	solid	20%	n.p.	3 (7)	131.3	Very severe						Southee (1998)
Iminodibenzyl	494-19-9	solid	20%	n.p.	1	0	Mild						Mild
Iminodibenzyl	494-19-9	solid	20%	n.p.	2	1	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	3	6	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	4	0	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	5	4	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	6	0	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	7	1	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	8	12	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	9	0	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	10	no data	n.a.	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	11	6	Mild	Gautheron et al. (1994)					
Iminodibenzyl	494-19-9	solid	20%	n.p.	12	-4	Nonirritant	Gautheron et al. (1994)					
Isobutanol	78-83-1	liquid	100%	99.9	1	54.4	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	2	74	Severe						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	3	67.7	Severe						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	4	41.78	Moderate						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	99.9	5	42.2	Moderate						Balls et al. (1995)
Isobutanol	78-83-1	liquid	100%	n.p.	-	-	Severe	Severe	Category 2A	-	Category II	R36	Casterton et al. (1996)
Isopropanol	67-63-0	liquid	100%	99.9	1	39.7	Moderate	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	2	59.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	3	72.3	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	4	78.5	Severe						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	5	39.3	Moderate						Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	n.p.	-	-	Moderate						Moderate
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	1	53	Moderate	Moderate	Category 2B		Category III	Nonirritant	Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	2	50	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	3	48	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	4	28	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	5	45	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	6	35	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	7	48	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	8	43	Moderate						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	9	63	Severe						Gautheron et al. (1994)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	11	89	Severe	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)					
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	12	48	Moderate						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	1	81	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	2	82	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	3	103	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	4	76	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	5	92	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	6	68	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	7	90	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	8	62	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	9	102	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	11	76	Severe						Gautheron et al. (1994)					
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	12	55	Moderate						Gautheron et al. (1994)					
Liquid Soap No. 2 (HZW) 25%	-	n.p.	10%	n.p.	-	5.6	Nonsevere						Nonsevere	Category 2B		Category III	Nonirritant	Gettings et al. (1996)
Liquid Soap No. 1 (HZB) 25%	-	n.p.	10%	n.p.	-	2.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	1	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	2	6	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	3	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	4	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	7	7	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	8	3	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	11	0	Mild						Gautheron et al. (1994)					
Magnesium carbonate	56378-72-4	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)					
Maneb	12427-38-2	solid	20%	90	1	67	Severe						Nonsevere	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	2	16.9	Mild											Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	3	21	Mild											Balls et al. (1995)
Maneb	12427-38-2	solid	20%	90	4	63.76	Severe	Balls et al. (1995)										
Maneb	12427-38-2	solid	20%	90	5	33.8	Moderate	Balls et al. (1995)										
Meat Room Degreaser (#3)	-	liquid	100%	n.p.	-	140.3	Severe	Severe					Swanson et al. (1995)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	2	-1	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	4	1	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	8	-8	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	9	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	10	0	Mild						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	11	-4	Nonirritant						Gautheron et al. (1994)					
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	12	-3	Nonirritant						Gautheron et al. (1994)					
Metal Cleaner (#20)	-	liquid	100%	n.p.	-	391.9	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)					
Methanol	67-56-1	liquid	100%	n.p.	1	88	Severe	Severe	Nonirritant		Category II	Nonirritant	Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	2	88	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	3	54	Moderate						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	4	71	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	5	81	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	6	108	Severe						Gautheron et al. (1994)					
Methanol	67-56-1	liquid	100%	n.p.	7	37	Moderate						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Methanol	67-56-1	liquid	100%	n.p.	8	19	Mild						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	9	99	Severe						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	11	179	Severe						Gautheron et al. (1994)
Methanol	67-56-1	liquid	100%	n.p.	12	102	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	1	61	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	2	69	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	3	66	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	4	47	Moderate						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	5	48	Moderate						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	6	62	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	7	65	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	8	62	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	9	57	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	11	74	Severe						Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	12	88	Severe						Gautheron et al. (1994)
Methyl acetate	79-20-9	liquid	100%	98	1	71.2	Severe						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	2	46.5	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	3	51.6	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	4	53.9	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	98	5	51.1	Moderate						Balls et al. (1995)
Methyl acetate	79-20-9	liquid	100%	n.p.	-	-	Moderate						Casteron et al. (1996)
Methyl cyanoacetate	105-34-0	liquid	100%	99	1	16.3	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	2	5.9	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	3	10.1	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	4	17.53	Mild						Balls et al. (1995)
Methyl cyanoacetate	105-34-0	liquid	100%	99	5	11	Mild						Balls et al. (1995)
Methyl cyclopentadiene dimer	-	liquid	100%	n.p.	-	0.7	Mild						Bailey et al. (2004)
Methylcyclopentane	96-37-7	liquid	100%	>99	1	3.8	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	2	4.6	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	3	1.4	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	4	1.71	Mild						Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	5	2.7	Mild						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1	93	Very severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2	67.4	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3	52.2	Moderate						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	4	78.71	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	5	60.8	Severe						Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	n.p.	-	-	Moderate						Casteron et al. (1996)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (1)	73.3	Severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	1 (2)	67.8	Severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (1)	108.7	Very severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	2 (2)	101.7	Very severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (1)	70.2	Severe						Southee (1998)
Methyl ethyl ketone	78-93-3	liquid	100%	99	3 (2)	73.5	Severe						Southee (1998)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	1	8.8	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	2	20.1	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	3	10.3	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	4	13.25	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	5	10.3	Mild						Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	liquid	100%	n.p.	-	-	Moderate						Casteron et al. (1996)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	1	22	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	2	25	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	3	27	Moderate	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	4	19	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	5	21	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	6	23	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	7	16	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	8	16	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	9	19	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	11	20	Mild						Gautheron et al. (1994)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	12	11	Mild						Gautheron et al. (1994)
1-Methylpropyl benzene	135-98-8	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Mild Shampoo (HZJ)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Mild Shampoo (HZJ) 25%	-	n.p.	10%	n.p.	-	0.1	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
MYRJ-45	-	surfactant	10%	n.p.	1	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	2	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	3	0	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	4	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	5	0	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	6	0	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	7	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	8	-4	Nonirritant						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	9	1	Mild						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	11	-3	Nonirritant						Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	12	-1	Nonirritant						Gautheron et al. (1994)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	1	120.8	Very severe						Very Severe
1-Naphthalene acetic acid	86-87-3	solid	20%	96	2	66.3	Severe	Balls et al. (1995)					
1-Naphthalene acetic acid	86-87-3	solid	20%	96	3	42	Moderate	Balls et al. (1995)					
1-Naphthalene acetic acid	86-87-3	solid	20%	96	4	88.73	Very severe	Balls et al. (1995)					
1-Naphthalene acetic acid	86-87-3	solid	20%	96	5	72.5	Severe	Balls et al. (1995)					
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	1	136	Very severe	Balls et al. (1995)					
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	2	144.9	Very severe	Very Severe	Category 1	1	Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	3	161	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	4	161.2	Very severe						Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	5	143	Very severe						Balls et al. (1995)
1-Nitropropane	108-03-2	liquid	100%	n.p.	1	11	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	2	8	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	3	9	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	4	4	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	5	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	7	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	8	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	9	17	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	10	4	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	11	6	Mild						Gautheron et al. (1994)
1-Nitropropane	108-03-2	liquid	100%	n.p.	12	7	Mild						Gautheron et al. (1994)
n-Octanol	111-87-5	liquid	100%	>99	1	43.4	Moderate						Moderate
n-Octanol	111-87-5	liquid	100%	>99	2	78.9	Severe	Balls et al. (1995)					
n-Octanol	111-87-5	liquid	100%	>99	3	39.8	Moderate	Balls et al. (1995)					
n-Octanol	111-87-5	liquid	100%	>99	4	14.54	Mild	Balls et al. (1995)					
n-Octanol	111-87-5	liquid	100%	>99	5	28	Moderate	Balls et al. (1995)					
Octanol	111-87-5	liquid	100%	n.p.	1	65	Severe	Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	2	33	Moderate	Gautheron et al. (1994)					

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Octanol	111-87-5	liquid	100%	n.p.	3	42	Moderate	Moderate	Category 2B		Category III	R36	Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	4	49	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	5	66	Severe						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	6	48	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	7	37	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	8	25	Mild						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	9	61	Severe						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	11	31	Moderate						Gautheron et al. (1994)					
Octanol	111-87-5	liquid	100%	n.p.	12	64	Severe						Gautheron et al. (1994)					
Parafluoraniiline	371-40-4	liquid	100%	99	1	29.5	Moderate						Moderate	SCNM		SCNM	Balls et al. (1995)	
Parafluoraniiline	371-40-4	liquid	100%	99	2	26.4	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	99	3	40.8	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	99	4	31.82	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	99	5	23.5	Moderate	Balls et al. (1995)										
Parafluoraniiline	371-40-4	liquid	100%	n.p.	-	-	Moderate	Casterton et al. (1996)										
Parafluoraniiline	371-40-4	liquid	100%	99	1 (1)	31	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	1 (2)	35	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	2 (1)	38.3	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	2 (2)	37.5	Moderate	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	3 (1)	22.1	Mild	Southee (1998)										
Parafluoraniiline	371-40-4	liquid	100%	99	3 (2)	28.9	Moderate	Southee (1998)										
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	1	61	Severe	Severe	Nonirritant		Category III	Nonirritant					Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	2	79	Severe										Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	3	75	Severe										Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	4	34	Moderate										Gautheron et al. (1994)	
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	5	70	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	6	46	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	7	54	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	8	44	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	9	50	Moderate						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	10	67	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	11	62	Severe						Gautheron et al. (1994)					
2,4-Pentanedione	123-54-6	liquid	100%	n.p.	12	76	Severe						Gautheron et al. (1994)					
Petroleum ether	8032-32-4	liquid	100%	n.p.	1	8	Mild						Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Petroleum ether	8032-32-4	liquid	100%	n.p.	2	13	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	3	11	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	4	1	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	5	2	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	6	5	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	7	7	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	8	0	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	9	2	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	10	3	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	11	5	Mild	Gautheron et al. (1994)										
Petroleum ether	8032-32-4	liquid	100%	n.p.	12	9	Mild	Gautheron et al. (1994)										
Petroleum wax	-	solid	100%	n.p.	-	0.3	Mild	Mild	Nonirritant		Category IV	Nonirritant						Bailey et al. (2004)
Phenylbutazone	50-33-9	solid	20%	n.p.	1	0	Mild	Mild	Nonirritant		Category IV	Nonirritant						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	3	1	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	4	0	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	6	1	Mild						Gautheron et al. (1994)					
Phenylbutazone	50-33-9	solid	20%	n.p.	7	0	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Phenylbutazone	50-33-9	solid	20%	n.p.	8	-6	Nonirritant						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	9	1	Mild						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	10	1	Mild						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	11	-3	Nonirritant						Gautheron et al. (1994)
Phenylbutazone	50-33-9	solid	20%	n.p.	12	2	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	1	7	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	2	12	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	3	15	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	4	9	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	5	28	Moderate						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	6	6	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	8	16	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	9	13	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	10	15	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	11	13	Mild						Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	12	15	Mild						Gautheron et al. (1994)
Polishing Scrub (H2T)	-	n.p.	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polishing Scrub (H2T) 100%	-	n.p.	10%	n.p.	-	3.7	Nonsevere	Nonsevere	Nonirritant		Category IV	Nonirritant	Gettings et al. (1996)
Polyalkenylsuccinate ester/amine salt	-	liquid	100%	n.p.	-	2.3	Mild	Mild	SCNM		Category III	SCNM	Bailey et al. (2004)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	1	0.6	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	2	2.5	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	3	-1.3	Nonirritant						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	4	1.08	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	5	2.8	Mild						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category IV	Nonirritant	Casterton et al. (1996)
Polyethylene glycol 600	-	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Pot and Pan Cleaner (#8)	-	liquid	100%	n.p.	-	-0.6	Nonirritant	Nonirritant					Swanson et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	1	16.2	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	2	22.9	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	3	12	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	4	17.38	Mild						Balls et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	5	6.5	Mild						Balls et al. (1995)
Process oil	-	liquid	100%	n.p.	-	2.7	Mild	Mild	Nonirritant		Category IV	Nonirritant	Bailey et al. (2004)
Promethazine hydrochloride	58-33-3	solid	20%	98	1	120.3	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	2	84.2	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	3	125.7	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	4	123.09	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	98	5	153.8	Very severe						Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	1	117	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	2	156	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	3	109	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	4	111	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	5	164	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	6	174	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	7	103	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	8	50	Moderate						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	9	139	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	11	94	Severe						Gautheron et al. (1994)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	12	19	Mild						Gautheron et al. (1994)
Propylene glycol	57-55-6	liquid	100%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	1	7	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	2	7	Mild						Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	3	14	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	4	4	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	5	6	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	6	9	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	7	6	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	8	11	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	9	6	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	11	12	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	12	5	Mild						Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (1)	11.2	Mild	Mild	Nonirritant		Category III	Nonirritant	Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	1 (2)	7.4	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (1)	5.2	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	2 (2)	3.6	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (1)	7.7	Mild						Southee (1998)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	3 (2)	6.2	Mild	Southee (1998)					
Pyridine	110-86-1	liquid	100%	>99.9	1	140.7	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	2	145.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	3	132.4	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	4	199.02	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	>99.9	5	122.7	Very severe						Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	n.p.	1	102	Severe	Severe	Category 1	4	Category II	R41	Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	2	123	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	3	186	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	4	79	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	5	102	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	6	77	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	7	124	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	8	132	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	9	105	Severe						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Pyridine	110-86-1	liquid	100%	n.p.	11	96	Severe	Gautheron et al. (1994)					
Pyridine	110-86-1	liquid	100%	n.p.	12	115	Severe	Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	1	0.3	Mild	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	2	0.4	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	3	2.1	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	4	1.85	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	5	3.1	Mild						Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	1	17	Mild	Moderate	Category 1	1	Category I	R41	Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	2	29	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	3	8	Mild						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	4	46	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	5	52	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	6	24	Mild						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	7	15	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	8	18	Moderate						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	9	58	Severe						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Quinacrine	69-05-6	solid	20%	n.p.	11	3	Mild	Gautheron et al. (1994)					
Quinacrine	69-05-6	solid	20%	n.p.	12	72	Severe	Gautheron et al. (1994)					
Shampoo No. 1 (HZC) 25%	-	n.p.	10%	n.p.	-	30.0	Severe	Severe	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)
Shampoo No. 2 (HZX)	-	n.p.	10%	n.p.	-	14.0	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)
Shampoo No. 3 (HZM) 25%	-	n.p.	10%	n.p.	-	4.3	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference					
Shampoo No. 4 (HZV) 25%	-	n.p.	10%	n.p.	-	8.4	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shampoo No. 5 (HZD) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shampoo No. 6 (HZN) 25%	-	n.p.	10%	n.p.	-	4.5	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shampoo No. 7 (HZA)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)					
Shampoo No. 7 (HZA) 100%	-	n.p.	10%	n.p.	-	6.6	Nonsevere	Nonsevere	Category 1	1	Category I	R41	Gettings et al. (1996)					
Shampoo No. 8 (HZG) 25%	-	n.p.	10%	n.p.	-	2.7	Nonsevere	Nonsevere	Nonirritant		Category III	Nonirritant	Gettings et al. (1996)					
Shower Gel (HZS)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)					
Shower Gel (HZS) 100%	-	n.p.	10%	n.p.	-	35.9	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)					
Skin Cleanser (HZI)	-	n.p.	100%	n.p.	-	-	Moderate	Moderate	Category 1	1	Category I	R41	Casterton et al. (1996)					
Skin Cleanser (HZI) 100%	-	n.p.	10%	n.p.	-	15.8	Severe	Severe	Category 1	1	Category I	R41	Gettings et al. (1996)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	1	167.4	Very severe	Very Severe	Category 2B		Category III	R36	Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	2	133.2	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	3	146.5	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	4	171.08	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	5	132.3	Very severe						Balls et al. (1995)					
Sodium hydroxide (1%)	1310-73-2	liquid	1%	n.p.	-	-	Severe	Severe	Category 2B		Category III	R36	Casterton et al. (1996)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	1	285.2	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	2	224.1	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	3	254.7	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	4	348.27	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	5	247.2	Very severe						Balls et al. (1995)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (1)	245.0	Very severe	Very Severe	Category 1	4	Category I	R41	Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	1 (2)	227.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (1)	241.3	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	2 (2)	235.5	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (1)	193.1	Very severe						Southee (1998)					
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	3 (2)	214.9	Very severe						Southee (1998)					
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	1	47.3	Moderate						Severe	Category 1	NC	Category I	R36	Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	2	93	Very severe											Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	3	63.2	Severe											Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	4	59.61	Severe											Balls et al. (1995)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	5	53.3	Moderate	Balls et al. (1995)										
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	n.p.	-	-	Moderate	Moderate	Category 1	NC	Category I	R36	Casterton et al. (1996)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (1)	5.4	Mild	Mild	Category 1	NC	Category I	SCNM	Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	1 (2)	5.2	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (1)	15.9	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	2 (2)	17.3	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (1)	8.7	Mild						Southee (1998)					
Sodium lauryl sulfate (15%)	151-21-3	liquid	10%	98	3 (2)	5.6	Mild						Southee (1998)					
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	1	31.7	Moderate						Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	2	31.7	Moderate											Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	3	27.3	Moderate	Balls et al. (1995)										
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	4	26.22	Moderate	Balls et al. (1995)										
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	5	12.3	Mild	Balls et al. (1995)										
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)					
Sodium lauryl sulfate (30 %)	151-21-3	liquid	30%	n.p.	-	-	Moderate	Moderate					Casterton et al. (1996)					
Sodium oxalate	62-76-0	solid	20%	>99	1	2.1	Mild	Mild	Category 1	4	Category I	R41	Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	2	7.6	Mild						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	3	5.8	Mild						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	4	49.59	Moderate						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	>99	5	4.9	Mild						Balls et al. (1995)					
Sodium oxalate	62-76-0	solid	20%	n.p.	1	2	Mild						Gautheron et al. (1994)					
Sodium oxalate	62-76-0	solid	20%	n.p.	2	2	Mild						Gautheron et al. (1994)					

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Sodium oxalate	62-76-0	solid	20%	n.p.	3	9	Mild	Mild	Category 1	4	Category I	R41	Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	4	5	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	5	3	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	6	2	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	7	4	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	8	3	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	9	3	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	10	9	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	11	11	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	n.p.	12	4	Mild						Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	99	1 (1)	10.3	Mild						Nonirritant
Sodium oxalate	62-76-0	solid	20%	99	1 (2)	4.4	Mild	Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	2 (1)	-0.3	Nonirritant	Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	2 (2)	-0.1	Nonirritant	Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	3 (1)	2.7	Nonirritant	Southee (1998)					
Sodium oxalate	62-76-0	solid	20%	99	3 (2)	4.5	Mild	Southee (1998)					
Sodium perborate	10486-00-7	solid	20%	98.6	1	143.6	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	2	118.4	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	3	96.2	Very severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	4	64.531	Severe						Balls et al. (1995)
Sodium perborate	10486-00-7	solid	20%	98.6	5	62.9	Severe						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	1	23.6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	2	7.9	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	3	14.2	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	4	20.65	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	5	8.9	Mild						Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	1	5	Mild	Mild	Nonirritant		Category II	Nonirritant	Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	2	1	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	3	2	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	4	6	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	5	0	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	6	4	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	7	2	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	8	19	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	9	3	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	11	18	Mild						Gautheron et al. (1994)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	12	6	Mild						Gautheron et al. (1994)
Thiadiazole alkyl derivative	-	liquid	100%	n.p.	-	10.9	Moderate	Moderate	SCNM		Category III	SCNM	Bailey et al. (2004)
Thiourea	62-56-6	solid	20%	>99	1	149.4	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	2	139.2	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	3	135.6	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	4	137.44	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	>99	5	99.1	Very severe						Balls et al. (1995)
Thiourea	62-56-6	solid	20%	n.p.	1	146	Severe	Severe	SCNM		SCNM	SCNM	Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	2	175	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	3	169	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	4	152	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	5	140	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	6	120	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	7	129	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	8	173	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	9	151	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	10	no data	n.a.						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Thiourea	62-56-6	solid	20%	n.p.	11	203	Severe						Gautheron et al. (1994)
Thiourea	62-56-6	solid	20%	n.p.	12	104	Severe						Gautheron et al. (1994)
Toilet Bowl Cleaner (#1)	-	liquid	100%	n.p.	-	13.5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Swanson et al. (1995)
Toilet Bowl Cleaner (#4)	-	liquid	100%	n.p.	-	15	Mild	Mild	Nonirritant		SCNM	Nonirritant	Swanson et al. (1995)
Toluene	108-88-3	liquid	100%	99	1	43.3	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	2	33.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	3	37.2	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	4	38.41	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	99	5	26.1	Moderate						Balls et al. (1995)
Toluene	108-88-3	liquid	100%	n.p.	-	-	Severe	Severe	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	1	81.9	Very severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	2	49.8	Moderate						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	3	75.3	Severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	4	92.97	Very severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	5	79.3	Severe						Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	1	272	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	2	225	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	3	296.9	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	4	323.08	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	5	203.7	Very severe						Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	n.p.	-	-	Severe	Severe	Category 1	4	Category I	R41	Casterton et al. (1996)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	1	47	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	2	42	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	3	78	Severe						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	4	28	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	5	42	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	6	47	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	7	48	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	8	24	Mild						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	9	91	Severe						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	11	28	Moderate						Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	12	47	Moderate						Gautheron et al. (1994)
Triethanolamine	102-71-6	liquid	100%	n.p.	1	2	Mild						Mild
Triethanolamine	102-71-6	liquid	100%	n.p.	2	4	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	3	0	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	4	0	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	5	-1	Nonirritant	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	6	1	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	7	1	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	8	3	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	9	3	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	10	no data	n.a.	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	11	5	Mild	Gautheron et al. (1994)					
Triethanolamine	102-71-6	liquid	100%	n.p.	12	6	Mild	Gautheron et al. (1994)					
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	1	25	Mild	Mild	Nonirritant		Category III	Nonirritant	Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	2	14	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	3	26	Moderate						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	4	11	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	5	27	Moderate						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	6	7	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	7	9	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	8	15	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	9	21	Mild						Gautheron et al. (1994)

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Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	10	10	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	11	7	Mild						Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	12	21	Mild						Gautheron et al. (1994)
Triton X-100 (1%)	9002-93-1	liquid	1%	n.p.	-	-	Mild	Mild					Casterton et al. (1996)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	1	85.7	Very severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	2	76	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	3	86.1	Very severe	Severe/Very Severe	Category 1	NC	Category II	R41	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	4	57.58	Severe						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	5	46.2	Moderate						Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	liquid	10%	n.p.	-	-	Severe	Severe	Category 1	NC	Category II	R41	Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	5%	98	1	74.3	Severe						Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	98	2	106.6	Very severe						Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	98	3	80.2	Very severe	Very Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	98	4	76.79	Very severe						Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	98	5	53.6	Moderate						Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	n.p.	-	-	Moderate	Moderate	Category 2A		Category III	Nonirritant	Casterton et al. (1996)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (1)	3.7	Mild						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	1 (2)	1.8	Mild						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (1)	5.8	Mild	Mild	Category 2B		Category III	R36	Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	2 (2)	3.4	Mild						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (1)	3.0	Nonirritant						Southee (1998)
Triton X-100 (5%)	9002-93-1	liquid	10%	98	3 (2)	1.9	Nonirritant						Southee (1998)
Triton X-155	9010-44-0	surfactant	10%	n.p.	1	-1	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	2	1	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	3	-1	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	4	0	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	5	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	6	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	7	0	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	8	2	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	9	3	Mild						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	10	no data	n.a.						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	11	-2	Nonirritant						Gautheron et al. (1994)
Triton X-155	9010-44-0	surfactant	10%	n.p.	12	0	Mild						Gautheron et al. (1994)
Tween 20	9005-64-5	liquid	n.p.	98	1	-0.6	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	2	-1.1	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	3	-1.6	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	4	2.711	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	n.p.	98	5	0.4	Mild						Balls et al. (1995)
Tween 20	9005-64-5	liquid	100%	98	1 (1)	0.3	Mild						Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	1 (2)	0.0	Mild						Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	2 (1)	0.4	Mild	Nonirritant	Nonirritant		Category III	Nonirritant	Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	2 (2)	0.4	Nonirritant						Southee (1998)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance Name

Substance	CASRN ¹	Form Tested	Concentration Tested	Purity (%)	Lab No.	<i>In Vitro</i> Score	<i>In Vitro</i> Classification ²	Consensus Classification ³	<i>In Vivo</i> GHS ^{4,5}	GHS Category 1 SubClass ⁶	<i>In Vivo</i> EPA ^{7,8}	<i>In Vivo</i> EU ^{9,10}	Reference
Tween 20	9005-64-5	liquid	100%	98	3 (1)	0.3	Nonirritant						Southee (1998)
Tween 20	9005-64-5	liquid	100%	98	3 (2)	0.0	Nonirritant						Southee (1998)
Tween 20	9005-64-5	liquid	100%	n.p.	-	-	Mild	Mild	Nonirritant		Category III	Nonirritant	Casterton et al. (1996)
Xylene	1330-20-7	liquid	100%	n.p.	-	-	Moderate	Moderate	Nonirritant		Category II	Nonirritant	Casterton et al. (1996)

¹CASRN=Chemical Abstract Services Registry Number

²*In Vitro* Classification represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance

³Consensus classification represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls

⁴GHS=Globally Harmonized System (UN [2003])

⁵Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye

⁶NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are both severe and persistent; and 4: corneal opacity score equal to 4 at any time; NC: not classified because none of the above criteria were met

⁷EPA=U.S. Environmental Protection Agency (EPA [1996]).

⁸Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr

⁹EU=European Union (EU [2001]).

¹⁰Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

¹¹SCNM=Study Criteria Not Met

¹²n.p.=Not provided

¹³n.a.=Not applicable

Appendix E

Intralaboratory Coefficient of Variation (CV) Analysis of BCOP

E1	BCOP Data from Southee 1998	E-3
E2	BCOP Data from Dr. Joseph Sina	E-17
E3	BCOP Data from Dr. Freddy Van Goethem	E-27

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Appendix E1

BCOP Data from Southee (1998)

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**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Ammonium nitrate - Lab 1 (1)	1	100%	6.0	0.078	7.2	
	2		2.0	0.022	2.3	
	3		5.0	0.011	5.2	
	mean		4.3	0.037	4.9	
	SD		2.1	0.036	2.5	
	%CV		48.0	97.1	50.3	
Ammonium nitrate - Lab 1 (2)	1	100%	5.7	0.038	6.3	
	2		5.7	0.094	7.1	
	3		3.7	0.045	4.4	
	mean		5.0	0.059	5.9	
	SD		1.2	0.031	1.4	
	%CV		22.9	51.7	23.4	
Ammonium nitrate - Lab 2 (1)	1	100%	2.3	0.123	4.1	
	2		2.3	0.221	5.6	
	3		0.3	0.116	2.0	
	mean		1.6	0.153	3.9	
	SD		1.2	0.059	1.8	
	%CV		70.7	38.3	46.4	
Ammonium nitrate - Lab 2 (2)	1	100%	1.7	0.057	2.6	
	2		1.7	0.139	3.8	
	3		2.7	0.126	4.6	
	mean		2.0	0.107	3.7	
	SD		0.6	0.044	1.0	
	%CV		28.4	41.1	27.5	
Ammonium nitrate - Lab 3 (1)	1	100%	4.0	0.126	5.9	
	2		3.0	0.111	4.7	
	3		4.0	0.063	4.9	
	mean		3.7	0.100	5.2	
	SD		0.6	0.033	0.6	
	%CV		15.7	32.9	12.4	
Ammonium nitrate - Lab 3 (2)	1	100%	4.0	0.191	6.9	
	2		4.0	0.078	5.2	
	3		5.0	0.207	8.1	
	mean		4.3	0.159	6.7	
	SD		0.6	0.070	1.5	
	%CV		13.3	44.3	21.6	
Benzalkonium chloride - Lab 1 (1)	1	100%	79.7	8.005	199.8	
	2		85.7	7.850	203.5	
	3		86.7	6.370	182.3	
	mean		84.0	7.408	195.2	
	SD		3.8	0.903	11.3	
	%CV		4.5	12.2	5.8	
Benzalkonium chloride - Lab 1 (2)	1	100%	89.3	3.326	139.2	
	2		84.3	3.519	137.1	
	3		83.3	3.070	129.4	
	mean		85.6	3.305	135.2	
	SD		3.2	0.225	5.2	
	%CV		3.8	6.8	3.8	
Benzalkonium chloride - Lab 1 (3)	1	100%	83.0	3.708	138.6	
	2		80.0	3.989	139.8	
	3		83.0	3.490	135.4	
	mean		82.0	3.729	137.9	
	SD		1.7	0.250	2.3	
	%CV		2.1	6.709	1.6	
Benzalkonium chloride - Lab 1 (4)	1	100%	82.0	5.8	168.6	
	2		82.0	3.539	135.1	
	3		91.0	4.987	165.8	
	mean		85.0	4.766	156.5	
	SD		5.2	1.132	18.6	
	%CV		6.1	23.8	11.9	
Benzalkonium chloride - Lab 1 (5)	1	100%	89.7	3.229	138.1	
	2		86.7	3.415	137.9	
	3		86.7	3.418	138.0	
	mean		87.7	3.354	138.0	
	SD		1.7	0.108	0.1	
	%CV		2.0	3.2	0.1	

**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Benzalkonium chloride - Lab 2 (1)	1	100%	95.0	3.919	153.8	
	2		80.0	4.237	143.6	
	3		89.0	5.122	165.8	
	mean		88.0	4.426	154.4	
	SD		7.5	0.623	11.1	
	%CV		8.6	14.1	7.2	
Benzalkonium chloride - Lab 2 (2)	1	100%	106.3	4.780	178.0	
	2		91.3	3.459	143.2	
	3		86.3	4.205	149.4	
	mean		94.6	4.148	156.9	
	SD		10.4	0.662	18.6	
	%CV		11.0	16.0	11.8	
Benzalkonium chloride - Lab 2 (3)	1	100%	86.0	4.324	150.9	
	2		80.0	4.246	143.7	
	3		95.0	4.187	157.8	
	mean		87.0	4.252	150.8	
	SD		7.5	0.069	7.1	
	%CV		8.7	1.6	4.7	
Benzalkonium chloride - Lab 2 (4)	1	100%	96.0	4.512	163.7	
	2		93.0	5.200	171.0	
	3		90.0	3.123	136.8	
	mean		93.0	4.278	157.2	
	SD		3.0	1.058	18.0	
	%CV		3.2	24.7	11.5	
Benzalkonium chloride - Lab 2 (5)	1	100%	97.0	4.035	157.5	
	2		97.0	4.296	161.4	
	3		101.0	3.584	154.8	
	mean		98.3	3.972	157.9	
	SD		2.3	0.360	3.3	
	%CV		2.3	9.1	2.1	
Benzalkonium chloride - Lab 3 (1)	1	100%	96.7	3.842	154.3	
	2		98.7	5.102	175.2	
	3		94.7	3.102	141.2	
	mean		96.7	4.015	156.9	
	SD		2.0	1.011	17.1	
	%CV		2.1	25.2	10.9	
Benzalkonium chloride - Lab 3 (2)	1	100%	106.3	3.321	156.1	
	2		86.3	6.381	182.0	
	3		85.3	4.456	152.1	
	mean		92.6	4.719	163.4	
	SD		11.8	1.547	16.2	
	%CV		12.8	32.8	9.9	
Benzalkonium chloride - Lab 3 (3)	1	100%	101.0	4.364	166.5	
	2		102.0	3.974	161.6	
	3		112.0	4.609	181.1	
	mean		105.0	4.316	169.7	
	SD		6.1	0.320	10.1	
	%CV		5.8	7.4	6.0	
Benzalkonium chloride - Lab 3 (4)	1	100%	99.3	3.727	155.2	
	2		91.3	5.637	175.9	
	3		95.3	4.127	157.2	
	mean		95.3	4.497	162.8	
	SD		4.0	1.007	11.4	
	%CV		4.2	22.4	7.0	
Benzalkonium chloride - Lab 3 (5)	1	100%	84.0	3.993	143.9	
	2		97.0	4.153	159.3	
	3		96.0	3.698	151.5	
	mean		92.3	3.948	151.6	
	SD		7.2	0.231	7.7	
	%CV		7.8	5.8	5.1	
Hexadecyl trimethyl ammonium bromide - Lab 1 (1)	1	10%	15.3	0.968	29.8	
	2		11.3	0.512	19.0	
	3		13.3	0.481	20.5	
	mean		13.3	0.654	23.1	
	SD		2.0	0.273	5.9	
	%CV		15.0	41.7	25.3	
Hexadecyl trimethyl ammonium bromide - Lab 1 (2)	1	10%	13.0	0.569	21.5	
	2		11.0	0.554	19.3	
	3		5.0	0.374	19.3	
	mean		9.7	0.499	20.0	
	SD		4.2	0.109	1.3	
	%CV		43.1	21.7	6.3	
Hexadecyl trimethyl ammonium bromide - Lab 2 (1)	1	10%	16.0	1.970	45.6	

**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
	2		10.0	0.771	21.6	
	3		15.0	1.454	36.8	Moderate
	mean		13.7	1.398	34.7	
	SD		3.2	0.601	12.1	
	%CV		23.5	43.0	35.0	
Hexadecy trimethyl ammonium bromide - Lab 2 (2)	1	10%	16.0	1.572	39.6	
	2		15.0	2.686	55.3	
	3		8.0	0.970	22.6	Moderate
	mean		13.0	1.743	39.2	
	SD		4.4	0.871	16.4	
	%CV		33.5	50.0	41.8	
Hexadecy trimethyl ammonium bromide - Lab 3 (1)	1	10%	18.3	0.988	33.1	
	2		16.3	0.846	29.0	
	3		17.3	1.039	32.9	Moderate
	mean		17.3	0.958	31.7	
	SD		1.0	0.100	2.3	
	%CV		5.8	10.4	7.3	
Hexadecy trimethyl ammonium bromide - Lab 3 (2)	1	10%	17.0	0.537	25.1	
	2		16.0	0.402	22.0	Moderate
	3		20.0	1.515	42.7	
	mean		17.7	0.818	29.9	
	SD		2.1	0.607	11.2	
	%CV		11.8	74.3	37.3	
Ethanol - Lab 1 (1)	1	100%	16.3	1.227	34.7	
	2		20.3	1.534	43.3	Moderate
	3		16.3	1.034	31.8	
	mean		17.6	1.265	36.6	
	SD		2.3	0.252	6.0	
	%CV		13.1	19.9	16.3	
Ethanol - Lab 1 (2)	1	100%	22.7	1.753	49.0	
	2		13.7	1.502	36.2	Moderate
	3		12.7	0.990	27.6	
	mean		16.4	1.415	37.6	
	SD		5.5	0.389	10.8	
	%CV		33.7	27.5	28.6	
Ethanol - Lab 1 (3)	1	100%	15.0	1.325	34.9	
	2		12.0	0.703	22.5	Moderate
	3		14.0	1.157	31.4	
	mean		13.7	1.062	29.6	
	SD		1.5	0.322	6.4	
	%CV		11.2	30.3	21.6	
Ethanol - Lab 1 (4)	1	100%	11.7	2.259	45.6	
	2		13.7	2.050	44.5	Moderate
	3		12.7	1.491	35.1	
	mean		12.7	1.933	41.7	
	SD		1.0	0.397	5.8	
	%CV		7.9	20.5	13.8	
Ethanol - Lab 1 (5)	1	100%	13.0	0.987	27.8	
	2		14.0	1.084	30.3	Moderate
	3		17.0	1.303	36.5	
	mean		14.7	1.125	31.5	
	SD		2.1	0.162	4.5	
	%CV		14.2	14.4	14.2	

**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Ethanol - Lab 2 (1)	1	100%	14.3	1.576	37.9	Moderate
	2		12.3	3.163	59.7	
	3		13.3	3.138	60.4	
	mean		13.3	2.626	52.7	
	SD		1.0	0.909	12.8	
	%CV		7.5	34.6	24.3	
Ethanol - Lab 2 (2)	1	100%	18.3	1.979	48.0	Severe
	2		18.3	2.231	51.8	
	3		14.3	3.303	63.8	
	mean		17.0	2.504	54.5	
	SD		2.3	0.703	8.2	
	%CV		13.6	28.1	15.1	
Ethanol - Lab 2 (3)	1	100%	22.0	2.511	59.7	Severe
	2		13.0	3.821	70.3	
	3		14.0	2.743	55.1	
	mean		16.3	3.025	61.7	
	SD		4.9	0.699	7.8	
	%CV		30.2	23.1	12.6	
Ethanol - Lab 2 (4)	1	100%	19.0	3.106	65.6	Severe
	2		16.0	2.859	58.9	
	3		17.0	2.606	56.1	
	mean		17.3	2.857	60.2	
	SD		1.5	0.250	4.9	
	%CV		8.8	8.8	8.1	
Ethanol - Lab 2 (5)	1	100%	14.0	2.444	50.7	Moderate
	2		13.0	3.126	59.9	
	3		17.0	2.339	52.1	
	mean		14.7	2.636	54.2	
	SD		2.1	0.427	5.0	
	%CV		14.2	16.2	9.1	
Ethanol - Lab 3 (1)	1	100%	18.3	0.853	31.1	Moderate
	2		17.3	2.756	58.6	
	3		14.3	2.471	51.4	
	mean		16.6	2.027	47.0	
	SD		2.1	1.026	14.3	
	%CV		12.5	50.6	30.3	
Ethanol - Lab 3 (2)	1	100%	16.3	1.866	44.3	Moderate
	2		21.3	1.761	47.7	
	3		16.3	1.866	44.3	
	mean		18.0	1.831	45.4	
	SD		2.9	0.061	2.0	
	%CV		16.1	3.3	4.3	
Ethanol - Lab 3 (3)	1	100%	17.3	1.726	43.2	Moderate
	2		18.3	1.592	42.2	
	3		22.3	1.701	47.8	
	mean		19.3	1.673	44.4	
	SD		2.6	0.071	3.0	
	%CV		13.7	4.3	6.7	
Ethanol - Lab 3 (4)	1	100%	19.0	1.301	38.5	Moderate
	2		23.0	1.374	43.6	
	3		24.0	2.073	55.1	
	mean		22.0	1.583	45.7	
	SD		2.6	0.426	8.5	
	%CV		12.0	26.9	18.6	
Ethanol - Lab 3 (5)	1	100%	18.3	2.700	58.8	Moderate
	2		17.3	2.515	55.0	
	3		20.3	1.970	49.9	
	mean		18.6	2.395	54.6	
	SD		1.5	0.380	4.5	
	%CV		8.2	15.8	8.2	
Imidazole - Lab 1 (1)	1	100%	89.0	3.312	138.7	Severe
	2		93.0	3.325	142.9	
	3		92.0	3.501	144.5	
	mean		91.3	3.379	142.0	
	SD		2.1	0.106	3.0	
	%CV		2.3	3.1	2.1	

**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Imidazole - Lab 1 (2)	1	100%	95.0	2.629	134.4	
	2		89.0	3.760	145.0	Severe
	3		80.0	3.528	132.9	
	mean		88.0	3.306	137.4	
	SD		7.5	0.597	6.6	
	%CV		8.6	18.1	4.8	
Imidazole - Lab 1 (3)	1	100%	62.7	1.940	91.8	
	2		75.7	1.963	105.1	Severe
	3		82.7	3.792	139.6	
	mean		73.7	2.565	112.2	
	SD		10.1	1.063	24.7	
	%CV		13.8	41.4	22.0	
Imidazole - Lab 1 (4)	1	100%	94.7	2.141	126.8	
	2		87.7	2.664	127.7	Severe
	3		75.7	4.213	138.9	
	mean		86.0	3.006	131.1	
	SD		9.6	1.078	6.7	
	%CV		11.2	35.8	5.1	
Imidazole - Lab 1 (5)	1	100%	114.7	2.972	159.3	
	2		85.7	3.390	136.6	Severe
	3		90.7	3.361	141.1	
	mean		97.0	3.241	145.7	
	SD		15.5	0.233	12.0	
	%CV		16.0	7.2	8.3	
Imidazole - Lab 2 (1)	1	100%	88.7	3.831	146.2	
	2		74.7	3.227	123.1	Severe
	3		93.7	3.412	144.9	
	mean		85.7	3.490	138.1	
	SD		9.8	0.309	13.0	
	%CV		11.5	8.9	9.4	
Imidazole - Lab 2 (2)	1	100%	95.0	3.032	140.5	
	2		96.0	3.715	151.7	Severe
	3		73.0	3.666	128.0	
	mean		88.0	3.471	140.1	
	SD		13.0	0.381	11.9	
	%CV		14.8	11.0	8.5	
Imidazole - Lab 2 (3)	1	100%	86.3	2.539	124.4	
	2		92.3	3.357	142.7	Severe
	3		80.3	3.825	137.7	
	mean		86.3	3.240	134.9	
	SD		6.0	0.651	9.5	
	%CV		7.0	20.1	7.0	
Imidazole - Lab 2 (4)	1	100%	86.3	4.085	147.6	
	2		101.3	3.416	152.5	Severe
	3		89.3	5.471	171.4	
	mean		92.3	4.324	157.2	
	SD		7.9	1.048	12.6	
	%CV		8.6	24.2	8.0	
Imidazole - Lab 2 (5)	1	100%	106.7	2.583	145.4	
	2		82.7	3.371	133.3	Severe
	3		74.7	3.969	134.2	
	mean		88.0	3.308	137.6	
	SD		16.7	0.695	6.7	
	%CV		18.9	21.0	4.9	
Imidazole - Lab 3 (1)	1	100%	73.0	3.756	129.3	
	2		76.0	2.956	120.3	Severe
	3		100.0	4.611	169.2	
	mean		83.0	3.774	139.6	
	SD		14.8	0.828	26.0	
	%CV		17.8	21.9	18.6	
Imidazole - Lab 3 (2)	1	100%	89.0	2.625	128.4	
	2		84.0	3.070	130.1	Severe
	3		102.0	4.000	162.0	
	mean		91.7	3.232	140.2	
	SD		9.3	0.702	18.9	
	%CV		10.1	21.7	13.5	

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Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	In Vitro Score ¹	Prediction
Imidazole - Lab 3 (3)	1	100%	77.7	3.604	131.8	Severe
	2		83.7	2.339	118.8	
	3		79.7	2.779	121.4	
	mean		80.4	2.907	124.0	
	SD		3.1	0.642	6.9	
	%CV		3.8	22.1	5.5	
Imidazole - Lab 3 (4)	1	100%	80.0	3.721	135.8	Severe
	2		84.0	3.106	130.6	
	3		83.0	2.451	119.8	
	mean		82.3	3.093	128.7	
	SD		2.1	0.635	8.2	
	%CV		2.5	20.5	6.3	
Imidazole - Lab 3 (5)	1	100%	68.3	2.741	109.4	Severe
	2		77.3	2.976	121.9	
	3		84.3	3.636	138.8	
	mean		76.6	3.118	123.4	
	SD		8.0	0.464	14.8	
	%CV		10.5	14.9	12.0	
NaOH - Lab 1 (1)	1	10%	190.7	5.354	271.0	Severe
	2		140.7	4.895	214.1	
	3		198.7	3.404	249.8	
	mean		176.7	4.551	245.0	
	SD		31.4	1.019	28.8	
	%CV		17.8	22.4	11.7	
NaOH - Lab 1 (2)	1	10%	171.0	3.483	223.2	Severe
	2		174.0	3.660	228.9	
	3		171.0	3.885	229.3	
	mean		172.0	3.676	227.1	
	SD		1.7	0.201	3.4	
	%CV		1.0	5.5	1.5	
NaOH - Lab 2 (1)	1	10%	189.0	4.228	252.4	Severe
	2		173.0	4.650	242.8	
	3		148.0	5.386	228.8	
	mean		170.0	4.755	241.3	
	SD		20.7	0.586	11.9	
	%CV		12.2	12.3	4.9	
NaOH - Lab 2 (2)	1	10%	180.0	4.122	241.8	Severe
	2		155.0	4.836	227.5	
	3		165.0	4.812	237.2	
	mean		166.7	4.590	235.5	
	SD		12.6	0.405	7.3	
	%CV		7.5	8.8	3.1	
NaOH - Lab 3 (1)	1	10%	139.0	5.039	214.6	Severe
	2		121.0	4.339	186.1	
	3		112.0	4.434	178.5	
	mean		124.0	4.604	193.1	
	SD		13.7	0.380	19.0	
	%CV		11.1	8.2	9.9	
NaOH - Lab 3 (2)	1	10%	149.3	3.535	202.3	Severe
	2		189.3	2.855	232.1	
	3		157.3	3.520	210.1	
	mean		165.3	3.303	214.8	
	SD		21.2	0.388	15.5	
	%CV		12.8	11.8	7.2	
Sodium oxalate - Lab 1 (1)	1	100%	-2.0	0.112	-0.3	Mild
	2		-2.0	0.020	-1.7	
	3		1.0	0.017	1.3	
	mean		-1.0	0.050	-0.2	
	SD		1.7	0.054	1.5	
	%CV		-173.2	108.7	-643.3	
Sodium oxalate - Lab 1 (2)	1	100%	-0.3	0.067	0.7	Mild
	2		-3.3	0.055	-2.5	
	3		0.7	0.044	1.4	
	mean		-1.0	0.055	-0.1	
	SD		2.1	0.012	2.1	
	%CV		-215.3	20.8	-1559.4	

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Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Sodium oxalate - Lab 2 (1)	1	100%	7.7	0.127	9.6	Mild
	2		7.7	0.112	9.4	
	3		9.7	0.144	11.9	
	mean		8.4	0.128	10.3	
	SD		1.2	0.016	1.4	
	%CV		13.8	12.5	13.5	
Sodium oxalate - Lab 2 (2)	1	100%	3.7	0.069	4.7	Mild
	2		2.7	0.044	3.4	
	3		3.7	0.099	5.2	
	mean		3.4	0.071	4.4	
	SD		0.6	0.028	0.9	
	%CV		17.1	39.0	21.0	
Sodium oxalate - Lab 3 (1)	1	100%	1.3	0.032	1.8	Mild
	2		2.3	0.088	3.6	
	3		2.3	0.032	2.8	
	mean		2.0	0.051	2.7	
	SD		0.6	0.032	0.9	
	%CV		29.4	63.8	33.0	
Sodium oxalate - Lab 3 (2)	1	100%	3.3	0.174	5.9	Mild
	2		2.3	0.145	4.5	
	3		1.3	0.130	3.3	
	mean		2.3	0.150	4.6	
	SD		1.0	0.022	1.3	
	%CV		43.5	14.9	28.5	
Parafluoroaniline - Lab 1 (1)	1	100%	15.0	1.777	41.7	Moderate
	2		14.0	1.965	43.5	
	3		11.0	1.248	29.7	
	mean		13.3	1.663	38.3	
	SD		2.1	0.372	7.5	
	%CV		15.6	22.4	19.6	
Parafluoroaniline - Lab 1 (2)	1	100%	13.3	0.908	26.9	Moderate
	2		21.3	1.970	50.9	
	3		13.3	1.419	34.6	
	mean		16.0	1.432	37.5	
	SD		4.6	0.531	12.3	
	%CV		28.9	37.081	32.7	
Parafluoroaniline - Lab 2 (1)	1	100%	14.3	0.930	28.3	Moderate
	2		16.3	1.521	39.1	
	3		15.3	0.681	25.5	
	mean		15.3	1.044	31.0	
	SD		1.0	0.431	7.2	
	%CV		6.5	41.3	23.2	
Parafluoroaniline - Lab 2 (2)	1	100%	14.3	0.922	28.1	Moderate
	2		20.3	1.332	40.3	
	3		14.3	1.476	36.4	
	mean		16.3	1.243	34.9	
	SD		3.5	0.287	6.2	
	%CV		21.3	23.1	17.8	
Parafluoroaniline - Lab 3 (1)	1	100%	11.0	0.913	24.7	Mild
	2		10.0	0.626	19.4	
	3		12.0	0.674	22.1	
	mean		11.0	0.738	22.1	
	SD		1.0	0.154	2.7	
	%CV		9.1	20.8	12.0	
Parafluoroaniline - Lab 3 (2)	1	100%	14.7	0.665	24.7	Moderate
	2		14.7	0.573	23.3	
	3		16.7	0.868	29.7	
	mean		15.4	0.702	25.9	
	SD		1.2	0.151	3.4	
	%CV		7.5	21.5	13.0	
Sodium lauryl sulfate - Lab 1 (1)	1	15%	0.7	0.596	9.6	Mild
	2		-0.3	0.933	13.7	
	3		1.7	1.507	24.3	
	mean		0.7	1.012	15.9	
	SD		1.0	0.461	7.6	
	%CV		142.9	45.5	47.8	

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Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Sodium lauryl sulfate - Lab 1 (2)	1	15%	0.7	0.998	15.7	Mild
	2		1.7	1.163	19.1	
	3		0.7	1.096	17.1	
	mean		1.0	1.086	17.3	
	SD		0.6	0.083	1.7	
	%CV		55.9	7.6	9.9	
Sodium lauryl sulfate - Lab 2 (1)	1	15%	-0.7	0.391	5.2	Mild
	2		-0.7	0.436	5.8	
	3		-0.7	0.398	5.3	
	mean		-0.7	0.408	5.4	
	SD		0.0	0.024	0.3	
	%CV		0.0	5.9	5.9	
Sodium lauryl sulfate - Lab 2 (2)	1	15%	0.3	0.157	2.7	Mild
	2		-0.7	0.367	4.8	
	3		0.3	0.519	8.1	
	mean		0.0	0.348	5.2	
	SD		0.6	0.182	2.7	
	%CV		-1732.1	52.3	52.3	
Sodium lauryl sulfate - Lab 3 (1)	1	15%	1.0	0.567	9.5	Mild
	2		0.0	0.594	8.9	
	3		1.0	0.392	6.9	
	mean		0.7	0.518	8.4	
	SD		0.6	0.110	1.4	
	%CV		86.6	21.2	16.1	
Sodium lauryl sulfate - Lab 3 (2)	1	15%	2.0	0.354	7.3	Mild
	2		1.0	0.230	4.5	
	3		1.0	0.266	5.0	
	mean		1.3	0.283	5.6	
	SD		0.6	0.064	1.5	
	%CV		43.3	22.5	26.7	
Butyl cellulosolve - Lab 1 (1)	1	100%	31.3	5.071	107.4	
	2		29.3	3.548	82.5	
	3		28.3	4.020	88.6	
	mean		29.6	4.213	92.8	
	SD		1.5	0.780	13.0	
	%CV		5.2	18.5	14.0	
Butyl cellulosolve - Lab 1 (2)	1	100%	30.0	5.013	105.2	Severe
	2		30.0	5.036	105.5	
	3		34.0	3.528	86.9	
	mean		31.3	4.526	99.2	
	SD		2.3	0.864	10.7	
	%CV		7.4	19.1	10.7	
Butyl cellulosolve - Lab 2 (1)	1	100%	41.3	5.148	118.5	Severe
	2		45.3	4.490	112.7	
	3		30.3	4.236	93.8	
	mean		39.0	4.625	108.3	
	SD		7.8	0.471	12.9	
	%CV		19.9	10.2	11.9	
Butyl cellulosolve - Lab 2 (2)	1	100%	38.3	4.829	110.7	
	2		45.3	4.106	106.9	
	3		45.3	4.832	117.8	
	mean		43.0	4.589	111.8	
	SD		4.0	0.418	5.5	
	%CV		9.4	9.1	4.9	
Butyl cellulosolve - Lab 3 (1)	1	100%	36.7	3.490	89.1	Severe
	2		37.7	4.865	110.7	
	3		38.7	3.085	85.0	
	mean		37.7	3.813	94.9	
	SD		1.0	0.933	13.8	
	%CV		2.7	24.5	14.5	
Butyl cellulosolve - Lab 3 (2)	1	100%	30.7	3.474	82.8	Severe
	2		40.7	3.204	88.8	
	3		41.7	5.414	122.9	
	mean		37.7	4.031	98.2	
	SD		6.1	1.206	21.6	
	%CV		16.1	29.9	22.0	

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Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
4-Carboxybenzaldehyde - Lab 1 (1)	1	100%	50.0	0.036	50.5	Moderate
	2		44.0	0.040	44.6	
	3		45.0	0.074	46.1	
	mean		46.3	0.050	47.1	
	SD		3.2	0.021	3.1	
	%CV		6.9	41.8	6.5	
4-Carboxybenzaldehyde - Lab 1 (2)	1	100%	44.7	0.044	45.4	Moderate
	2		49.7	0.057	50.6	
	3		44.7	0.072	45.8	
	mean		46.4	0.058	47.3	
	SD		2.9	0.014	2.9	
	%CV		6.2	24.3	6.1	
4-Carboxybenzaldehyde - Lab 2 (1)	1	100%	57.7	0.022	58.0	Moderate
	2		54.7	-0.001	54.7	
	3		48.7	0.016	48.9	
	mean		53.7	0.012	53.9	
	SD		4.6	0.012	4.6	
	%CV		8.5	96.7	8.6	
4-Carboxybenzaldehyde - Lab 2 (2)	1	100%	49.7	0.000	49.7	Moderate
	2		49.7	0.001	49.7	
	3		43.7	0.004	43.8	
	mean		47.7	0.002	47.7	
	SD		3.5	0.002	3.4	
	%CV		7.3	124.9	7.1	
4-Carboxybenzaldehyde - Lab 3 (1)	1	100%	37.3	0.031	37.8	Moderate
	2		42.3	0.003	42.3	
	3		46.3	0.005	46.4	
	mean		42.0	0.013	42.2	
	SD		4.5	0.016	4.3	
	%CV		10.7	120.2	10.2	
4-Carboxybenzaldehyde - Lab 3 (2)	1	100%	45.3	0.030	45.8	Moderate
	2		37.3	0.041	37.9	
	3		41.3	0.035	41.8	
	mean		41.3	0.035	41.8	
	SD		4.0	0.006	4.0	
	%CV		9.7	15.6	9.4	
Methyl ethyl ketone - Lab 1 (1)	1	100%	64.3	2.734	105.3	Severe
	2		59.3	2.640	98.9	
	3		59.3	4.174	121.9	
	mean		61.0	3.183	108.7	
	SD		2.9	0.860	11.9	
	%CV		4.7	27.0	10.9	
Methyl ethyl ketone - Lab 1 (2)	1	100%	54.3	1.909	82.9	Severe
	2		65.3	2.155	97.6	
	3		66.3	3.880	124.5	
	mean		62.0	2.648	101.7	
	SD		6.7	1.074	21.1	
	%CV		10.7	40.6	20.8	
Methyl ethyl ketone - Lab 2 (1)	1	100%	45.3	1.658	70.2	Severe
	2		54.3	2.408	90.4	
	3		43.3	1.052	59.1	
	mean		47.6	1.706	73.2	
	SD		5.9	0.679	15.9	
	%CV		12.3	39.8	21.7	
Methyl ethyl ketone - Lab 2 (2)	1	100%	46.3	0.989	61.1	Severe
	2		50.3	1.386	71.1	
	3		47.3	1.584	71.1	
	mean		48.0	1.320	67.8	
	SD		2.1	0.303	5.8	
	%CV		4.3	23.0	8.5	
Methyl ethyl ketone - Lab 3 (1)	1	100%	55.0	1.277	74.2	Severe
	2		51.0	1.218	69.3	
	3		61.0	0.420	67.3	
	mean		55.7	0.972	70.3	
	SD		5.0	0.479	3.6	
	%CV		9.0	49.3	5.1	

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Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Methyl ethyl ketone - Lab 3 (2)	1	100%	55.7	1.227	74.1	Severe
	2		52.7	0.947	66.9	
	3		54.7	1.660	79.6	
	mean		54.4	1.278	73.5	
	SD		1.5	0.359	6.4	
	%CV		2.8	28.1	8.7	
TritonX100 - Lab 1 (1)	1	5%	1.7	0.388	7.5	Mild
	2		0.7	0.158	3.1	
	3		1.7	0.347	6.9	
	mean		1.4	0.298	5.8	
	SD		0.6	0.123	2.4	
	%CV		42.2	41.2	40.9	
TritonX100 - Lab 1 (2)	1	5%	0.7	0.162	3.1	Mild
	2		-0.3	0.191	2.6	
	3		-0.3	0.324	4.6	
	mean		0.0	0.226	3.4	
	SD		0.6	0.086	1.0	
	%CV		1732.1	38.3	30.3	
TritonX100 - Lab 2 (1)	1	5%	3.3	0.025	3.7	Mild
	2		4.3	0.026	4.7	
	3		2.3	0.019	2.6	
	mean		3.3	0.023	3.7	
	SD		1.0	0.004	1.1	
	%CV		30.3	16.2	28.6	
TritonX100 - Lab 2 (2)	1	5%	0.3	0.040	0.9	Mild
	2		2.3	0.036	2.8	
	3		1.3	0.029	1.7	
	mean		1.3	0.035	1.8	
	SD		1.0	0.006	1.0	
	%CV		76.9	15.9	53.0	
TritonX100 - Lab 3 (1)	1	5%	3.7	0.033	4.2	Mild
	2		1.7	0.015	1.9	
	3		2.7	0.021	3.0	
	mean		2.7	0.023	3.0	
	SD		1.0	0.009	1.2	
	%CV		37.0	39.8	37.9	
TritonX100 - Lab 3 (2)	1	5%	0.7	0.035	1.2	Mild
	2		1.7	0.052	2.5	
	3		2.7	0.027	2.1	
	mean		1.7	0.038	1.9	
	SD		1.0	0.013	0.7	
	%CV		58.8	33.6	34.4	
Propyl-4-hydroxybenzoate - Lab 1 (1)	1	100%	4.0	0.006	4.1	Mild
	2		4.0	0.007	4.1	
	3		7.0	0.027	7.4	
	mean		5.0	0.013	5.2	
	SD		1.7	0.012	1.9	
	%CV		34.6	88.8	36.6	
Propyl-4-hydroxybenzoate - Lab 1 (2)	1	100%	4.7	0.006	4.8	Mild
	2		3.7	0.034	4.2	
	3		1.7	0.009	1.8	
	mean		3.4	0.016	3.6	
	SD		1.5	0.015	1.6	
	%CV		45.4	94.1	44.1	
Propyl-4-hydroxybenzoate - Lab 2 (1)	1	100%	7.7	0.001	7.7	Mild
	2		11.7	0.018	12.0	
	3		12.7	0.084	14.0	
	mean		10.7	0.034	11.2	
	SD		2.6	0.044	3.2	
	%CV		24.7	127.7	28.7	
Propyl-4-hydroxybenzoate - Lab 2 (2)	1	100%	7.7	0.016	7.9	Mild
	2		6.7	0.051	7.5	
	3		6.7	0.001	6.7	

**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
	mean		7.0	0.023	7.4	
	SD		0.6	0.026	0.6	
	%CV		8.2	113.2	8.3	
Propyl-4-hydroxybenzoate - Lab 3 (1)	1	100%	5.3	0.034	5.8	
	2		4.3	0.037	4.9	Mild
	3		12.3	0.012	12.5	
	mean		7.3	0.028	7.7	
	SD		4.4	0.014	4.2	
	%CV		59.7	49.3	53.7	
Propyl-4-hydroxybenzoate - Lab 3 (2)	1	100%	5.3	0.099	6.8	
	2		5.3	0.008	5.4	Mild
	3		6.3	0.014	6.5	
	mean		5.6	0.040	6.2	
	SD		0.6	0.051	0.7	
	%CV		10.2	126.2	11.8	
Tween20 - Lab 1 (1)	1	100%	0.7	0.001	0.7	
	2		-0.3	-0.001	-0.3	Mild
	3		0.7	0.003	0.7	
	mean		0.4	0.001	0.4	
	SD		0.6	0.002	0.6	
	%CV		157.5	200.0	157.5	
Tween20 - Lab 1 (2)	1	100%	0.7	0.003	0.7	
	2		-0.3	0.010	-0.2	Mild
	3		0.7	-0.005	0.6	
	mean		0.4	0.003	0.4	
	SD		0.6	0.008	0.5	
	%CV		157.5	281.5	134.5	
Tween20 - Lab 2 (1)	1	100%	0.3	0.016	0.5	
	2		0.3	-0.005	0.2	Mild
	3		0.3	-0.003	0.3	
	mean		0.3	0.003	0.3	
	SD		0.0	0.012	0.2	
	%CV		0.0	434.6	45.8	
Tween20 - Lab 2 (2)	1	100%	1.3	0.000	1.3	
	2		0.0	0.000	0.0	Mild
	3		0.3	0.015	0.5	
	mean		0.5	0.005	0.6	
	SD		0.7	0.009	0.7	
	%CV		127.6	173.2	109.3	
Tween20 - Lab 3 (1)	1	100%	0.0	0.042	0.6	
	2		0.0	0.007	0.1	Mild
	3		0.0	0.017	0.3	
	mean		0.0	0.022	0.3	
	SD		0.0	0.018	0.3	
	%CV		0.0	81.9	75.5	
Tween20 - Lab 3 (2)	1	100%	0.0	0.000	0.0	
	2		0.0	0.000	0.0	Mild
	3		1.0	0.026	1.4	
	mean		0.3	0.009	0.5	
	SD		0.6	0.015	0.8	
	%CV		173.2	173.2	173.2	
Glycerol - Lab 1 (1)	1	100%	0.3	0.019	0.6	
	2		0.3	0.006	0.4	Mild
	3		1.3	0.010	1.5	
	mean		0.6	0.012	0.8	
	SD		0.6	0.007	0.6	
	%CV		91.2	57.1	70.3	
Glycerol - Lab 1 (2)	1	100%	1.0	0.015	1.2	
	2		1.0	0.011	1.2	Mild
	3		0.0	-0.002	1.0	
	mean		0.7	0.008	1.1	
	SD		0.6	0.009	0.1	
	%CV		86.6	111.1	10.2	

**Intralaboratory CV Analysis of BCOP -
Southee 1998**

Substance - Lab No. (Experiment No.)	Cornea number	Concentration	Opacity	Permeability	<i>In Vitro</i> Score ¹	Prediction
Glycerol - Lab 2 (1)	1	100%	0.0	0.000	0.0	Mild
	2		1.3	0.000	1.2	
	3		0.3	0.000	0.3	
	mean		0.5	0.000	0.5	
	SD		0.7	0.000	0.6	
	%CV		127.6	0.0	124.9	
Glycerol - Lab 2 (2)	1	100%	1.3	-0.006	1.2	Mild
	2		0.3	-0.004	0.2	
	3		0.3	-0.006	0.2	
	mean		0.6	-0.005	0.5	
	SD		0.6	0.001	0.6	
	%CV		91.2	-21.7	108.3	
Glycerol - Lab 3 (1)	1	100%	0.7	-0.007	0.6	Mild
	2		0.7	0.002	0.7	
	3		1.7	-0.004	1.6	
	mean		1.0	-0.003	1.0	
	SD		0.6	0.005	0.6	
	%CV		55.9	-152.8	57.0	
Glycerol - Lab 3 (2)	1	100%	0.7	-0.001	0.7	Mild
	2		0.7	0.002	0.7	
	3		0.7	0.020	1.0	
	mean		0.7	0.007	0.8	
	SD		0.0	0.011	0.2	
	%CV		0.0	162.3	21.7	
Abbreviations: CV = Coefficient of variation; SD =Standard deviation.						
¹ <i>In Vitro</i> Score = Opacity + (15 x permeability value)						

Appendix E2

BCOP Data from Dr. Joseph Sina

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**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
Dimethyl ethylimidazo pyridine	1	10%/32	11	0.044	11.66	
	2		-3	0.063	-2.06	
	3		5	0.068	6.02	
	4		-3	0.055	-2.18	
	mean		3	0.058	3.36	Mild
	SD		7	0.010	6.73	
	%CV		272	18.2	200.2	
Sodium bitartrate	1	20%/RT	16	0.002	16.03	
	2		8	0.008	8.12	
	3		6	0.020	6.30	
	4		17	0.000	17.00	
	mean		12	0.008	11.86	Mild
	SD		6	0.009	5.44	
	%CV		47	120.0	45.8	
Quinaldine (2-methylquinoline)	1	100%/32	17	0.211	20.17	
	2		23	0.250	26.75	
	3		22	0.507	29.61	
	mean		21	0.323	25.51	Moderate
	SD		3	0.161	4.84	
	%CV		16	49.8	19.0	
	N-Acetyl- <i>p</i> -anisidine	1	20%/RT	7	0.014	7.21
2			11	0.013	11.20	
3			-3	0.005	-2.93	
4			-2	0.000	-2.00	
mean			3	0.008	3.37	Mild
SD			7	0.007	6.94	
%CV			211	83.5	205.9	
1,3-Benzenedicarboxaldehyde	1	20%/32	11	0.019	11.29	
	2		1	0.006	1.09	
	3		10	0.091	11.37	
	4		9	0.051	9.77	
	mean		8	0.042	8.38	Mild
	SD		5	0.038	4.91	
	%CV		59	90.8	58.7	
	1	20%/RT	8	0.018	8.27	
	2		13	0.058	13.87	
	3		3	0.008	3.12	
	4		8	0.035	8.53	
	mean		8	0.030	8.45	Mild
	SD		4	0.022	4.39	
	%CV		51	73.6	52.0	
1	20%/32	24	0.217	27.26		
2		31	0.037	31.56		
3		23	0.255	26.83		
4		31	0.162	33.43		
mean		27	0.168	29.77	Moderate	
SD		4	0.095	3.24		
%CV		16	56.7	10.9		
Triethylammonium iodide	1	20%/RT	21	0.089	22.34	
	2		27	0.042	27.63	
	3		26	0.049	26.74	
	4		18	0.076	19.14	
	mean		23	0.064	23.96	Mild
	SD		4	0.022	3.96	
	%CV		18	34.7	16.5	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
Dicyclohexylcarbodiimide	1	20%/RT	23	0.010	23.15	
	2		22	0.032	22.48	
	3		16	0.037	16.56	
	4		18	0.034	18.51	
	mean		20	0.028	20.17	Mild
	SD		3	0.012	3.16	
	%CV		17	43.7	15.7	
L-Proline, N-carboxyanhydride	1	20%/RT	8	0.007	8.11	
	2		12	0.008	12.12	
	3		-5	0.009	-4.87	
	4		5	0.014	5.21	
	mean		5	0.010	5.14	Mild
	SD		7	0.003	7.25	
	%CV		145	32.7	141.0	
Substituted propanediol	1	20%/RT	50	1.538	73.07	
	2		52	1.552	75.28	
	3		48	2.428	84.42	
	4		46	1.625	70.38	
	mean		49	1.786	75.79	Severe
	SD		3	0.430	6.10	
	%CV		5	24.1	8.0	
3-Trichlorovinylaniline HCL	1	20%/32	398	0.001	398.02	
	2		404	0.001	404.02	
	3		406	0.000	406.00	
	4		408	0.002	408.03	
	mean		404	0.001	404.02	Severe
	SD		4	0.001	4.32	
	%CV		1	81.6	1.1	
Methyl chlorobenzyl butylthio propyl indolyl dimethylpropanoate	1	20%/RT	15	0.005	15.08	
	2		18	0.002	18.03	
	3		8	0.002	8.03	
	4		5	0.001	5.02	
	mean		12	0.003	11.54	Mild
	SD		6	0.002	6.04	
	%CV		52	69.3	52.4	
Nitropyridinone	1	20%/RT	11	0.043	11.65	
	2		12	0.035	12.53	
	3		5	0.025	5.38	
	4		6	0.002	6.03	
	mean		9	0.026	8.89	Mild
	SD		4	0.018	3.71	
	%CV		41	67.7	41.7	
	1	20%/32	-5	0.036	-4.46	
	2		2	0.027	2.41	
	3		-9	0.023	-8.66	
	4		-4	0.003	-3.96	
	mean		-4	0.022	-3.67	Mild
	SD		5	0.014	4.56	
	%CV		-114	62.6	-124.5	
alpha-Naphthyl-pyranone	1	20%/RT	1	0.026	1.39	
	2		12	0.020	12.30	
	3		-1	0.013	-0.81	
	4		11	0.018	11.27	
	mean		6	0.019	6.04	Mild
	SD		7	0.005	6.71	
	%CV		117	27.9	111.1	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
Cyclic peptide	1	20%/32	5	0.087	6.31	
	2		2	0.086	3.29	
	3		-5	0.057	-4.15	
	4		5	0.025	5.38	
	mean		2	0.064	2.71	Mild
	SD		5	0.029	4.74	
	%CV		270	46.0	175.1	
Chloroquinoliny methyl ester carboxylic acid	1	20%/RT	38	0.246	41.69	
	2		39	0.325	43.88	
	3		50	0.378	55.67	
	4		25	0.409	31.14	
	mean		38	0.340	43.09	Moderate
	SD		10	0.071	10.06	
	%CV		27	21.0	23.4	
7-Chloroquinaldine	1	20%/RT	4	0.002	4.03	
	2		8	0.000	8.00	
	3		3	0.000	3.00	
	4		6	0.000	6.00	
	mean		5	0.001	5.26	Mild
	SD		2	0.001	2.21	
	%CV		42	200.0	42.1	
	1	20%/32	7	0.044	7.66	
	2		14	0.029	14.44	
	3		8	0.057	8.86	
	4		11	0.043	11.65	
	mean		10	0.043	10.65	Mild
	SD		3	0.011	3.03	
	%CV		32	26.5	28.4	
alpha-Pyranone, 7,7-dioxide	1	20%/RT	0	0.045	0.68	
	2		0	0.072	1.08	
	3		6	0.136	8.04	
	4		2	0.090	3.35	
	mean		2	0.086	3.29	Mild
	SD		3	0.038	3.38	
	%CV		141	44.6	102.9	
Methyl boronic acid	1	20%/RT	10	0.144	12.16	
	2		21	0.143	23.15	
	3		28	0.164	30.46	
	4		19	0.114	20.71	
	mean		20	0.141	21.62	Mild
	SD		7	0.021	7.55	
	%CV		38	14.6	34.9	
	1	20%/32	20	0.305	24.58	
	2		14	0.164	16.46	
	3		21	0.383	26.75	
	4		28	0.303	32.55	
	mean		21	0.289	25.08	Moderate
	SD		6	0.091	6.66	
	%CV		28	31.6	26.6	
1,1-Diphenyl prolinol (sulfate salt)	1	20%/RT	11	1.730	36.95	
	2		17	0.790	28.85	
	3		7	1.144	24.16	
	4		10	2.405	46.08	
	mean		11	1.517	34.01	Severe
	SD		4	0.707	9.62	
	%CV		37	46.6	28.3	
4-(2-Quinolylmethoxy)aniline	1	20%/32	23	0.000	23.00	
	2		-3	0.000	-3.00	
	3		-6	0.001	-5.99	
	4		-3	0.019	-2.72	
	mean		3	0.005	2.83	Mild
	SD		14	0.009	13.53	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
	%CV		494	186.9	479.0	
Sulfone amine	1	20%/RT	11	0.018	11.27	
	2		14	0.008	14.12	
	3		8	0.015	8.23	
	4		24	0.004	24.06	
	mean		14	0.011	14.42	Mild
	SD		7	0.006	6.86	
	%CV		49	56.9	47.6	
<i>p</i> -Nitrobenzyl 2-diazo acetoacetate	1	20%/RT	0	0.028	0.42	
	2		15	0.012	15.18	
	3		24	0.016	24.24	
	4		19	0.039	19.59	
	mean		15	0.024	14.86	Mild
	SD		10	0.012	10.31	
	%CV		71	51.5	69.4	
alpha-Pyranol, 7,7-dioxide	1	20%/RT	12	0.035	12.53	
	2		11	0.033	11.50	
	3		7	0.025	7.38	
	4		-1	0.014	-0.79	
	mean		7	0.027	7.65	Mild
	SD		6	0.010	6.05	
	%CV		82	35.6	79.1	
	1	20%/32	20	0.156	22.34	
	2		29	0.228	32.42	
	3		38	0.115	39.73	
	mean		29	0.166	31.50	Mild
	SD		9	0.057	8.73	
	%CV		31	34.4	27.7	
	Triethylamine hydroiodide	1	20%/RT	29	0.021	29.32
2			32	0.059	32.89	
3			33	0.064	33.96	
4			29	0.038	29.57	
mean			31	0.046	31.43	Moderate
SD			2	0.020	2.34	
%CV			7	43.6	7.4	
Substituted cephalosporanic acid	1	20%/RT	11	0.006	11.09	
	2		17	0.056	17.84	
	3		10	0.017	10.26	
	4		12	0.001	12.02	
	mean		13	0.020	12.80	Mild
	SD		3	0.025	3.44	
	%CV		25	124.6	26.8	
	1	20%/32	-3	0.006	-2.91	
	2		-6	0.000	-6.00	
	3		-6	0.010	-5.85	
	4		-3	0.012	-2.82	
	mean		-5	0.007	-4.40	Mild
	SD		2	0.005	1.77	
	%CV		-38	75.6	-40.2	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
4-Benzoxycarbonicamino-2-hydroxy-butanoic acid	1	20%/RT	392	0.001	392.02	
	2		395	0.006	395.09	
	3		397	0.008	397.12	
	4		399	0.000	399.00	
	mean		396	0.004	395.81	Severe
	SD		3	0.004	2.99	
	%CV		1	103.0	0.8	
N-Sulfonamido hydroxyacetophenone	1	20%/RT	4	0.006	4.09	
	2		3	0.040	3.60	
	3		12	0.026	12.39	
	4		-10	0.002	-9.97	
	mean		2	0.019	2.53	Mild
	SD		9	0.018	9.26	
	%CV		405	96.0	366.2	
	1	20%/32	-8	0.021	-7.69	
	2		-12	0.012	-11.82	
	3		-8	0.015	-7.78	
	4		4	0.001	4.02	
	mean		-6	0.012	-5.82	Mild
	SD		7	0.008	6.83	
	%CV		-115	68.4	-117.5	
Cyclic peptide	1	20%/32	7	0.011	7.17	
	2		4	0.007	4.11	
	3		10	0.013	10.20	
	4		10	0.017	10.26	
	mean		8	0.012	7.93	Mild
	SD		3	0.004	2.93	
	%CV		37	34.7	36.9	
4-Bromo-2,5-dimethylphenol	1	20%/32	54	4.006	114.09	
	2		54	4.708	124.62	
	3		61	5.000	136.00	
	4		76	4.914	149.71	
	mean		61	4.657	131.11	Severe
	SD		10	0.451	15.29	
	%CV		17	9.7	11.7	
2-Amino-3,6-dimethylphenol, hydrobromide salt	1	20%/32	162	0.252	165.78	
	2		141	0.228	144.42	
	3		138	0.294	142.41	
	4		145	0.272	149.08	
	mean		147	0.262	150.42	Severe
	SD		11	0.028	10.61	
	%CV		7	10.8	7.1	
Mixture of 2-chloromethyl-4,7-dimethylbenzoxazole and 2-bromomethyl dimethylbenzoxazole	1	20%/32	14	0.001	14.02	
	2		17	0.000	17.00	
	3		19	0.000	19.00	
	4		22	0.016	22.24	
	mean		18	0.004	18.06	Mild
	SD		3	0.008	3.46	
	%CV		19	184.6	19.1	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
R-Hydroxy ester of benzoic acid compound	1	20%/32	-14	0.050	-13.25	
	2		-10	0.009	-9.87	
	3		-12	0.020	-11.70	
	4		-14	0.022	-13.67	
	mean		-13	0.025	-12.12	Mild
	SD		2	0.017	1.73	
	%CV		-15	69.2	-14.2	
<i>t</i> -Butyl-3-oxo-6-methoxyhexanoate	1	100%/32	7	0.008	7.12	
	2		17	0.000	17.00	
	3		19	0.191	21.87	
	mean		14	0.066	15.33	Mild
	SD		6	0.108	7.51	
	%CV		45	162.9	49.0	
	Methyl 3-oxo-6-methoxyhexanoate	1	100%/32	44	1.795	70.93
2			38	1.935	67.03	
3			34	0.824	46.36	
4			34	0.863	46.95	
mean			38	1.354	57.81	Severe
SD			5	0.593	12.99	
%CV			13	43.8	22.5	
+-Butyl-3R-hydroxy-6-methoxyhepanoate	1	100%/32	12	1.165	29.48	
	2		8	1.160	25.40	
	3		3	0.734	14.01	
	4		13	0.615	22.23	
	mean		9	0.919	22.78	Mild
	SD		5	0.286	6.56	
	%CV		51	31.1	28.8	
Aglycone; natural product	1	20%/32	14	0.005	14.08	
	2		3	0.016	3.24	
	3		11	0.000	11.00	
	4		17	0.005	17.08	
	mean		11	0.007	11.35	Mild
	SD		6	0.007	5.95	
	%CV		54	104.0	52.4	
Carbic anhydride	1	20%/32	192	0.000	192.00	
	2		185	0.000	185.00	
	3		209	0.000	209.00	
	4		221	0.000	221.00	
	mean		202	0.000	201.75	Severe
	SD		16	0.000	16.32	
	%CV		8	0.0	8.1	
3-Bromo-7-methyl-9-flurenone	1	20%/32	-2	0.019	-1.72	
	2		2	0.011	2.17	
	3		-6	0.009	-5.87	
	4		-5	0.007	-4.90	
	mean		-3	0.012	-2.58	Mild
	SD		4	0.005	3.62	
	%CV		-131	45.7	-140.6	
<i>tert</i> -Butyl-6-methoxy-3-S-(2-thiophenethio) hexanoate	1	100%/32	5	0.000	5.00	
	2		-3	0.000	-3.00	
	3		2	0.000	2.00	
	4		2	0.000	2.00	
	mean		2	0.000	1.50	Mild
	SD		3	0.000	3.32	
	%CV		221	0.0	221.1	
Cyanopyridinone	1	20%/32	-5	0.016	-4.76	
	2		-8	0.018	-7.73	
	3		-1	0.007	-0.90	
	4		-4	0.003	-3.96	
	mean		-5	0.011	-4.34	Mild
	SD		3	0.007	2.81	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Joseph Sina**

Substance	Cornea number	Concentration/ Incubation temp.	Opacity	Permeability	<i>In vitro</i> score ¹	Prediction
	%CV		-64	65.1	-64.8	
S-Hydroxy ester of benzoic acid compound	1	20%/32	12	0.021	12.32	
	2		18	0.000	18.00	
	3		20	0.000	20.00	
	4		33	0.000	33.00	
	mean		21	0.005	20.83	Mild
	SD		9	0.011	8.74	
	%CV		43	200.0	42.0	
Cyano methylpyridine	1	20%/32	8	0.037	8.56	
	2		17	0.025	17.38	
	3		21	0.013	21.20	
	4		15	0.000	15.00	
	mean		15	0.019	15.53	Mild
	SD		5	0.016	5.30	
	%CV		36	84.7	34.2	
Carbonitrile	1	20%/32	21	0.180	23.70	
	2		22	0.200	25.00	
	3		20	0.241	23.62	
	4		12	0.187	14.81	
	mean		19	0.202	21.78	
	SD		5	0.027	4.69	
	%CV		24	13.5	21.5	Mild
Abbreviations: CV = Coefficient of variation; RT = Room temperature; SD = Standard deviation.						
¹ <i>In Vitro</i> Score = Opacity + (15 x permeability value)						

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Appendix E3

BCOP Data from Dr. Freddy Van Goethem

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**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
2-Ethoxyethanol	100%	1	61.3	1.444	83	
		2	64	1.498	86.5	
		3	60	1.666	85	
		4	64	1.304	83.6	
		5	61.3	1.534	84.3	
		6	59.7	1.646	84.3	
		mean	61.717	1.515	84.450	Severe
		s.d.	1.886	0.134	1.214	
	%CV	3.1%	8.9%	1.4%		
Cyclohexanone	100%	1	80.8	3.954	140.1	
		2	76.2	5.393	157.1	
		3	70.2	4.373	135.8	
		4	75.5	3.903	134	
		5	80.5	4.081	141.7	
		6	76.5	4.341	141.6	
		mean	76.617	4.341	141.717	Severe
		s.d.	3.878	0.551	8.171	
	%CV	5.1%	12.7%	5.8%		
Gluconolactone	20%	1	88.7	0.171	91.2	
		2	86.7	0.181	89.4	
		3	78	0.143	80.1	
		4	78.7	0.21	81.8	
		5	88	0.1	89.5	
		6	91.3	0.118	93.1	
		mean	85.233	0.154	87.517	Severe
		s.d.	5.543	0.041	5.290	
	%CV	6.5%	26.8%	6.0%		
2,4-Pentanedione	100%	1	44.3	0.075	45.5	
		2	47.3	0.046	48	
		3	50.7	0.133	52.7	
		4	48.3	0.123	50.2	
		5	54.3	0.055	55.2	
		6	49.3	0.074	50.4	
		mean	49.033	0.084	50.333	Moderate
		s.d.	3.363	0.036	3.409	
	%CV	6.9%	42.4%	6.8%		
Promethazine hydrochloride	20%	1	119	0.261	122.9	
		2	134.3	0.564	142.8	
		3	144	0.051	144.8	
		4	140.7	0.539	148.8	
		5	143	0.179	145.7	
		6	128.7	0.128	130.6	
		mean	134.950	0.287	139.267	Severe
		s.d.	9.733	0.216	10.182	
	%CV	7.2%	75.3%	7.3%		
Deoxycholic acid, sodium salt	10%	1	12.2	5.181	89.9	
		2	14.8	5.49	97.2	
		3	11.8	6.097	103.3	
		4	16.8	5.204	94.9	
		5	16.5	6.444	113.2	
		6	10.8	5.895	99.3	
		mean	13.817	5.719	99.633	Severe
		s.d.	2.563	0.511	8.008	
	%CV	18.6%	8.9%	8.0%		
Furan	100%	1	24	1.886	52.3	
		2	22.7	2.274	56.8	
		3	19.7	1.815	46.9	
		4	19.3	1.771	45.9	
		5	21	1.93	49.9	
		6	17	2.143	49.1	
		mean	20.617	1.970	50.150	Moderate
		s.d.	2.513	0.197	3.966	
	%CV	12.2%	10.0%	7.9%		
Benzethonium chloride	10%	1	83.7	6.937	187.7	
		2	87.7	4.716	158.4	
		3	85.7	4.452	152.5	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
		4	83.7	5.911	172.3	
		5	79	4.769	150.5	
		6	88	5.736	174	
		mean	84.633	5.420	165.900	Severe
		s.d.	3.327	0.949	14.524	
		%CV	3.9%	17.5%	8.8%	
Hexadecyltrimethylammonium	10%	1	17.7	3.159	65.1	
		2	18.7	3.957	78	
		3	24.7	2.627	64.1	
		4	13.7	3.438	65.2	
		5	18.7	3.271	67.7	
		6	16.7	4.176	79.3	
		mean	18.367	3.438	69.900	Severe
		s.d.	3.615	0.562	6.893	
		%CV	19.7%	16.3%	9.9%	
Quinacrine	20%	1	52.3	0.024	52.7	
		2	58	0.041	58.6	
		3	64	0.097	65.4	
		4	53.3	0.018	53.6	
		5	51.7	0.085	52.9	
		6	62.7	0.112	64.3	
		mean	57.000	0.063	57.917	Severe
		s.d.	5.410	0.040	5.800	
		%CV	9.5%	63.9%	10.0%	
1-Nitropropane	100%	1	18.5	-0.002	18.5	
		2	14.5	0.002	14.5	
		3	16.8	-0.001	16.8	
		4	18.5	0.045	19.2	
		5	15.5	0.004	15.6	
		6	15.2	0	15.2	
		mean	16.500	0.008	16.633	Mild
		s.d.	1.719	0.018	1.885	
		%CV	10.4%	228.2%	11.3%	
Octanol	100%	1	19.2	2.582	57.9	
		2	32.5	1.946	61.7	
		3	28.2	2.265	62.1	
		4	31.2	2.685	71.4	
		5	30.5	2.091	61.9	
		6	24.8	1.7	50.3	
		mean	27.733	2.212	60.883	Severe
		s.d.	4.981	0.377	6.851	
		%CV	18.0%	17.1%	11.3%	
N-Lauroylsarcosine, sodium salt	10%	1	8.7	3.117	55.4	
		2	8.7	3.764	65.1	
		3	8.3	3.981	68.1	
		4	6.7	4.415	72.9	
		5	6.7	3.227	55.1	
		6	7.7	3.411	58.8	
		mean	7.800	3.653	62.567	Severe
		s.d.	0.927	0.496	7.282	
		%CV	11.9%	13.6%	11.6%	
Allyl alcohol	100%	1	116.7	1.552	139.9	
		2	112.3	1.953	141.6	
		3	90.3	1.856	118.2	
		4	97.7	1.578	121.3	
		5	80	1.945	109.2	
		6	67.3	2.804	109.4	
		mean	94.050	1.948	123.267	Severe
		s.d.	18.902	0.455	14.370	
		%CV	20.1%	23.4%	11.7%	
Butyrolactone	100%	1	35	0.38	40.7	
		2	33.3	0.506	40.9	
		3	31	0.291	35.4	
		4	31.7	0.747	42.9	
		5	39.7	0.721	50.5	
		6	34.7	0.326	39.6	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
		mean	34.233	0.495	41.667	Moderate
		s.d.	3.112	0.199	4.992	
		%CV	9.1%	40.2%	12.0%	
1-Phenyl-3-pyrazolidone	20%	1	11.5	0.156	13.8	
		2	11.5	0.093	12.9	
		3	9.8	0.11	11.5	
		4	11.2	0.114	12.9	
		5	9.8	0.145	12	
		6	12.5	0.237	16.1	
		mean	11.050	0.143	13.200	Mild
		s.d.	1.063	0.052	1.630	
		%CV	9.6%	36.4%	12.3%	
Methanol	100%	1	76.8	1.552	100.1	
		2	64.5	0.917	78.3	
		3	71.2	2.088	102.5	
		4	70.8	1.795	97.8	
		5	78.2	1.333	98.2	
		6	80.8	2.5	118.3	
		mean	73.717	1.698	99.200	Severe
		s.d.	5.993	0.560	12.777	
		%CV	8.1%	33.0%	12.9%	
Thiourea	20%	1	86	4.373	151.6	
		2	71	3.379	121.7	
		3	79	4.357	144.4	
		4	94	4.342	159.1	
		5	91	6.263	184.9	
		6	93.7	3.524	146.5	
		mean	85.783	4.373	151.367	Severe
		s.d.	9.187	1.028	20.672	
		%CV	10.7%	23.5%	13.7%	
Ethanol	100%	1	29.8	1.627	54.2	
		2	21.2	1.907	49.8	
		3	21.5	1.686	46.8	
		4	23.8	1.394	44.7	
		5	19.5	1.011	34.7	
		6	18.2	1.73	44.1	
		mean	22.333	1.559	45.717	Moderate
		s.d.	4.123	0.316	6.555	
		%CV	18.5%	20.3%	14.3%	
Ethyl acetoacetate	100%	1	28.3	0.215	31.6	
		2	25.3	0.043	26	
		3	20.7	0.06	21.6	
		4	23.3	0.307	27.9	
		5	25.3	0.023	25.7	
		6	21	0.049	21.7	
		mean	23.983	0.116	25.750	Moderate
		s.d.	2.907	0.117	3.809	
		%CV	12.1%	100.3%	14.8%	
Pyridine	100%	1	47.5	5.145	124.7	
		2	43.8	3.653	98.6	
		3	40.8	3.044	86.5	
		4	42.2	3.207	90.3	
		5	42.8	4.309	107.5	
		6	49.5	4.733	120.5	
		mean	44.433	4.015	104.683	Severe
		s.d.	3.357	0.849	15.705	
		%CV	7.6%	21.1%	15.0%	
Dimethyl sulfoxide	100%	1	6.7	0.218	9.9	
		2	5.3	0.159	7.7	
		3	8.7	0.196	11.6	
		4	4	0.291	8.4	
		5	5.7	0.23	9.1	
		6	7.7	0.134	9.7	
		mean	6.350	0.205	9.400	Mild
		s.d.	1.704	0.056	1.354	
		%CV	26.8%	27.1%	14.4%	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
2-Methoxyethanol	100%	1	48.7	0.879	61.8	
		2	39.7	0.685	49.9	
		3	52.7	0.751	63.9	
		4	37.7	0.732	48.6	
		5	52.7	1.044	68.3	
		6	39	0.713	49.7	
		mean	45.083	0.801	57.033	Severe
		s.d.	7.066	0.137	8.632	
%CV	15.7%	17.1%	15.1%			
Methylisobutyl ketone	100%	1	11.5	0.504	19.1	
		2	14.5	0.395	20.4	
		3	8.5	0.359	13.9	
		4	7.5	0.94	21.6	
		5	13.5	0.335	18.5	
		6	11.5	0.74	22.6	
		mean	11.167	0.546	19.350	Mild
		s.d.	2.733	0.244	3.073	
%CV	24.5%	44.7%	15.9%			
Dibenzoyl-L-tartaric acid	20%	1	90	0.523	97.9	
		2	81	0.425	87.4	
		3	53.7	0.453	60.5	
		4	63.7	0.485	70.9	
		5	87.7	0.194	90.6	
		6	75.3	0.416	81.6	
		mean	75.233	0.416	81.483	Severe
		s.d.	14.166	0.116	13.711	
%CV	18.8%	27.8%	16.8%			
Imidazole	20%	1	41.7	2.096	73.1	
		2	32.7	1.416	53.9	
		3	27.7	1.412	48.9	
		4	52	1.386	72.8	
		5	36.7	1.68	61.9	
		6	51.3	1.597	75.3	
		mean	40.350	1.598	64.317	Severe
		s.d.	9.893	0.271	11.151	
%CV	24.5%	17.0%	17.3%			
2-Aminophenol	20%	1	9.2	0.093	10.6	
		2	10.8	0.056	11.7	
		3	12.2	0.065	13.1	
		4	10.8	0.039	11.4	
		5	12.8	0.083	14.1	
		6	9.5	0.526	17.4	
		mean	10.883	0.144	13.050	Mild
		s.d.	1.426	0.188	2.473	
%CV	13.1%	131.1%	18.9%			
1,2,4-Trimethylbenzene	100%	1	12.2	0.34	17.3	
		2	13.8	0.532	21.8	
		3	12.5	0.383	18.3	
		4	12.8	0.786	24.6	
		5	9.8	1.216	28.1	
		6	13.8	0.212	17	
		mean	12.483	0.578	21.183	Mild
		s.d.	1.473	0.369	4.490	
%CV	11.8%	63.8%	21.2%			
1,2,3-Trichloropropane	100%	1	6	6.151	98.3	
		2	11.3	4.191	74.2	
		3	6.3	4.491	73.7	
		4	7	7.751	123.3	
		5	8.3	4.511	76	
		6	7.3	6.271	101.4	
		mean	7.700	5.561	91.150	Severe
		s.d.	1.940	1.398	20.056	
%CV	25.2%	25.1%	22.0%			
Aluminum hydroxide	20%	1	8.7	0.012	8.9	
		2	9.7	0.004	9.7	
		3	10	0.015	10.2	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
		4	13	0.011	13.2	
		5	6	0.022	6.3	
		6	11	0.006	11.1	
		mean	9.733	0.012	9.900	Mild
		s.d.	2.339	0.006	2.299	
		%CV	24.0%	55.5%	23.2%	
Diacetone alcohol	100%	1	32.5	4.507	100.1	
		2	31.2	4.119	92.9	
		3	34.8	6.509	132.5	
		4	25.5	3.775	82.1	
		5	32.8	3.064	78.8	
		6	29.8	2.74	70.9	
		mean	31.100	4.119	92.883	Severe
		s.d.	3.212	1.341	21.997	
		%CV	10.3%	32.6%	23.7%	
Laurylsulfobetaine	10%	1	14.3	6.259	108.2	
		2	19.3	4.404	85.4	
		3	19	7.4	130	
		4	10	3.743	66.2	
		5	13.3	5.543	96.5	
		6	21.3	7.102	127.9	
		mean	16.200	5.742	102.367	Severe
		s.d.	4.334	1.462	24.819	
		%CV	26.8%	25.5%	24.2%	
2,4-Dichloro-5-sulfamoylbenzoic acid	20%	1	24	-0.011	23.8	
		2	21	-0.014	20.8	
		3	15.3	-0.011	15.2	
		4	11.7	-0.003	11.6	
		5	22	-0.012	21.8	
		6	22	-0.008	21.9	
		mean	19.333	-0.010	19.183	Mild
		s.d.	4.761	0.004	4.723	
		%CV	24.6%	-39.3%	24.6%	
Propyl-4-hydroxybenzoate	20%	1	8	0.008	8.1	
		2	4	0.169	6.5	
		3	6.3	0.063	7.3	
		4	4	0.014	4.2	
		5	4.7	0.089	6	
		6	4	0.053	4.8	
		mean	5.167	0.066	6.150	Mild
		s.d.	1.650	0.059	1.476	
		%CV	31.9%	89.3%	24.0%	
3-Glycidoxypropyltrimethoxysilane	100%	1	19.5	0.213	22.7	
		2	21.2	0.015	21.4	
		3	20.5	0.005	20.6	
		4	12.5	0.111	14.2	
		5	10.5	0.023	10.8	
		6	15.5	0.025	15.9	
		mean	16.617	0.065	17.600	Mild
		s.d.	4.472	0.082	4.693	
		%CV	26.9%	125.3%	26.7%	
Triethanolamine	100%	1	3.2	0.029	3.6	
		2	3.2	0.03	3.6	
		3	1.8	0.016	2.1	
		4	3.5	0.043	4.1	
		5	2.8	0.018	3.1	
		6	1.2	0.016	1.4	
		mean	2.617	0.025	2.983	Mild
		s.d.	0.913	0.011	1.030	
		%CV	34.9%	42.3%	34.5%	
Phenylbutazone	20%	1	0.3	-0.005	0.3	
		2	0.3	-0.012	0.1	
		3	0.3	-0.015	0.1	
		4	1	-0.007	0.9	
		5	0.7	0.005	0.7	
		6	1.3	-0.013	1.1	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
		mean	0.650	-0.008	0.533	Mild
		s.d.	0.428	0.007	0.427	
		%CV	65.8%	-93.6%	80.1%	
Sodium oxalate	20%	1	0.3	0.092	1.7	
		2	1	0.028	1.4	
		3	2.3	0.108	3.9	
		4	1.7	0.128	3.6	
		5	2	0.15	4.2	
		6	2.7	0.115	4.4	
		mean	1.667	0.104	3.200	Mild
		s.d.	0.882	0.042	1.310	
		%CV	52.9%	40.4%	40.9%	
Tetraaminopyrimidine sulfate	20%	1	2.7	-0.009	2.5	
		2	3	0.002	3	
		3	3	-0.009	2.9	
		4	1	0.007	1.1	
		5	1	-0.007	0.9	
		6	4.7	-0.004	4.6	
		mean	2.567	-0.003	2.500	Mild
		s.d.	1.404	0.007	1.367	
		%CV	54.7%	-196.0%	54.7%	
Magnesium carbonate	20%	1	1	0.02	1.3	
		2	0	0.015	0.2	
		3	0	0.023	0.4	
		4	1	0.012	1.2	
		5	0	0.015	0.2	
		6	1	0.014	1.2	
		mean	0.500	0.017	0.750	Mild
		s.d.	0.548	0.004	0.536	
		%CV	109.5%	25.1%	71.4%	
Betaine monohydrate	20%	1	6.7	0.015	6.9	
		2	1	0.026	1.4	
		3	1	0.027	1.4	
		4	5	0.02	5.3	
		5	1.7	0.055	2.5	
		6	3	0.029	3.4	
		mean	3.067	0.029	3.483	Mild
		s.d.	2.339	0.014	2.219	
		%CV	76.3%	48.5%	63.7%	
Triton X-155	10%	1	2.7	0.003	2.7	
		2	3.7	-0.006	3.6	
		3	4.7	0	4.7	
		4	0.7	0.004	0.7	
		5	1.7	0.02	2	
		6	4.7	0.032	5.1	
		mean	3.033	0.009	3.133	Mild
		s.d.	1.633	0.014	1.669	
		%CV	53.8%	161.4%	53.3%	
EDTA, di-potassium salt	20%	1	0.3	0.024	0.7	
		2	1	0.02	1.3	
		3	0.3	-0.004	0.3	
		4	0.3	-0.004	0.3	
		5	1	0.024	1.4	
		6	1.7	0	1.7	
		mean	0.767	0.010	0.950	Mild
		s.d.	0.572	0.014	0.599	
		%CV	74.5%	140.3%	63.1%	
BRIJ-35	10%	1	1.7	0.012	1.8	
		2	0.7	0.001	0.7	
		3	0.7	0	0.7	
		4	2	-0.006	1.9	
		5	0.7	-0.008	0.6	
		6	0.7	-0.009	0.5	
		mean	1.083	-0.002	1.033	Mild
		s.d.	0.601	0.008	0.638	
		%CV	55.5%	-471.9%	61.7%	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
Petroleum ether	100%	1	3.2	0.006	3.3	
		2	0.5	0.02	0.8	
		3	3.8	0.035	4.4	
		4	2.2	0.008	2.3	
		5	2.8	0.006	2.9	
		6	-1.2	0.012	-1	
		mean	1.883	0.015	2.117	Mild
s.d.	1.885	0.011	1.934			
%CV	100.1%	78.2%	91.4%			
Anthracene	20%	1	3	0.001	3	
		2	0.3	-0.009	0.2	
		3	1.7	0.005	1.7	
		4	0.3	0.004	0.4	
		5	2.7	0.007	2.8	
		6	0.3	0.01	0.5	
		mean	1.383	0.003	1.433	Mild
s.d.	1.262	0.007	1.253			
%CV	91.3%	220.1%	87.4%			
Dimethylbiguanide	20%	1	0	0.016	0.2	
		2	2	0.014	2.2	
		3	1	0.036	1.5	
		4	-1.7	0.034	-1.2	
		5	-0.7	0.457	6.2	
		6	3.3	0.026	3.7	
		mean	0.650	0.097	2.100	Mild
s.d.	1.829	0.177	2.617			
%CV	281.5%	181.7%	124.6%			
MYRJ-45	10%	1	2.8	0.012	3	
		2	-1.2	0.001	-1.1	
		3	0.2	0.005	0.2	
		4	-0.5	0.002	-0.5	
		5	0.5	0.001	0.5	
		6	0.5	0.009	0.6	
		mean	0.383	0.005	0.450	Mild
s.d.	1.356	0.005	1.407			
%CV	353.6%	92.1%	312.6%			
Hexane	100%	1	0.7	0.002	0.7	
		2	4.3	0.002	4.4	
		3	2.3	0	2.3	
		4	-0.3	0.007	-0.2	
		5	-0.3	0.003	-0.3	
		6	1.3	0.002	1.4	
		mean	1.333	0.003	1.383	Mild
s.d.	1.759	0.002	1.775			
%CV	131.9%	87.7%	128.3%			
2-Mercaptopyrimidine	20%	1	0	-0.005	-0.1	
		2	0	-0.004	-0.1	
		3	0	-0.006	-0.1	
		4	0	0.001	0	
		5	0	-0.005	-0.1	
		6	-1	-0.004	-1.1	
		mean	-0.167	-0.004	-0.250	Mild
s.d.	0.408	0.002	0.418			
%CV	-244.9%	-64.8%	-167.3%			
Iminodibenzyl	20%	1	0	0.002	0	
		2	0	0.002	0	
		3	0	-0.002	0	
		4	0	-0.003	0	
		5	1	0.001	1	
		6	0	-0.004	-0.1	
		mean	0.167	-0.001	0.150	Mild
s.d.	0.408	0.003	0.418			
%CV	244.9%	-398.7%	278.9%			
DL-Glutamic acid	20%	1	0.3	-0.004	0.3	
		2	-0.7	0.003	-0.6	
		3	0.3	-0.012	0.2	

**Intralaboratory CV Analysis of BCOP -
Data from Dr. Freddy Van Goethem**

Substance	Concentration	Cornea number	Opacity	Permeability	<i>In Vitro</i> Score ¹	<i>In Vitro</i> Classification
		4	-0.7	-0.005	-0.7	
		5	0.3	-0.006	0.2	
		6	-0.7	-0.008	-0.8	
		mean	-0.200	-0.005	-0.233	Mild
		s.d.	0.548	0.005	0.516	
		%CV	-273.9%	-93.1%	-221.3%	

Abbreviations: CV = Coefficient of variation; SD = Standard deviation

¹*In Vitro* Score = Opacity + (15 x permeability value)

Appendix F

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

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**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	In Vitro Endpoint	No. Samples Tested In Vitro	Interlaboratory Correlation of In Vitro Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
A	BCOPP9	60	a	1.000				
A	BCOPP10	60	b	0.777	1.000			
A	BCOPP11	60	c	0.886	0.862	1.000		
A	BCOPP12	60	d	0.797	0.683	0.859	1.000	
A	BCOPP13	60	e	0.856	0.788	0.906	0.892	1.000
A	BCOPO9	60	a	1.000				
A	BCOPO10	60	b	0.924	1.000			
A	BCOPO11	60	c	0.934	0.898	1.000		
A	BCOPO12	60	d	0.946	0.905	0.978	1.000	
A	BCOPO13	60	e	0.970	0.936	0.953	0.955	1.000
A	BCOPI9	60	a	1.000				
A	BCOPI10	60	b	0.894	1.000			
A	BCOPI11	60	c	0.922	0.896	1.000		
A	BCOPI12	60	d	0.924	0.867	0.957	1.000	
A	BCOPI13	60	e	0.955	0.901	0.947	0.958	1.000
A	BCOPI9b	60	a	1.000				
A	BCOPI10b	60	b	0.898	1.000			
A	BCOPI11b	60	c	0.913	0.913	1.000		
A	BCOPI12b	60	d	0.908	0.848	0.916	1.000	
A	BCOPP13b	60	e	0.939	0.885	0.938	0.938	1.000
A	HETQ14	49	a	1.000				
A	HETQ15	40	b	0.790	1.000			
A	HETQ16	47	c	0.473	0.521	1.000		
A	HETQ17	41	d	0.550	0.734	0.664	1.000	
A	HETS14	11	a	1.000				
A	HETS15	13	b	0.174	1.000			
A	HETS16	13	c	-0.171	-0.171	1.000		
A	HETS17	17	d	-0.103	0.808	0.031	1.000	
A	HETQ14b	49	a	1.000				
A	HETQ15b	40	b	0.627	1.000			
A	HETQ16b	47	c	0.709	0.638	1.000		
A	HETQ17b	41	d	0.449	0.814	0.528	1.000	
A	HETS14b	11	a	1.000				
A	HETS15b	13	b	*	1.000			
A	HETS16b	13	c	-0.043	-0.316	1.000		
A	HETS17b	41	d	*	*	*	*	
A	ICES 22	60	a	1.000				
A	ICES 27	60	b	0.721	1.000			

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
A	ICES 24	59	c	0.750	0.715	1.000		
A	ICES 25	58	d	0.627	0.668	0.734	1.000	
A	ICEO 22	60	a	1.000				
A	ICEO 27	60	b	0.700	1.000			
A	ICEO 24	60	c	0.759	0.716	1.000		
A	ICEO 25	60	d	0.752	0.679	0.732	1.000	
A	ICEF 22	60	a	1.000				
A	ICEF 27	60	b	0.693	1.000			
A	ICEF 24	59	c	0.768	0.525	1.000		
A	ICEF 25	60	d	0.719	0.654	0.690	1.000	
A	ICEC 22	60	a	1.000				
A	ICEC 27	60	b	0.829	1.000			
A	ICEC 24	60	c	0.849	0.759	1.000		
A	ICEC 25	60	d	0.844	0.801	0.853	1.000	
A	IREA 26	60	a	1.000				
A	IREA 23	60	b	0.441	1.000			
A	IREA 28	60	c	0.585	0.695	1.000		
A	IREA 29	60	d	0.619	0.587	0.677	1.000	
A	IREB 26	60	a	1.000				
A	IREB 23	60	b	0.728	1.000			
A	IREB 28	60	c	0.714	0.688	1.000		
A	IREB 29	60	d	0.688	0.617	0.808	1.000	
A	IREC 26	58	a	1.000				
A	IREC 23	60	b	0.524	1.000			
A	IREC 28	58	c	0.485	0.414	1.000		
A	IREC 29	60	d	0.625	0.681	0.819	1.000	
A	IRED 26	58	a	1.000				
A	IRED 23	60	b	0.623	1.000			
A	IRED 28	58	c	0.707	0.618	1.000		
A	IRED 29	60	d	0.813	0.698	0.882	1.000	
A	IRESUM 26	60	a	1.000				
A	IRESUM 23	59	b	0.502	1.000			
A	IRESUM 28	60	c	0.574	0.834	1.000		
A	IRESUM 29	54	d	0.689	0.709	0.798	1.000	
B	BCOPP9	30	a	1.000				
B	BCOPP10	30	b	0.733	1.000			
B	BCOPP11	30	c	0.864	0.818	1.000		
B	BCOPP12	30	d	0.760	0.521	0.807	1.000	

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
B	BCOPP13	30	e	0.880	0.666	0.870	0.840	1.000
B	BCOPO9	30	a	1.000				
B	BCOPO10	30	b	0.945	1.000			
B	BCOPO11	30	c	0.971	0.932	1.000		
B	BCOPO12	30	d	0.962	0.927	0.964	1.000	
B	BCOPO13	30	e	0.959	0.938	0.946	0.928	1.000
B	BCOPI9	30	a	1.000				
B	BCOPI10	30	b	0.906	1.000			
B	BCOPI11	30	c	0.952	0.936	1.000		
B	BCOPI12	30	d	0.929	0.855	0.944	1.000	
B	BCOPI13	30	e	0.950	0.864	0.949	0.948	1.000
B	BCOPI9b	30	a	1.000				
B	BCOPI10b	30	b	0.888	1.000			
B	BCOPI11b	30	c	0.936	0.938	1.000		
B	BCOPI12b	30	d	0.892	0.823	0.916	1.000	
B	BCOPP13b	30	e	0.930	0.850	0.952	0.926	1.000
B	HETQ14	25	a	1.000				
B	HETQ15	17	b	0.711	1.000			
B	HETQ16	23	c	0.355	0.387	1.000		
B	HETQ17	18	d	0.456	0.760	0.679	1.000	
B	HETS14	5	a	*				
B	HETSd15	9	b	*	1.000			
B	HETS16	7	c	*	0.949	1.000		
B	HETS17	11	d	*	0.831	0.420	1.000	
B	HETQ14b	25	a	1.000				
B	HETQ15b	17	b	0.727	1.000			
B	HETQ16b	23	c	0.645	0.594	1.000		
B	HETQ17b	18	d	0.927	0.470	0.535	1.000	
B	ICES 22	30	a	1.000				
B	ICES 27	30	b	0.808	1.000			
B	ICES 24	29	c	0.722	0.789	1.000		
B	ICES 25	29	d	0.691	0.795	0.789	1.000	
B	ICEO 22	30	a	1.000				
B	ICEO 27	30	b	0.775	1.000			
B	ICEO 24	30	c	0.775	0.821	1.000		
B	ICEO 25	30	d	0.847	0.812	0.771	1.000	
B	ICEF 22	30	a	1.000				
B	ICEF 27	30	b	0.803	1.000			

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	In Vitro Endpoint	No. Samples Tested In Vitro	Interlaboratory Correlation of In Vitro Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
B	ICEF 24	29	c	0.846	0.692	1.000		
B	ICEF 25	30	d	0.676	0.727	0.704	1.000	
B	ICEC 22	30	a	1.000				
B	ICEC 27	30	b	0.892	1.000			
B	ICEC 24	30	c	0.881	0.860	1.000		
B	ICEC 25	30	d	0.881	0.896	0.858	1.000	
B	IREA 26	30	a	1.000				
B	IREA 23	30	b	0.503	1.000			
B	IREA 28	30	c	0.624	0.814	1.000		
B	IREA 29	30	d	0.608	0.706	0.701	1.000	
B	IREB 26	30	a	1.000				
B	IREB 23	30	b	0.754	1.000			
B	IREB 28	30	c	0.699	0.746	1.000		
B	IREB 29	30	d	0.690	0.674	0.912	1.000	
B	IREC 26	29	a	1.000				
B	IREC 23	30	b	0.606	1.000			
B	IREC 28	28	c	0.655	0.439	1.000		
B	IREC 29	30	d	0.777	0.733	0.855	1.000	
B	IRED 26	29	a	1.000				
B	IRED 23	30	b	0.663	1.000			
B	IRED 28	28	c	0.799	0.598	1.000		
B	IRED 29	30	d	0.855	0.747	0.939	1.000	
B	IRESUM 26	30	a	1.000				
B	IRESUM 23	29	b	0.568	1.000			
B	IRESUM 28	30	c	0.595	0.955	1.000		
B	IRESUM 29	25	d	0.835	0.749	0.799	1.000	
C	BCOPP9	18	a	1.000				
C	BCOPP10	18	b	0.915	1.000			
C	BCOPP11	18	c	0.932	0.893	1.000		
C	BCOPP12	18	d	0.785	0.688	0.894	1.000	
C	BCOPP13	18	e	0.901	0.889	0.963	0.922	1.000
C	BCOPO9	18	a	1.000				
C	BCOPO10	18	b	0.959	1.000			
C	BCOPO11	18	c	0.913	0.896	1.000		
C	BCOPO12	18	d	0.942	0.928	0.991	1.000	
C	BCOPO13	18	e	0.982	0.972	0.961	0.978	1.000
C	BCOPI9	18	a	1.000				
C	BCOPI10	18	b	0.946	1.000			

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
C	BCOPI11	18	c	0.898	0.879	1.000		
C	BCOPI12	18	d	0.937	0.915	0.980	1.000	
C	BCOPI13	18	e	0.981	0.964	0.947	0.978	1.000
C	BCOPI9b	18	a	1.000				
C	BCOPI10b	18	b	0.943	1.000			
C	BCOPI11b	18	c	0.864	0.877	1.000		
C	BCOPI12b	18	d	0.949	0.916	0.923	1.000	
C	BCOPI13b	18	e	0.971	0.954	0.905	0.968	1.000
C	HETQ14	12	a	1.000				
C	HETQ15	11	b	0.944	1.000			
C	HETQ16	12	c	0.809	0.745	1.000		
C	HETQ17	11	d	0.621	0.580	0.782	1.000	
C	HETS14	6	a	1.000				
C	HETS15	4	b	0.096	1.000			
C	HETS16	6	c	-0.159	-0.910	1.000		
C	HETS17	4	d	-0.288	0.852	-0.094	1.000	
C	HETQ14b	12	a	1.000				
C	HETQ15b	11	b	0.692	1.000			
C	HETQ16b	12	c	0.816	0.642	1.000		
C	HETQ17b	11	d	0.626	0.830	0.562	1.000	
C	ICES 22	18	a	1.000				
C	ICES 27	18	b	0.671	1.000			
C	ICES 24	18	c	0.757	0.599	1.000		
C	ICES 25	17	d	0.514	0.210	0.732	1.000	
C	ICEO 22	18	a	1.000				
C	ICEO 27	18	b	0.498	1.000			
C	ICEO 24	18	c	0.704	0.414	1.000		
C	ICEO 25	18	d	0.786	0.442	0.851	1.000	
C	ICEF 22	18	a	1.000				
C	ICEF 27	18	b	0.433	1.000			
C	ICEF 24	18	c	0.847	0.371	1.000		
C	ICEF 25	18	d	0.745	0.517	0.763	1.000	
C	ICEC 22	18	a	1.000				
C	ICEC 27	18	b	0.705	1.000			
C	ICEC 24	18	c	0.844	0.569	1.000		
C	ICEC 25	18	d	0.763	0.595	0.905	1.000	
C	IREA 26	18	a	1.000				
C	IREA 23	18	b	0.413	1.000			

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
C	IREA 28	18	c	0.599	0.722	1.000		
C	IREA 29	18	d	0.656	0.480	0.634	1.000	
C	IREB 26	18	a	1.000				
C	IREB 23	18	b	0.629	1.000			
C	IREB 28	18	c	0.683	0.552	1.000		
C	IREB 29	18	d	0.607	0.409	0.575	1.000	
C	IREC 26	17	a	1.000				
C	IREC 23	18	b	0.169	1.000			
C	IREC 28	18	c	0.276	0.456	1.000		
C	IREC 29	18	d	0.210	0.392	0.748	1.000	
C	IRED 26	17	a	1.000				
C	IRED 23	18	b	0.490	1.000			
C	IRED 28	18	c	0.704	0.689	1.000		
C	IRED 29	18	d	0.790	0.615	0.874	1.000	
C	IRESUM 26	18	a	1.000				
C	IRESUM 23	18	b	0.481	1.000			
C	IRESUM 28	18	c	0.555	0.861	1.000		
C	IRESUM 29	18	d	0.628	0.964	0.896	1.000	
D	BCOPP9	12	a	1.000				
D	BCOPP10	12	b	0.835	1.000			
D	BCOPP11	12	c	0.932	0.912	1.000		
D	BCOPP12	12	d	0.843	0.966	0.922	1.000	
D	BCOPP13	12	e	0.766	0.924	0.921	0.958	1.000
D	BCOPO9	12	a	1.000				
D	BCOPO10	12	b	0.957	1.000			
D	BCOPO11	12	c	0.971	0.981	1.000		
D	BCOPO12	12	d	0.947	0.972	0.957	1.000	
D	BCOPO13	12	e	0.967	0.995	0.985	0.973	1.000
D	BCOPI9	12	a	1.000				
D	BCOPI10	12	b	0.914	1.000			
D	BCOPI11	12	c	0.951	0.952	1.000		
D	BCOPI12	12	d	0.915	0.989	0.936	1.000	
D	BCOPI13	12	e	0.915	0.959	0.947	0.966	1.000
D	BCOPI9b	12	a	1.000				
D	BCOPI10b	12	b	0.914	1.000			
D	BCOPI11b	12	c	0.951	0.952	1.000		
D	BCOPI12b	12	d	0.915	0.989	0.936	1.000	
D	BCOPI13b	12	e	0.915	0.959	0.947	0.966	1.000

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
D	HETQ14	12	a	1.000				
D	HETQ15	12	b	0.793	1.000			
D	HETQ16	12	c	0.438	0.779	1.000		
D	HETQ17	12	d	0.816	0.876	0.579	1.000	
D	HETQ14b	12	a	1.000				
D	HETQ15b	12	b	0.721	1.000			
D	HETQ16b	12	c	0.670	0.768	1.000		
D	HETQ17b	12	d	0.420	0.966	0.721	1.000	
D	ICES 22	12	a	1.000				
D	ICES 27	12	b	0.741	1.000			
D	ICES 24	12	c	0.920	0.696	1.000		
D	ICES 25	12	d	0.641	0.392	0.543	1.000	
D	ICEO 22	12	a	1.000				
D	ICEO 27	12	b	0.618	1.000			
D	ICEO 24	12	c	0.719	0.759	1.000		
D	ICEO 25	12	d	0.438	0.834	0.483	1.000	
D	ICEF 22	12	a	1.000				
D	ICEF 27	12	b	0.663	1.000			
D	ICEF 24	12	c	0.636	0.546	1.000		
D	ICEF 25	12	d	0.950	0.748	0.664	1.000	
D	ICEC 22	12	a	1.000				
D	ICEC 27	12	b	0.827	1.000			
D	ICEC 24	12	c	0.854	0.805	1.000		
D	ICEC 25	12	d	0.870	0.759	0.724	1.000	
D	IREA 26	12	a	1.000				
D	IREA 23	12	b	0.433	1.000			
D	IREA 28	12	c	0.317	0.567	1.000		
D	IREA 29	12	d	0.678	0.462	0.480	1.000	
D	IREB 26	12	a	1.000				
D	IREB 23	12	b	0.786	1.000			
D	IREB 28	12	c	0.894	0.789	1.000		
D	IREB 29	12	d	0.814	0.736	0.845	1.000	
D	IREC 26	12	a	1.000				
D	IREC 23	12	b	0.091	1.000			
D	IREC 28	12	c	-0.148	0.269	1.000		
D	IREC 29	12	d	-0.010	0.527	0.835	1.000	
D	IRED 26	12	a	1.000				
D	IRED 23	12	b	0.647	1.000			

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
D	IREC 28	12	c	0.405	0.635	1.000		
D	IREC 29	12	d	0.686	0.589	0.758	1.000	
D	IRESUM 26	12	a	1.000				
D	IRESUM 23	12	b	0.363	1.000			
D	IRESUM 28	12	c	0.769	0.498	1.000		
D	IRESUM 29	11	d	0.665	0.614	0.872	1.000	
E	BCOPP9	20	a	1.000				
E	BCOPP10	20	b	0.773	1.000			
E	BCOPP11	20	c	0.926	0.843	1.000		
E	BCOPP12	20	d	0.878	0.563	0.889	1.000	
E	BCOPP13	20	e	0.932	0.670	0.934	0.886	1.000
E	BCOPO9	20	a	1.000				
E	BCOPO10	20	b	0.941	1.000			
E	BCOPO11	20	c	0.908	0.887	1.000		
E	BCOPO12	20	d	0.912	0.903	0.977	1.000	
E	BCOPO13	20	e	0.966	0.930	0.952	0.942	1.000
E	BCOPI9	20	a	1.000				
E	BCOPI10	20	b	0.902	1.000			
E	BCOPI11	20	c	0.897	0.872	1.000		
E	BCOPI12	20	d	0.880	0.852	0.960	1.000	
E	BCOPI13	20	e	0.945	0.884	0.943	0.942	1.000
E	BCOPI9b	20	a	1.000				
E	BCOPI10b	20	b	0.881	1.000			
E	BCOPI11b	20	c	0.887	0.869	1.000		
E	BCOPI12b	20	d	0.870	0.776	0.889	1.000	
E	BCOPP13b	20	e	0.921	0.824	0.925	0.930	1.000
E	HETQ14	9	a	1.000				
E	HETQ15	0	b	*	*			
E	HETQ16	7	c	0.500	*	1.000		
E	HETQ17	1	d	*	*	*	*	
E	HETS14	11	a	1.000				
E	HETS15	13	b	0.174	1.000			
E	HETS16	13	c	-0.171	-0.171	1.000		
E	HETS17	17	d	-0.103	0.808	0.031	1.000	
E	HETQ14b	9	a	1.000				
E	HETQ15b	0	b	*	*			
E	HETQ16b	7	c	0.985	*	1.000		
E	HETQ17b	1	d	*	*	*	*	

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	In Vitro Endpoint	No. Samples Tested In Vitro	Interlaboratory Correlation of In Vitro Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
E	ICES 22	20	a	1.000				
E	ICES 27	20	b	0.869	1.000			
E	ICES 24	20	c	0.847	0.734	1.000		
E	ICES 25	19	d	0.778	0.722	0.811	1.000	
E	ICEO 22	20	a	1.000				
E	ICEO 27	20	b	0.595	1.000			
E	ICEO 24	20	c	0.752	0.602	1.000		
E	ICEO 25	20	d	0.868	0.649	0.752	1.000	
E	ICEF 22	20	a	1.000				
E	ICEF 27	20	b	0.729	1.000			
E	ICEF 24	20	c	0.864	0.678	1.000		
E	ICEF 25	20	d	0.739	0.869	0.674	1.000	
E	ICEC 22	20	a	1.000				
E	ICEC 27	20	b	0.806	1.000			
E	ICEC 24	20	c	0.874	0.752	1.000		
E	ICEC 25	20	d	0.883	0.816	0.880	1.000	
E	IREA 26	20	a	1.000				
E	IREA 23	20	b	0.195	1.000			
E	IREA 28	20	c	0.394	0.908	1.000		
E	IREA 29	20	d	0.405	0.543	0.468	1.000	
E	IREB 26	20	a	1.000				
E	IREB 23	20	b	0.782	1.000			
E	IREB 28	20	c	0.629	0.649	1.000		
E	IREB 29	20	d	0.569	0.524	0.672	1.000	
E	IREC 26	19	a	1.000				
E	IREC 23	20	b	0.335	1.000			
E	IREC 28	20	c	0.670	0.404	1.000		
E	IREC 29	20	d	0.559	0.628	0.829	1.000	
E	IRED 26	19	a	1.000				
E	IRED 23	20	b	0.540	1.000			
E	IRED 28	20	c	0.791	0.685	1.000		
E	IRED 29	20	d	0.798	0.689	0.949	1.000	
E	IRESUM 26	20	a	1.000				
E	IRESUM 23	19	b	0.199	1.000			
E	IRESUM 28	20	c	0.191	0.991	1.000		
E	IRESUM 29	15	d	0.432	0.606	0.635	1.000	
F	BCOPP9	14	a	1.000				
F	BCOPP10	14	b	0.731	1.000			

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
F	BCOPP11	14	c	0.901	0.864	1.000		
F	BCOPP12	14	d	0.795	0.903	0.896	1.000	
F	BCOPP13	14	e	0.699	0.846	0.875	0.933	1.000
F	BCOPO9	14	a	1.000				
F	BCOPO10	14	b	0.984	1.000			
F	BCOPO11	14	c	0.985	0.959	1.000		
F	BCOPO12	14	d	0.989	0.968	0.987	1.000	
F	BCOPO13	14	e	0.984	0.988	0.955	0.976	1.000
F	BCOPI9	14	a	1.000				
F	BCOPI10	14	b	0.917	1.000			
F	BCOPI11	14	c	0.975	0.920	1.000		
F	BCOPI12	14	d	0.974	0.914	0.974	1.000	
F	BCOPI13	14	e	0.969	0.926	0.954	0.980	1.000
F	BCOPI9b	14	a	1.000				
F	BCOPI10b	14	b	0.899	1.000			
F	BCOPI11b	14	c	0.970	0.928	1.000		
F	BCOPI12b	14	d	0.955	0.921	0.962	1.000	
F	BCOPP13b	14	e	0.946	0.918	0.976	0.972	1.000
F	HETQ14	14	a	1.000				
F	HETQ15	14	b	0.880	1.000			
F	HETQ16	14	c	0.776	0.730	1.000		
F	HETQ17	14	d	0.712	0.842	0.765	1.000	
F	HETQ14b	14	a	*				
F	HETQ15b	14	b	*	1.000			
F	HETQ16b	14	c	*	0.591	1.000		
F	HETQ17b	14	d	*	0.974	0.590	1.000	
F	ICES 22	14	a	1.000				
F	ICES 27	14	b	0.617	1.000			
F	ICES 24	13	c	0.757	0.856	1.000		
F	ICES 25	13	d	0.539	0.889	0.821	1.000	
F	ICEO 22	14	a	1.000				
F	ICEO 27	14	b	0.797	1.000			
F	ICEO 24	14	c	0.796	0.907	1.000		
F	ICEO 25	14	d	0.794	0.868	0.717	1.000	
F	ICEF 22	14	a	1.000				
F	ICEF 27	14	b	0.781	1.000			
F	ICEF 24	13	c	0.604	0.543	1.000		
F	ICEF 25	14	d	0.901	0.689	0.772	1.000	

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
F	ICEC 22	14	a	1.000				
F	ICEC 27	14	b	0.873	1.000			
F	ICEC 24	14	c	0.877	0.905	1.000		
F	ICEC 25	14	d	0.907	0.913	0.868	1.000	
F	IREA 26	14	a	1.000				
F	IREA 23	14	b	0.648	1.000			
F	IREA 28	14	c	0.733	0.712	1.000		
F	IREA 29	14	d	0.789	0.596	0.817	1.000	
F	IREB 26	14	a	1.000				
F	IREB 23	14	b	0.808	1.000			
F	IREB 28	14	c	0.862	0.812	1.000		
F	IREB 29	14	d	0.789	0.746	0.906	1.000	
F	IREC 26	13	a	1.000				
F	IREC 23	14	b	0.914	1.000			
F	IREC 28	12	c	0.464	0.682	1.000		
F	IREC 29	14	d	0.805	0.815	0.845	1.000	
F	IRED 26	13	a	1.000				
F	IRED 23	14	b	0.776	1.000			
F	IRED 28	12	c	0.613	0.575	1.000		
F	IRED 29	14	d	0.868	0.696	0.781	1.000	
F	IRESUM 26	14	a	1.000				
F	IRESUM 23	14	b	0.770	1.000			
F	IRESUM 28	14	c	0.863	0.811	1.000		
F	IRESUM 29	14	d	0.884	0.800	0.957	1.000	
G	BCOPP9	26	a	1.000				
G	BCOPP10	26	b	0.733	1.000			
G	BCOPP11	26	c	0.801	0.856	1.000		
G	BCOPP12	26	d	0.781	0.612	0.801	1.000	
G	BCOPP13	26	e	0.893	0.794	0.858	0.845	1.000
G	BCOPO9	26	a	1.000				
G	BCOPO10	26	b	0.961	1.000			
G	BCOPO11	26	c	0.935	0.955	1.000		
G	BCOPO12	26	d	0.949	0.961	0.967	1.000	
G	BCOPO13	26	e	0.961	0.964	0.913	0.940	1.000
G	BCOPI9	26	a	1.000				
G	BCOPI10	26	b	0.873	1.000			
G	BCOPI11	26	c	0.875	0.939	1.000		
G	BCOPI12	26	d	0.897	0.851	0.902	1.000	

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
G	BCOPI13	26	e	0.953	0.891	0.898	0.956	1.000
G	BCOPI9b	26	a	1.000				
G	BCOPI10b	26	b	0.873	1.000			
G	BCOPI11b	26	c	0.875	0.939	1.000		
G	BCOPI12b	26	d	0.897	0.851	0.902	1.000	
G	BCOPP13b	26	e	0.953	0.891	0.898	0.956	1.000
G	HETQ14	26	a	1.000				
G	HETQ15	26	b	0.755	1.000			
G	HETQ16	26	c	0.221	0.450	1.000		
G	HETQ17	26	d	0.492	0.692	0.704	1.000	
G	HETQ14b	26	a	1.000				
G	HETQ15b	26	b	0.721	1.000			
G	HETQ16b	26	c	0.771	0.638	1.000		
G	HETQ17b	26	d	0.675	0.765	0.591	1.000	
G	ICES 22	26	a	1.000				
G	ICES 27	26	b	0.779	1.000			
G	ICES 24	26	c	0.690	0.736	1.000		
G	ICES 25	26	d	0.626	0.461	0.560	1.000	
G	ICEO 22	26	a	1.000				
G	ICEO 27	26	b	0.757	1.000			
G	ICEO 24	26	c	0.770	0.695	1.000		
G	ICEO 25	26	d	0.719	0.692	0.764	1.000	
G	ICEF 22	26	a	1.000				
G	ICEF 27	26	b	0.607	1.000			
G	ICEF 24	26	c	0.748	0.394	1.000		
G	ICEF 25	26	d	0.594	0.494	0.654	1.000	
G	ICEC 22	26	a	1.000				
G	ICEC 27	26	b	0.856	1.000			
G	ICEC 24	26	c	0.830	0.745	1.000		
G	ICEC 25	26	d	0.778	0.751	0.803	1.000	
G	IREA 26	26	a	1.000				
G	IREA 23	26	b	0.496	1.000			
G	IREA 28	26	c	0.685	0.518	1.000		
G	IREA 29	26	d	0.709	0.625	0.704	1.000	
G	IREB 26	26	a	1.000				
G	IREB 23	26	b	0.525	1.000			
G	IREB 28	26	c	0.628	0.526	1.000		
G	IREB 29	26	d	0.664	0.470	0.824	1.000	

**Interlaboratory Correlation Coefficients from the
EC/HO Validation Study (Balls et al. 1995)**

Chemical Category	<i>In Vitro</i> Endpoint	No. Samples Tested <i>In Vitro</i>	Interlaboratory Correlation of <i>In Vitro</i> Data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
G	IREC 26	26	a	1.000				
G	IREC 23	26	b	0.137	1.000			
G	IREC 28	26	c	0.245	0.214	1.000		
G	IREC 29	26	d	0.342	0.101	0.808	1.000	
G	IREC 26	26	a	1.000				
G	IREC 23	26	b	0.539	1.000			
G	IREC 28	26	c	0.712	0.507	1.000		
G	IREC 29	26	d	0.790	0.613	0.906	1.000	
G	IRESUM 26	26	a	1.000				
G	IRESUM 23	26	b	0.527	1.000			
G	IRESUM 28	26	c	0.693	0.793	1.000		
G	IRESUM 29	25	d	0.626	0.696	0.716	1.000	

A = Full set of chemicals; B= Water soluble; C = Water insoluble; D = Surfactants; E = Solids; F = Solutions; G = Liquids

The numbers 1-38 against each endpoint in the Table refer to the laboratories which conducted each particular test. Laboratory 36 left the study without submitting any results

* = No data

BCOPP = Permeability; BCOPO = Opacity; BCOPI = Index; BCOPIb = Index, cut-off at 200

HETQ = Q Score; HETS = S Score; HETQB = Q Score; cutoff at 2; HETSB = S Score, cutoff at 2

ICES = Swelling; ICEO = Opacity; ICEF = Fluorescein retention; ICEC = Irritation Index

IREA = Opacity (1 hr); IREB = Opacity (4 hr); IREC = Swelling (1 hr); IRED = Swelling (4 hr); IRESUM = Summary score

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Appendix G

**Additional BCOP Studies Received in Response to
Federal Register Notices (Vol. 69, No. 57, pp. 13859-13861) and
(Vol. 70, No. 38, pp. 9661-9662)**

- G1 Dataset Received from S.C. Johnson & Son, Inc. in Support of Cuellar et al. (2004) Poster Presentation..... G-3**
- G2 Dataset Received from S.C. Johnson & Son, Inc. in Support of Cuellar et al. (2002) Poster Presentation..... G-43**
- G3 Dataset Received from S.C. Johnson & Son, Inc. in Support of Gran et al. (2003) Poster Presentation G-61**
- G4 Dataset Received from L'OREAL Advanced Research for an In-house Porcine Corneal Opacity and Permeability Assay G-91**
- G5 Supporting Analyses Received from IIVS for Gettings et al. (1996) Study G-101**
- G6 Dataset Received from Johnson & Johnson Pharmaceutical Research and Development – A Division of Janssen Pharmaceutica N.V. (Laboratory No. 9 in Gautheron et al. 1994) G-191**
- G7 Dataset Received from Johnson & Johnson Pharmaceutical Research and Development – A Division of Janssen Pharmaceutica N.V. (BCOP Tests With Young vs. Old Corneas) G-251**

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Appendix G1

**Dataset Received from S.C. Johnson & Son, Inc. in Support of
Cuellar et al. (2004) Poster Presentation**

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A FAMILY COMPANY

S.C. Johnson & Son, Inc.
Worldwide Consumer Products, RD & E
Global Safety Assessment and Regulatory Affairs, Product Toxicology
MS 139 1525 Howe Street, Racine WI 53403

August 27, 2004

Christina Inhof, MSPH
Senior Project Coordinator/Technical Writer ILS, Inc.
NICEATM
P.O. Box 12233
NIEHS MD EC-17
Research Triangle Park, NC 27709

Christina,

Hi! How are you? I am happy to be submitting data on solvents and simple fragrance formulations, which were discussed in the poster citation listed below:

Cuellar, N., Lloyd, P.H., Swanson J.E., Merrill, J.C., Mun, G., Harbell, J.W. and Bonnette, K.L. (2004) Phase Two: Evaluating the eye irritancy of solvents in a simple fragrance mixture with the bovine corneal opacity and permeability (BCOP) assay. *The Toxicologist* 78(S-1): Abstract No. 1306.

Included with this submission are the following documents:

1. Cover letter
2. Poster text
3. Poster graphs
4. Histology slides
5. Coded formula spreadsheet

Study Protocols:

Modified Draize protocol was used for the in-vivo studies. Four animals were treated per sample (3 for histopathology and 1 animal for recovery). Each animal received a 0.1 ml dose of the formula in the conjunctival sac of the right eye. The left eye served as the untreated control. All animals were scored at 1, 4, and 24 hours after dosing. Histology was conducted on 3 of the 4 animals.

Standard BCOP protocol was used for the in-vitro work at IIVS. The first BCOP study required exposure times of 1 and 3 minutes with a post exposure of 20 hours to compliment the timing in the animal. The second BCOP study utilized a 3-minute exposure time with

post exposures of 2 to 4 hours to understand effects using standard post exposure times. Histology was conducted on all corneas. Since the 1-minute exposure did not produce extensive lesions, only the 3-minute exposure was evaluated in the second study. Only the 3-minute exposure data are reported in this poster.

Formula Spreadsheet:

The formulas listed in this spreadsheet are coded similarly to formulas listed in the poster. Test material number is the unique sample number and the group name denotes formula description. Raw materials are listed followed by their percentages in each formula.

Poster:

Fragrance poster not included. John Harbell previously sent it to you.

Poster Text:

A word document consisting of poster text and tables is included in this submission for ease of reading. The poster contained a wealth of information, thus limited visibility. This document highlights where the graphs and histology slides should be inserted for ease of understanding. Please note: Table one has improved coloring/formatting on the poster.

Poster Graphs:

Poster graphs should be referenced on page 10.

Histology Slides:

Histology slides should be referenced on page 12.

Data Worksheet:

The data worksheet is not included for this submission. GHS and EPA classification of results was not possible due to lack of animals. Only 1 of the 4 animals was carried out for recovery purposes. The remaining 3 animals were used for histopathology.

Summary:

Solvents have a major impact on the ocular irritation potential of fragrance mixtures. Both the degree and the time-course of the irritation can be impacted by the solvent. Over the three harvest times, the BCOP assay was able to identify histological changes that characterize the treatment groups into severe (ethanol alone), moderate (2-stages), and mild categories. One treatment group (fragrance + DPG) was over predicted by the BCOP compared to the in vivo assay. The time course of the tissue scores in vivo was similar to

August 30, 2004

the time course of the histological changes in BCOP. The BCOP model was more consistent in its response to a given treatment than the in vivo model.

If you have any questions or comments on this data set, please feel free to contact either Judith Swanson or myself at the following:

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Sincere regards,

A handwritten signature in cursive script that reads "Nicole Cuellar". The signature is written in black ink and is positioned above the typed name and title.

Nicole Cuellar
Sr. Research Toxicologist

POSTER TEXT FOR S.C. JOHNSON SUBMISSION DATED AUGUST 27, 2004

TITLE:

PHASE TWO: EVALUATING THE EYE IRRITANCY OF SOLVENTS IN A SIMPLE FRAGRANCE MIXTURE WITH THE BOVINE CORNEAL OPACITY AND PERMEABILITY (BCOP) ASSAY

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ABSTRACT:

Fragrances are complex mixtures used in many consumer products. Organic solvents, such as ethanol, are major components of fragrance formulations functioning mainly as solubilizers and fragrance delivery mechanisms. In Phase One (Cuellar et al, 2003), the BCOP assay and primary eye irritation study (EPA-OPPTS 870.2400) were conducted using simple fragrance mixtures containing six commonly used solvents. The corneal depth of injury was assessed histologically both in vitro and in vivo. In the BCOP assay, corneas were exposed for 1 and 3 minutes, rinsed and incubated for 20 hours before the opacity and permeability endpoints were assessed. In vivo, animals were scored at 1, 4, and 24 hours. Individual solvents impacted the level of irritation of these formulations. Phase Two evaluated the time course of lesion development after exposure in the BCOP assay and determined those early lesion that would be predictive of damage observed after 20+ hours in vitro and in vivo. Bovine corneas were exposed for 3 minutes, rinsed, and incubated for 2 or 4 hours before the endpoints were assessed and tissue taken for histology. In vivo, certain solvents increased the rate of lesion development but not the overall intensity or duration compared to the fragrance alone. Other solvents decreased the overall intensity and duration. The BCOP assay showed a generally similar pattern of lesion development. Those combinations that showed opacity at 4 hours in vivo, showed epithelial and stromal lesion in the BCOP by 4 hours post-exposure. Fragrance alone was slower to develop opacity in vivo and required the 20 hour post-exposure to produce appreciable lesions in vitro. These data suggest that our standard post exposure (2 hour) can be predictive of irritation potential of fragrance/solvent mixtures.

INTRODUCTION:

The Bovine Corneal Opacity and Permeability (BCOP) Assay is routinely used by S.C. Johnson and Son as a tool for evaluating air fresheners for potential ocular irritation. Depending on the type of air freshener, other components may be added to solubilize a fragrance or to facilitate fragrance delivery mechanisms. In Phase I of this study (Cuellar et al., 2003), the BCOP assay and the primary eye irritation assay (EPA OPPTS 870.2400) were conducted using simple fragrance mixtures containing six commonly used solvents. As with Cuellar et al. (2002), Cuellar et al. (2003) found that solvents had an impact on the ocular irritation potential of fragrance mixtures. Based on this information, we examined the use of the BCOP at our standard post exposure times (2 and 4 hour) in comparison with Phase I post exposure times both in vitro (20 hour) and in vivo (24 hour) for rate, degree and intensity of irritation potential of the same fragrance mixtures.

Histological examination is necessary to understand the degree and depth of injury associated with the permeability and opacity measurements with diverse chemical classes or mixtures (Curren et al., 2000). Depth of injury has been shown to be a predictor of the degree and duration (reversibility) of ocular injury by Maurer et al. (2002) and Jester et al. (1998). Histological evaluation was used in Cuellar et al. (2002) to define the degree of injury to a reference sample and also to set the upper bound limit for other formulations of that type. Cuellar et al. (2003), demonstrated that permeability and opacity scores in the BCOP assay and the MAS scores in vivo paralleled the depth of injury and cellular changes seen histologically from both BCOP and in vivo samples. In Phase II of this study, we evaluated the progression of lesion development after exposure in the BCOP assay. Additionally, we determined specific early lesions that would be predictive of damage observed after 20+ hours in vitro and in vivo in the same fragrance mixtures.

MATERIALS AND METHODS:

Phase	In – vitro (BCOP)	In-vivo
One	3 & 10 minute exposure, 20 hour post-exposure	1, 4, & 24 hour scored
Two	3 minute exposure, 2 & 4 hour post-exposure	Not repeated

IN VITRO - BCOP:

Bovine Eyes

The BCOP assay was performed following the methods of Sina et al. (1995). Bovine eyes were obtained from a local abattoir as a by-product from freshly slaughtered animals. The eyes were grossly examined for damage and those exhibiting defects were discarded. The corneas were excised such that a 2 to 3 mm rim of sclera was present around the cornea. The corneas were mounted in the holders and the two chambers filled with Minimum Essential Medium Eagle (MEM) without phenol red, supplemented with 1% fetal bovine serum (complete MEM). The corneal holders were incubated at $32 \pm 1^\circ\text{C}$ for a minimum of 1 hour.

Bovine Corneal Opacity and Permeability Assay

After a minimum of 1 hour of incubation, the medium replaced in both chambers and the opacity was determined for each cornea using a Spectro Designs OP-KIT opacimeter. Three corneas, whose opacity readings were close to the median opacity for all the corneas, were selected as the negative control corneas. The medium was then removed from the anterior chamber and replaced with either the test article, positive control, or negative control.

Testing Procedure

Each test article was administered neat to the BCOP test system. An aliquot of 750 μl of either the test article, positive control (100% ethanol), or negative control (deionized water) was introduced into the anterior chamber while slightly rotating the holder to ensure uniform distribution over the cornea. Six corneas were used for each test article (three corneas per each post-exposure incubation period of 2 or 4 hours) were exposed for three minutes at $32 \pm 1^\circ\text{C}$. Six corneas were treated with the negative control (three corneas per each post-exposure incubation period of 2 and 4 hours) were exposed for ten minutes at $32 \pm 1^\circ\text{C}$. Three corneas were treated with the positive control for 10 minutes $32 \pm 1^\circ\text{C}$. After the exposure periods, the test or control article treatments were removed. The corneal surface was washed at least three times to ensure total removal of the test or control articles. The corneas exposed were returned to the incubator for approximately 2 hours (test articles, positive and negative controls) and 4 hours (test articles and negative controls). After this incubation (2 or 4 hours), the final measure of opacity was obtained. Corneas cultured for 4 hours were refeed immediately prior to the final measure of opacity. The values obtained at this second opacity measurement are presented in the report and were used in calculating the corneal opacity.

After the second opacity measurement was performed, the medium was removed from both chambers of the holder. The posterior chamber was refilled with complete MEM, and 1 ml of a 4 mg/ml fluorescein solution was added to the anterior chamber. The corneas were then incubated in a horizontal position (anterior side up) for approximately 90 minutes at $32 \pm 1^\circ\text{C}$. After the incubation, an aliquot of 360 μl from each chamber was placed into the designated well on a 96-well plate. The optical density at 490 nm (OD_{490}) was determined using a Molecular Devices V_{max} kinetic microplate reader.

Opacity Measurement: The change in opacity for each cornea was calculated by subtracting the pre-treatment opacity readings from the final opacity readings. The corrected opacity value of each cornea was calculated by subtracting the average change in opacity of the negative control corneas from that of each treated cornea. The mean opacity values of each treatment group were then calculated.

Permeability Measurement: The corrected OD₄₉₀ was calculated by subtracting the mean OD₄₉₀ of the negative control corneas from the OD₄₉₀ value of each treated cornea. The mean OD₄₉₀ values of each treatment group were then calculated.

Histology

The corneas were placed in individual, prelabelled cassettes and fixed for at least 24 hours in 10% buffered formalin. The fixed corneas were transferred to Pathology Associates - A Charles River Company (Frederick, MD) for embedding, sectioning and staining. Each slide was then stained with hematoxylin and eosin. Slides were returned to the Institute for In Vitro Sciences, Inc. for evaluation. Photomicrographs and thickness measurements were prepared using a Spot Insight (Spot Diagnostic Instruments) digital camera and associated software.

IN VIVO:

The acute eye irritation study was conducted in accordance with the US EPA, Health Effects Test Guidelines (OPPTS 870.2400). Four New Zealand White rabbits were treated per sample (three animals for histopathology and one animal for recovery). Each animal received a 0.1mL dose of the appropriate test article in the conjunctival sac of the right eye. The left eye of each animal remained untreated and served as the control. Eyes were macroscopically scored at 1, 4, and 24 hours after dosing for both histopathology and recovery animals according to the Ocular Grading System based on Draize (1959). The group mean irritation score was then calculated for each scoring interval based on the number of animals initially dosed in each group. The calculated group mean ocular irritation scores for each interval were used to classify the test article according to the Ocular Evaluation Criteria of Kay and Calandra (1962).

Histology:

The test and control eyes were collected, identified, and placed in 10% neutral buffered formalin for fixation. The sections were processed histologically (embedded in paraffin, cut, and stained with hematoxylin and eosin). The histology was conducted by HistoTechniques (Powell, Ohio). The resulting slides were examined by a board certified pathologist (Dr. J. Dale Thurman, Senior Director of Pathology). No tissues were retained or examined for the recovery animals. Subsequently, slides were scored for cellular changes (paralleling those scored for bovine corneas) and photographed by one of us (JHW). These observations are reported in Table 1.

RESULTS:

The histological results of the BCOP and acute eye irritation assay for thirteen treatment groups are presented in Tables 1-3. The numerical scores of the BCOP and acute eye irritation assay for the thirteen treatment groups are graphically presented in Figures 1-6. The thirteen treatment groups include fragrance only, six solvents only, and six solvent/fragrance mixtures. The simple fragrance alone consists of 25% of each of the following fragrance components: benzyl acetate, linalool, dihydroxymyrcenol, and Verdox. The solvents consist of 100% of each of the following solvents: ethanol (ETOH), Dowanol DPM (DPM), Isopar M, dipropylene glycol (DPG), carbitol, and benzyl benzoate (BB). The solvent/fragrance mixtures (solvent + F, e.g. ETOH+F) consist of 80% fragrance mixture (20% of each fragrance component) and 20% of each solvent. Fragrance components and solvents were chosen because they are more frequently used in fragrance formulations.

Table 1 shows the depth of injury, cellular change and opacity score x area score for each animal for the thirteen treatment groups. Characteristic lesions are grouped together by severity of injury and cellular change from Group I (least irritating) to Group IV (most irritating). Days to clear for the recovery animal is listed below.

Table 1. In-Vivo Histological Summary

Group	Characteristic Lesions	Opacity Score x Area Score for each animal					
		2x4	2x3	2x2	2x1	1x1	0x0
IV	1) Complete or nearly complete loss of epithelium over the cornea 2) Marked inflammatory infiltrate extending well into the corneal stroma 3) Loss of keratocytes in the upper stroma 4) Increased frequency of enlarged keratocytes in the mid stroma	ETOH ETOH ETOH					
III	1) Focal, full thickness loss of epithelium 2) Marked inflammatory infiltrate restricted to the edge of the cornea 3) Increased frequency of enlarged keratocytes in the upper stroma under the epithelial lesion	Frag- rance ETOH+F DPM+F	DPG+F Carbitol +F	Frag- rance Carbitol+ F BB+F	Frag- rance Carbitol+F DPM DPM		
II	1) Small focus of epithelial loss or thinning 2) Limited inflammatory infiltrate 3) Slight increase in enlarged keratocytes		DPM Carbitol	Carbitol	ETOH+F DPM+F Carbitol	Isopar M+F BB+F	DPG+F DPG
I	1) Epithelium was intact or just slightly thinned 2) Little or no inflammatory infiltrate 3) No enlarged keratocytes						Isopar M Isopar M DPG DPG BB BB BB ETOH+F DPM+F Isopar M+F Isopar M+F DPG+F BB+F ETOH Isopar M

Days to clear (for the remaining animal in the treatment group)

>28 days - ETOH

7 Days - Fragrance, ETOH+F, DPM+F, Carbitol +F

3 Days – DPG+F, DPM, DPG, Carbitol

2 Days – Isopar+F, BB+F

1 Day – Isopar M, BB

Table 2 demonstrates the description of the characteristic lesions seen in the epithelial layer of the corneas of the 13 treatment samples in the BCOP assay at three different post-exposure times (2, 4, and 20 hours). Corneas are grouped by severity of the depth of injury and cellular changes from Group E (most irritating) to Group A (least irritating).

Table 2. Summary of the epithelial layer changes in the BCOP

In Vitro	Characteristic Lesions	2-hour post-exposure	4-hour post-exposure	20-hour post-exposure
Group E	Full thickness loss or separation on >50% of the corneal surface	ETOH	ETOH	ETOH DPM + F (2) Carbitol + F
Group D	Full thickness loss/separation on <50% of the corneal surface but substantial damage to wing and basal cell layers	ETOH+F(2) DPG+F Carbitol+F	ETOH+F Carbitol+F(2))	Fragrance ETOH+F DPG+F (2) DPM+F (1)
Group C	Little or no full thickness loss but damage well into the wing and basal cell layers (may include nuclear changes and cytoplasmic vacuolization)	ETOH+F(1) DPM+F DPM Carbitol	DPM+F DPG+F Carbitol+ F(1) DPM Carbitol	DPG+F(1) BB+F DPM Carbitol
Group B	Loss of the full squamous cell layer with occasional damage into the wing cell layer. No full thickness loss	Fragrance Isopar M+F	Fragrance	Isopar M+F
Group A	Similar to the time-matched negative control epithelium or with some loss/loosening of the surface squamous epithelial layers	BB+F Isopar M DPG BB	Isopar M+F BB+F Isopar M DPG BB	Isopar M DPG BB

Table 3 demonstrates the description of the characteristic lesions seen in the stroma of the corneas of the 13 treatment samples in the BCOP assay at three different post-exposure times (2, 4, and 20 hours). Corneas are grouped by severity of the depth of injury and cellular changes from Group E (most irritating) to Group A (least irritating).

Table 3. Summary of the Stromal Lesions in the BCOP.

In Vitro	Characteristic Lesions	2-hour post-exposure	4-hour post-exposure	20-hour post-exposure
Group E	1) Thickness: Appreciably thicker than the time-matched controls 2) Stromal matrix vacuolization: Marked to 50% depth 3) Keratocytes: a. Upper stroma: Marked cell loss and/or increase in nuclear changes (degeneration, pyknosis, vacuolization or abnormal chromatin condensation) to \leq 50% depth b. Nuclear enlargement/ cytoplasmic eosinophilia: Marked or Moderate to \geq 50% depth		ETOH	ETOH
Group D	1) Thickness: Thicker than the time-matched controls 2) Stromal matrix vacuolization: Some marked but moderate to 50% depth 3) Keratocytes: a. Upper stroma: Moderate cell loss and/or increase in nuclear changes (degeneration, pyknosis, vacuolization or abnormal chromatin condensation) to \leq 25% depth b. Nuclear enlargement/ cytoplasmic eosinophilia: Moderate/Marked to 50% depth		ETOH+F DPG+F Carbitol+F(2)	Fragrance ETOH+F DPM+F Carbitol+F
Group C	1) Thickness: Thicker than the time-matched controls 2) Stromal matrix vacuolization: Moderate to \leq 50% depth 3) Keratocytes: a. Upper stroma: Slight cell loss and/or increase in nuclear changes (degeneration, pyknosis, vacuolization or abnormal chromatin condensation) to \leq 25% depth b. Nuclear enlargement/ cytoplasmic eosinophilia: Moderate to \leq 50% depth	Carbitol+F DPM Carbitol	DPM+F DPM Carbitol	DPG+F Carbitol DPM
Group B	1) Thickness: Slightly thicker than the time-matched controls 2) Stromal matrix vacuolization: Moderate to \leq 30% depth 3) Keratocytes: a. Upper stroma: Normal (no cell loss or nuclear degeneration) b. Nuclear changes (enlargement)/ cytoplasmic eosinophilia: Moderate increase to \leq 30% depth	ETOH+F ETOH		BB+F
Group A	1) Thickness: Similar to the time-matched controls 2) Stromal matrix vacuolization: Slight or less increase to \leq 30% depth 3) Keratocytes:	Fragrance DPM+F Isopar M+F DPG+F	Fragrance Isopar M+F DPG+F Carbitol+F(1)	Isopar M + F Isopar M DPG BB

In Vitro	Characteristic Lesions	2-hour post-exposure	4-hour post-exposure	20-hour post-exposure
	a. Upper stroma: Normal (no cell loss or nuclear degeneration) b. Nuclear changes (enlargement)/ cytoplasmic eosinophilia: Slight or less increase to $\leq 20\%$ depth	BB+F Isopar M DPG BB	BB+F Isopar M DPG BB	

GRAPHICAL RESULTS: Appended Below

Figure 1. In-vivo Results – Opacity

Figure 2. In-vivo Results – Opacity X Area

Figure 3. In-vivo Results - MAS scores

Figure 4. BCOP Opacity Scores

Figure 5. BCOP Permeability Scores

Figure 6. BCOP In vitro Scores

RESULTS:

- Alone, the fragrance induced only slight corneal changes until 24 hours after treatment in vivo. In the BCOP assay, the similar time course was observed.
- Impact of Solvent:
 1. The addition of ethanol or DPM to the fragrance increased the in-vivo corneal scores (opacity and area) at 4 hours compared to the fragrance alone.
 2. The addition of ethanol, DPM, DPG, or carbitol to the fragrance increased the BCOP opacity and permeability scores (and histological changes) at 2 and 4 hours compared to fragrance alone.
 3. The addition of IsoPar M to the fragrance showed a strong mitigating effect on the overall irritancy of the fragrance in-vivo and BCOP assays.
 4. The addition of BB to the fragrance slowed the onset and reduced the overall irritation (in vivo) and BCOP opacity and permeability scores (and histological changes).
- The rapid onset of irritancy to the cornea (in-vivo) of ethanol, DPM, and carbitol was correctly predicted by the BCOP at 2 hours based on both the scores (opacity and permeability) and histological changes in the epithelium. The full expression of stromal changes took 4 hours in the BCOP (e.g., ethanol).
- Irritation Levels:
 1. Severe irritation was defined by sustained high Draize scores, high in-vitro scores, significant tissue damage (Group IV and E) and no recovery.
 2. Moderate irritation was defined at two levels with moderate tissue damage (Group III, II & D-B):
 - one level defined by moderate Draize and in-vitro scores, and seven days to clear and
 - second level defined by moderate Draize and in-vitro scores and three days to clear.
 3. Mild irritation was defined by mild Draize and in-vitro scores, minimal tissue damage (Group I & A) and rapid recovery (<3 days).
- Based on the histological changes over the three harvest times, the BCOP was able to distinguish a) the severe irritation potential of ethanol, b) the moderate irritation potentials of fragrance alone, fragrance + ethanol, fragrance + DPM, and fragrance + carbitol, c) the moderate but more rapidly clearing irritation of DPM and carbitol alone, d) the mild irritation of fragrance + Isopar M and fragrance + BB, and e) the very mild Isopar M, DPG, and BB alone. The exception is fragrance + DPG where the in vitro response was much more pronounced than the in vivo response.

In Vivo Histology : Appended below

Figures 7-8 show animal corneas treated with test substance.

Figure 7. In Vivo Group 1: BB & Isopar M

- (A) Center of the cornea, no changes observed (magnification 230x)
- (B) Area, away from limbus, showing separation of squamous epithelium (magnification 430x)

Figure 8. In Vivo Group 4: ETOH.

- (A) Central cornea showing loss of epithelium, inflammation, and marked increase in larger dark staining keratocyte nuclei in area of inflammatory infiltrate. Note - the cells were not in the upper 20% of the stroma (magnification 170x)
- (B) Area in denuded area showing keratocyte changes and swelling (magnification 430x)

BCOP Histology

Figures 9-12 show corneas treated for 3 minutes, at varying post exposure times with test substance in the BCOP.

Figure 9. BCOP Fragrance alone: 3-minute exposure, 2-hour post-exposure

- (A) Epithelium – Loss of surface squamous epithelium and some necrotic cells within the wing and basal layers (magnification 230x)(Epithelial Group B)
- (B) Stroma – Very similar to the time-matched negative control-treated corneas (magnification 430x)(Stromal Group A)

Figure 10. BCOP Fragrance alone: 3-minute exposure, 20-hour post-exposure

- (A) Epithelium – Loss of the squamous epithelium and marked nuclear pyknosis and cytoplasmic eosinophilia in the wing cell layer (magnification 230x) (Epithelial Group D)
- (B) Stroma – Marked collagen matrix vacuolization to 20% depth and keratocyte nuclear swelling and cytoplasmic eosinophilia (magnification 430x) (Stromal Group D)

Figure 11. BCOP ETOH alone: 3-minute exposure, 2-hour post-exposure

- (A) Epithelium – Marked cellular damage and separation between the basal cells and basal lamina (magnification 230x) (Epithelial Group E)
- (B) Stroma – Moderate collagen matrix vacuolization to mid depth and moderate increase in keratinocytes with nuclear pyknosis in the upper 25% of the stroma (magnification 430x) (Stromal Group B)

Figure 12. BCOP ETOH alone: 3-minute exposure, 4-hour post-exposure

- (A) Epithelium - Marked cellular damage and separation between the basal cells and basal lamina (magnification 230x) (Epithelial Group E)
- (B) Stroma – Marked collagen matrix vacuolization and a decrease in viable keratocytes extended to 30% depth. Marked keratocyte nuclear enlargement cytoplasmic eosinophilia was present at mid depth but is not shown in this micrograph (magnification 430x) (Stromal Group E)

CONCLUSIONS:

- Over the three harvest times, the BCOP assay was able to identify histological changes that characterize the treatment groups into severe (ethanol alone), moderate (2-stages), and mild categories. One treatment group (fragrance + DPG) was over predicted by the BCOP compared to the in vivo assay.
- Solvents have a major impact on the ocular irritation potential of fragrance mixtures. Both the degree and the time-course of the irritation can be impacted by the solvent.
- The time course of the tissue scores in vivo was similar to the time course of the histological changes in BCOP.
- When injury was significant enough, morphological changes in the keratocytes, specifically keratocyte nuclear enlargement (activation), were detectable in both the BCOP and in-vivo-treated corneas. Fini (1999) and collaborators have reported that certain morphological changes in keratocytes are associated with phenotypic changes (activation) and subsequent undesirable fibrotic scarring.
- BCOP model was more consistent in its response to a given treatment than the in vivo model (Table 1-3).

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ACKNOWLEDGEMENTS

The authors wish to thank the general staffs at both the Institute for In Vitro Sciences, Inc. and the Charles River Laboratories, Inc. for their assistance on this project.

Figure 1. In Vivo Opacity Scores

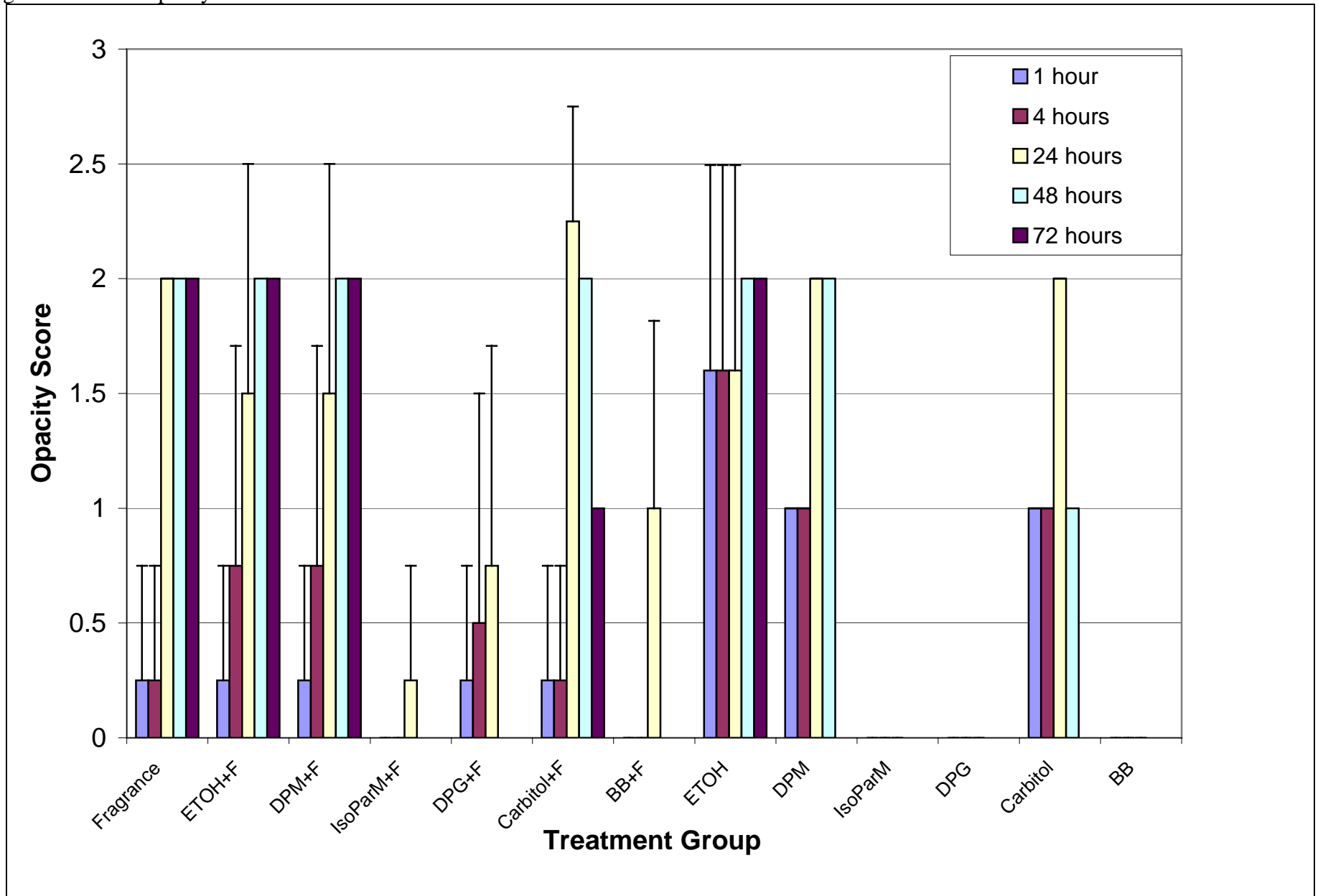


Figure 2. In Vivo Corneal Scores (Opacity x Area)

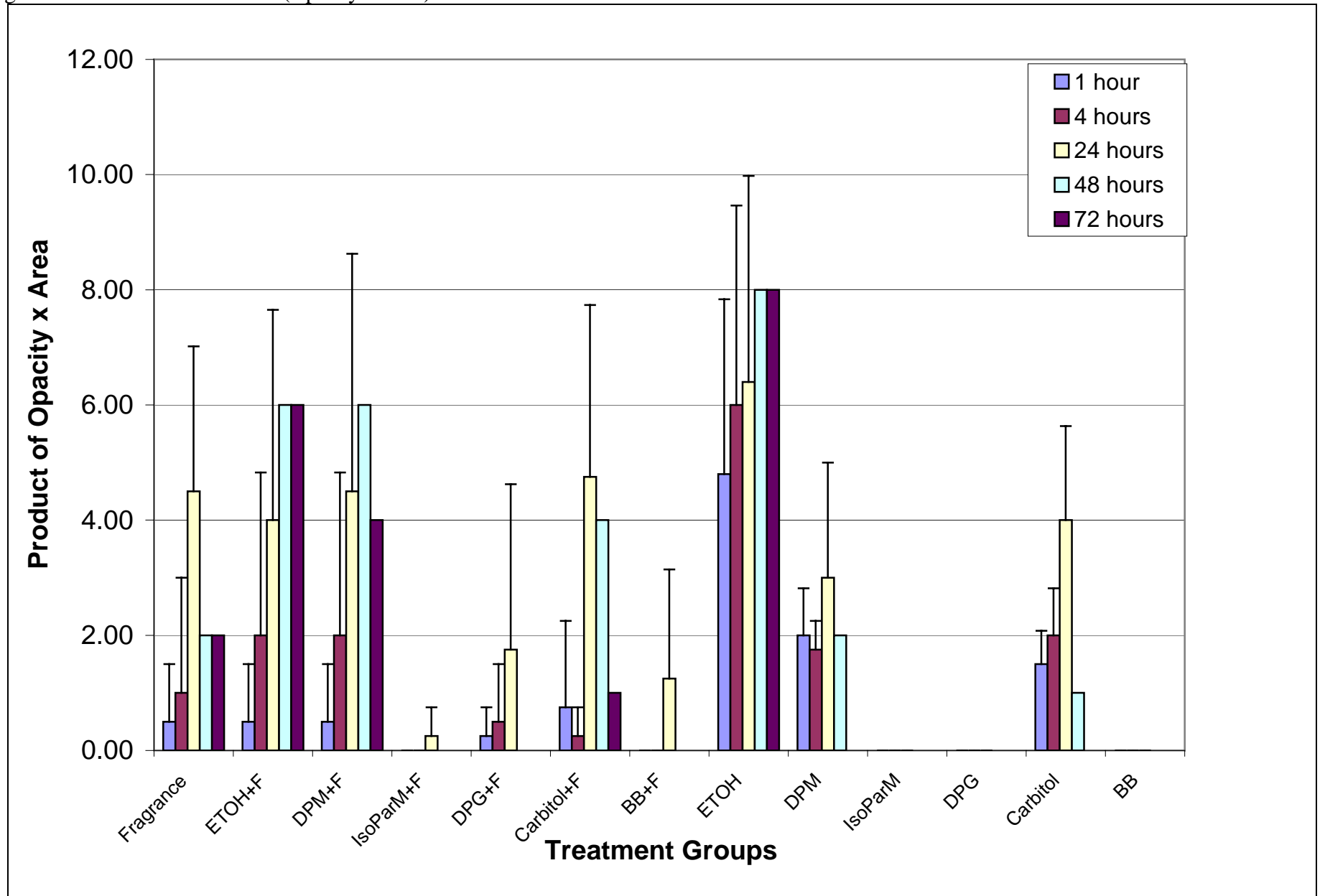


Figure 3. In Vivo MAS Scores

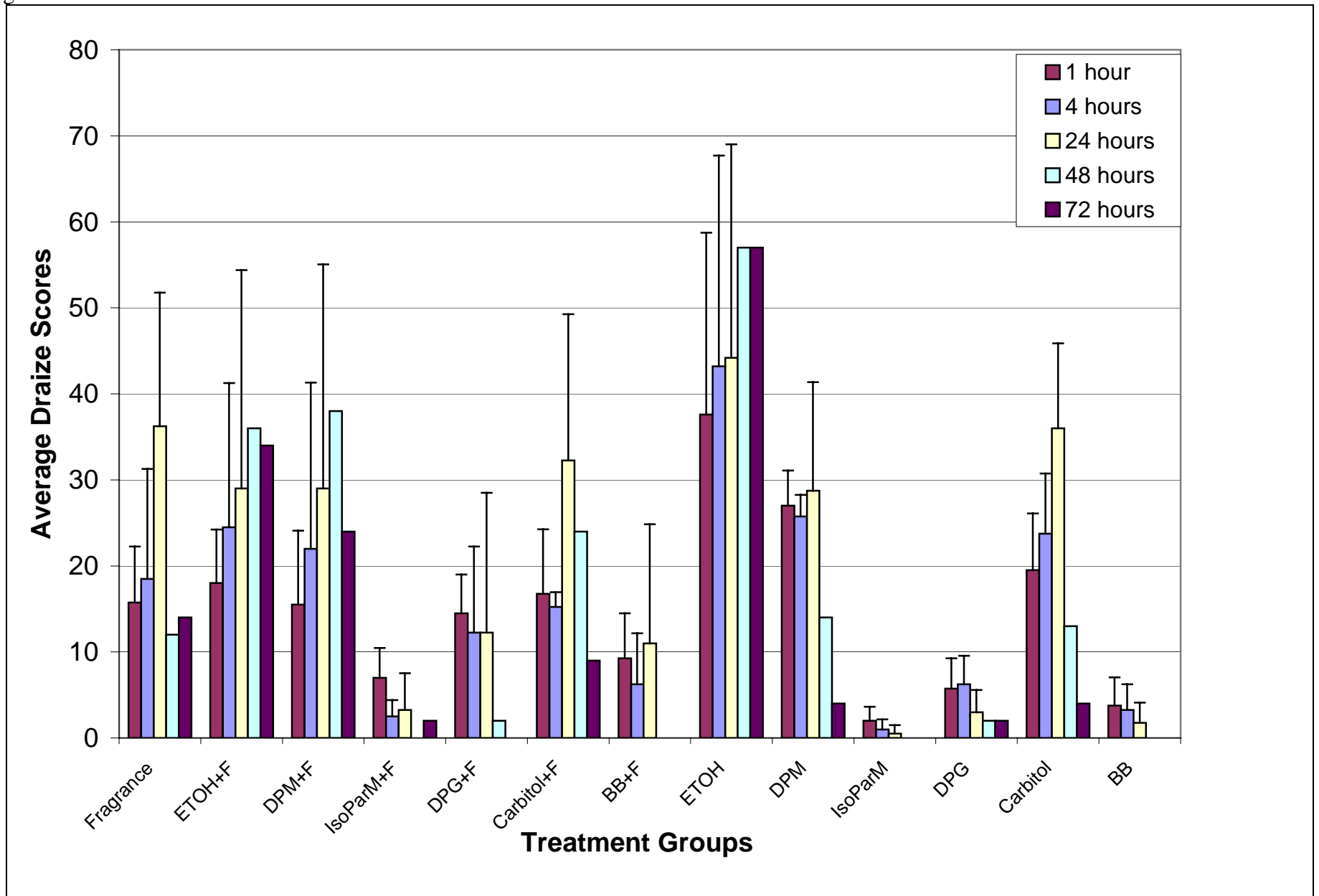


Figure 4. BCOP Opacity Scores

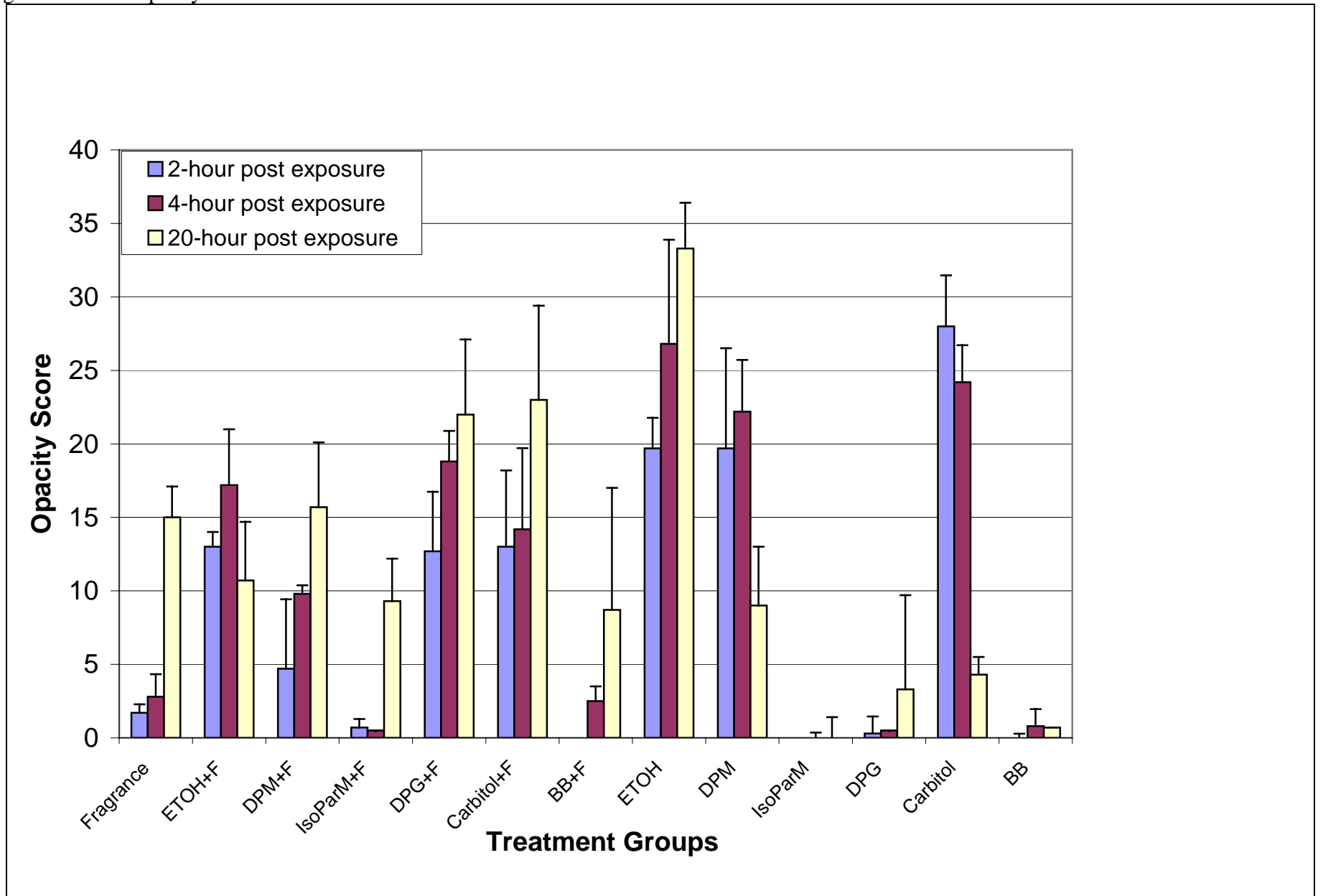


Figure 5. BCOP Permeability Scores

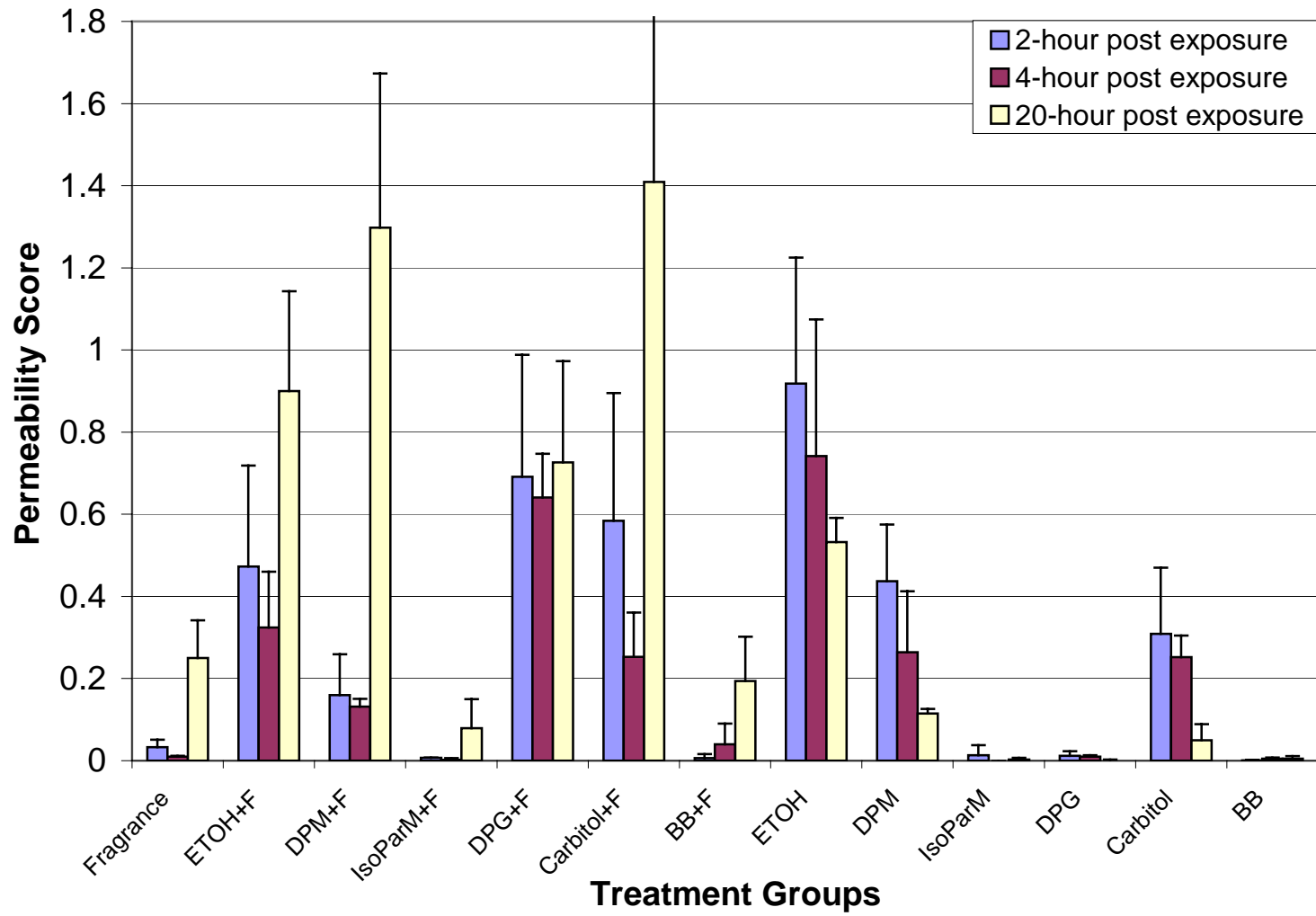


Figure 6. BCOP In Vitro Scores

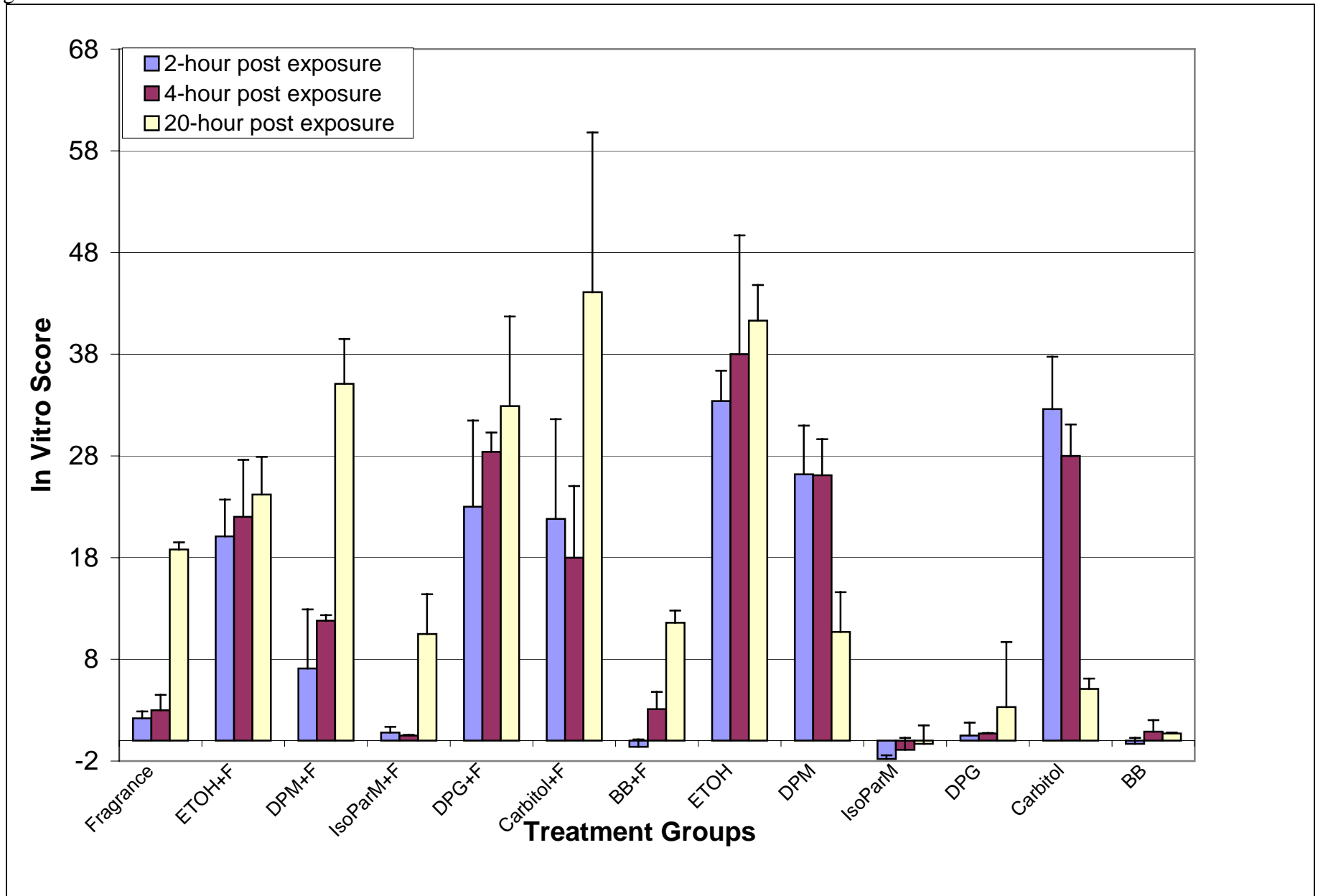
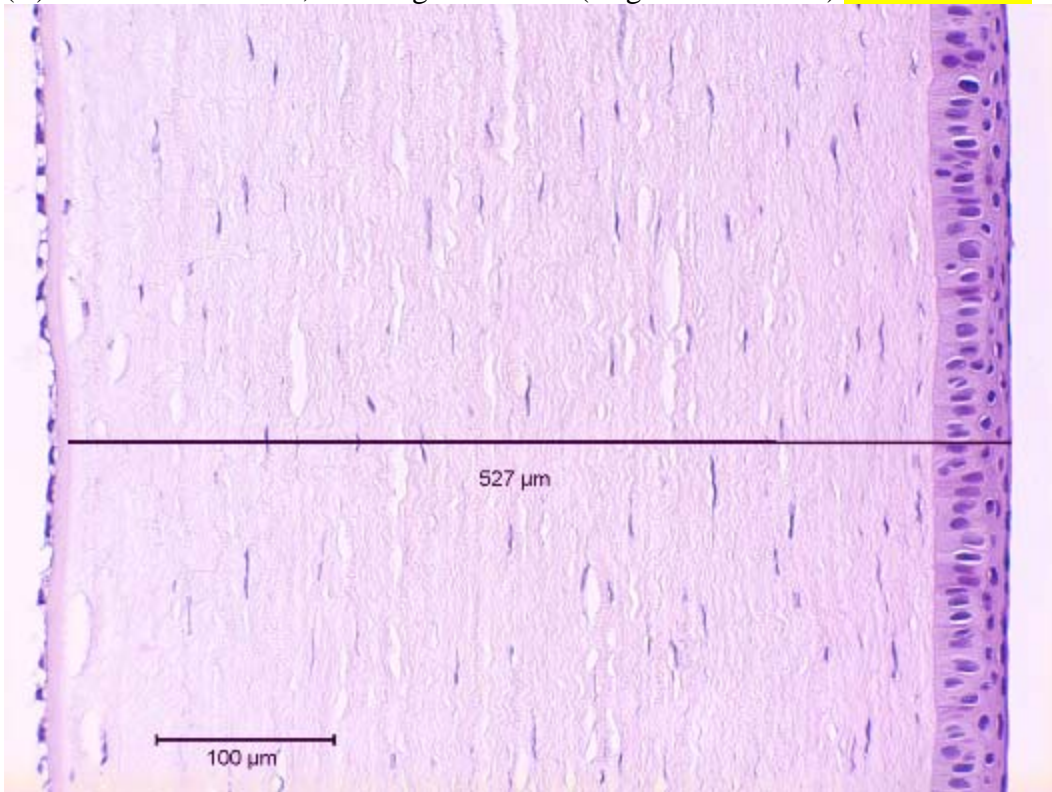


Figure 7. In Vivo Group 1: BB & Isopar M

(A) Center of the cornea, no changes observed (magnification 230x) [File 100902-77](#)

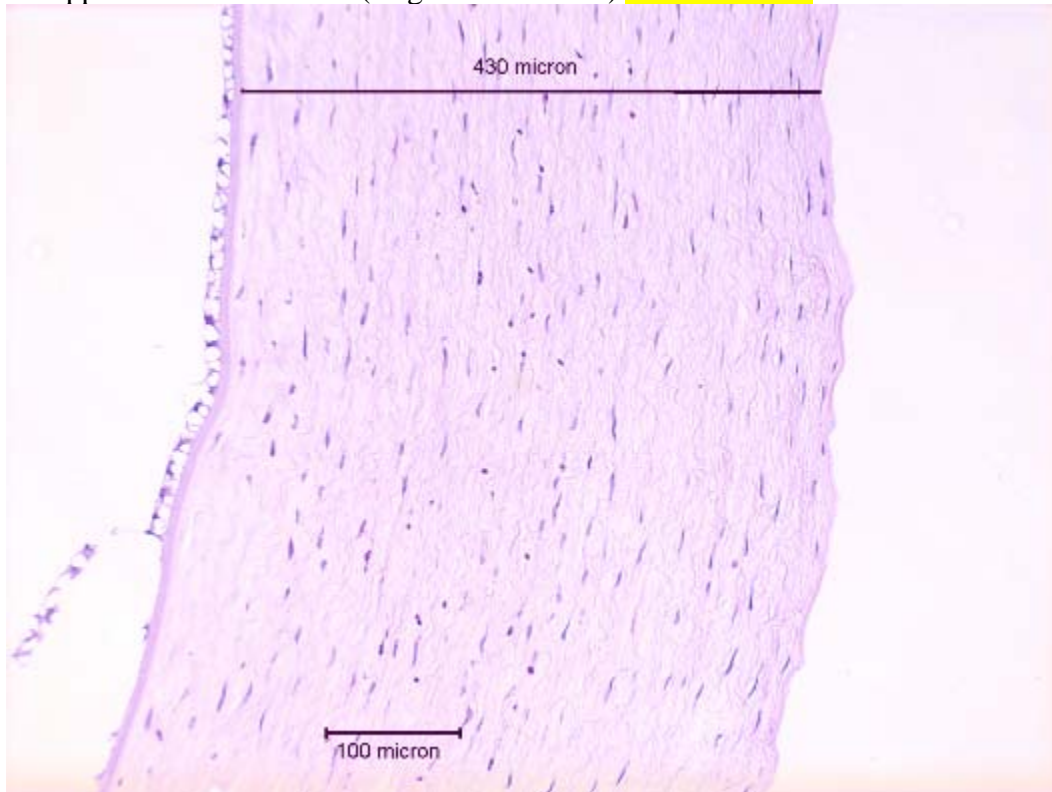


(B) Area, away from limbus, showing separation of squamous epithelium (magnification 430x) **File 100902-61**



Figure 8. In Vivo Group 4: ETOH.

(A) Central cornea showing loss of epithelium, inflammation, and marked increase in larger dark staining keratocyte nuclei in area of inflammatory infiltrate. Note - the cells were not in the upper 20% of the stroma (magnification 170x) [File 100902-41](#)



(B) Area in denuded area showing keratocyte changes and swelling (magnification 430x) File 100902-42

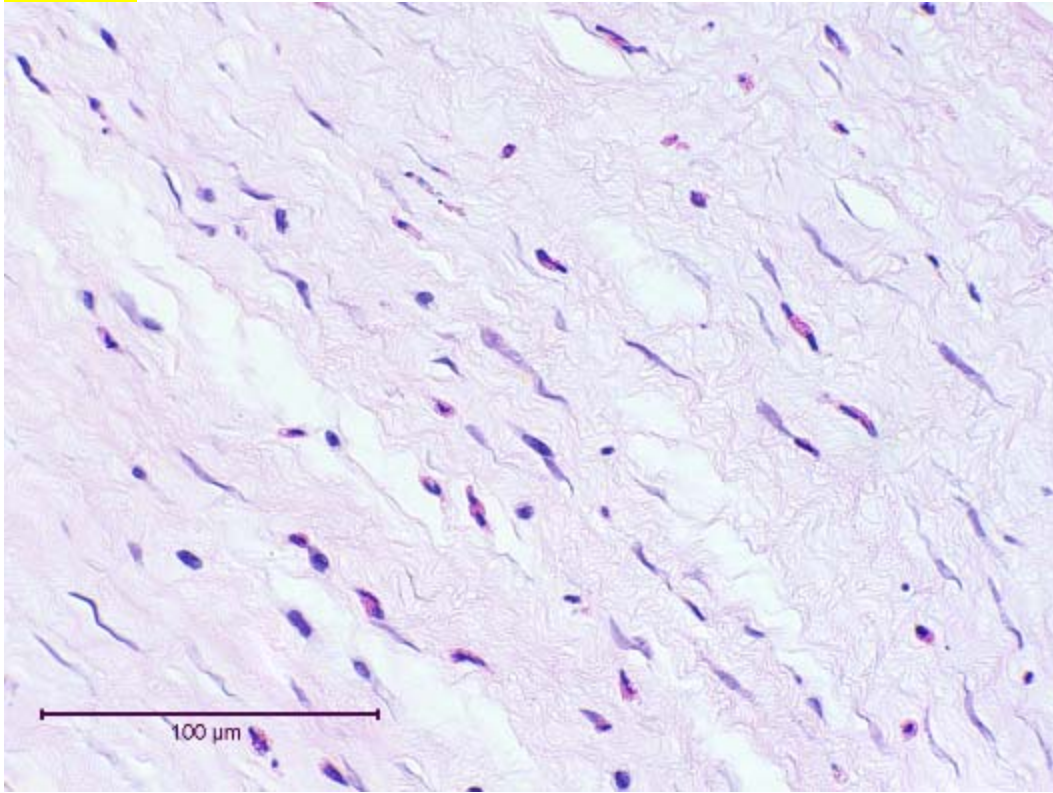
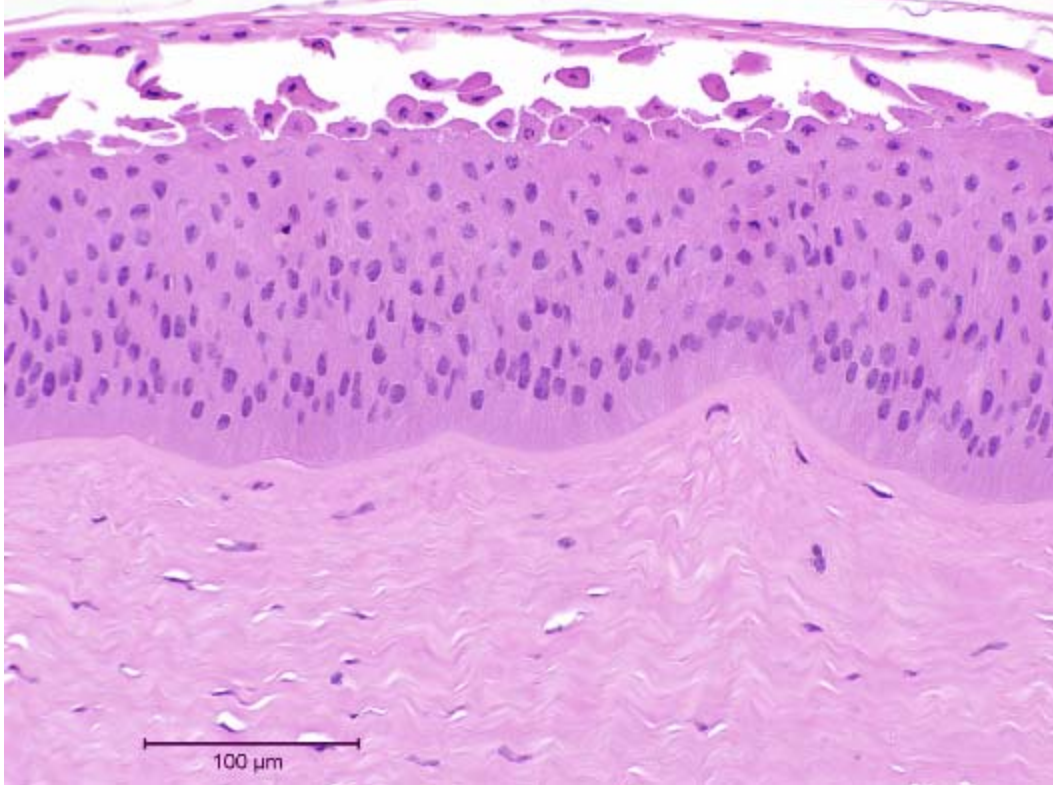


Figure 9. BCOP Fragrance alone: 3-minute exposure, 2-hour post-exposure

(A) Epithelium – Loss of surface squamous epithelium and some necrotic cells within the wing and basal layers (magnification 230x)(Epithelial Group B) [File 082903-08](#)



(B) Stroma – Very similar to the time-matched negative control-treated corneas (magnification 430x)(Stromal Group A) [File 082903-10](#)

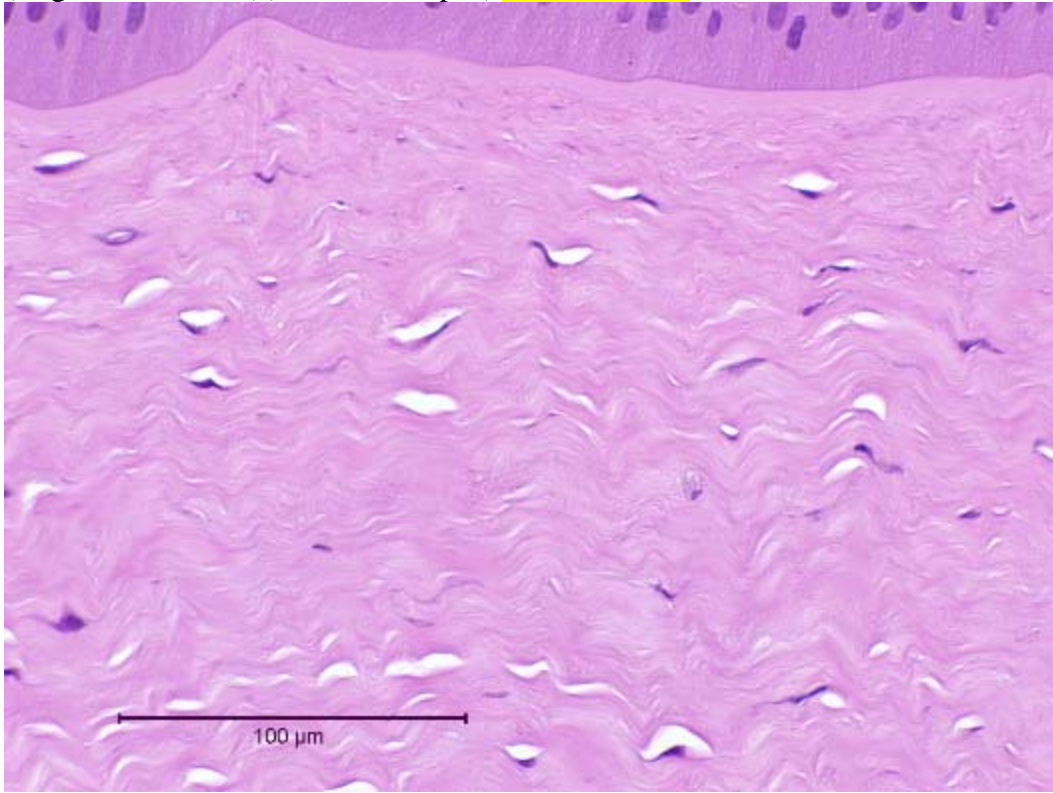
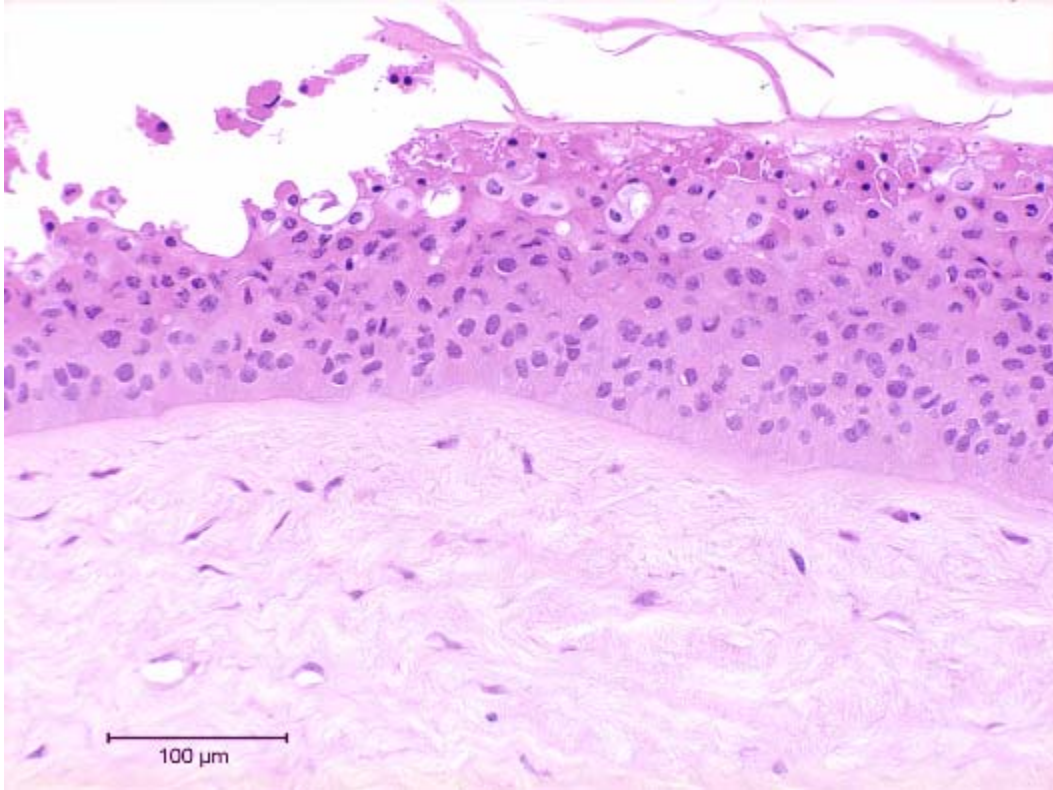


Figure 10. BCOP Fragrance alone: 3-minute exposure, 20-hour post-exposure

(A) Epithelium – Loss of the squamous epithelium and marked nuclear pyknosis and cytoplasmic eosinophilia in the wing cell layer (magnification 230x) (Epithelial Group D) [File 111702-12](#)



(B) Stroma – Marked collagen matrix vacuolization to 20% depth and keratocyte nuclear swelling and cytoplasmic eosinophilia (magnification 430x) (Stromal Group D) **File 111702-14**

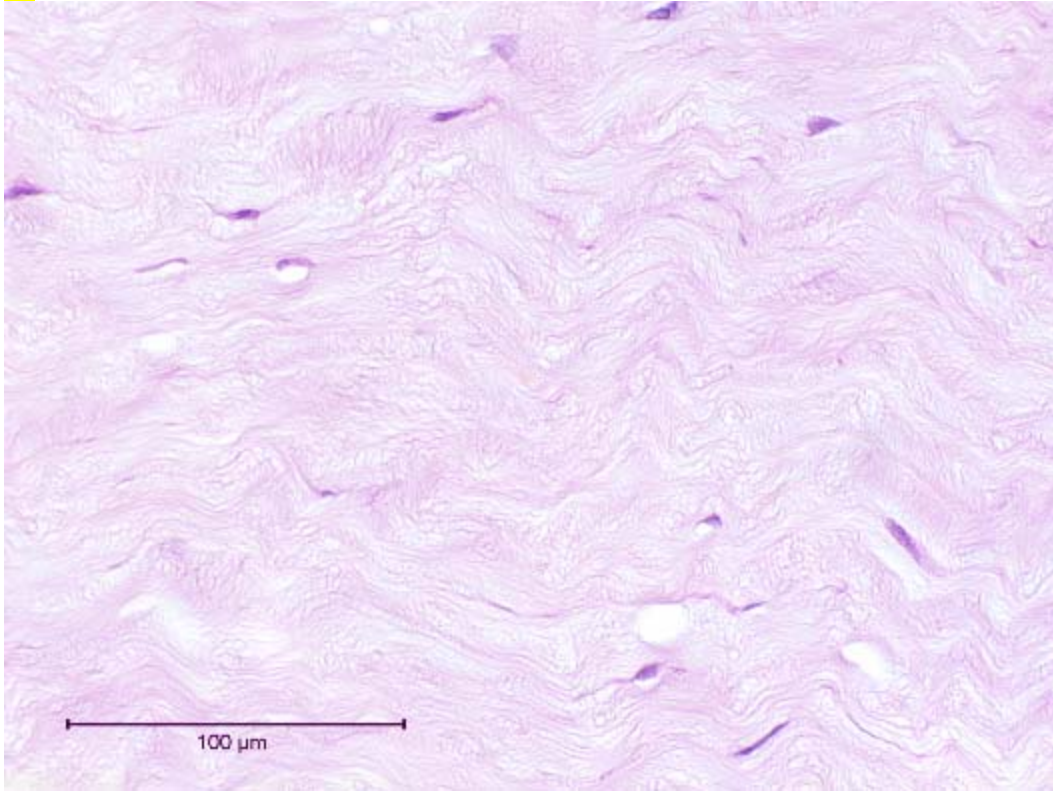
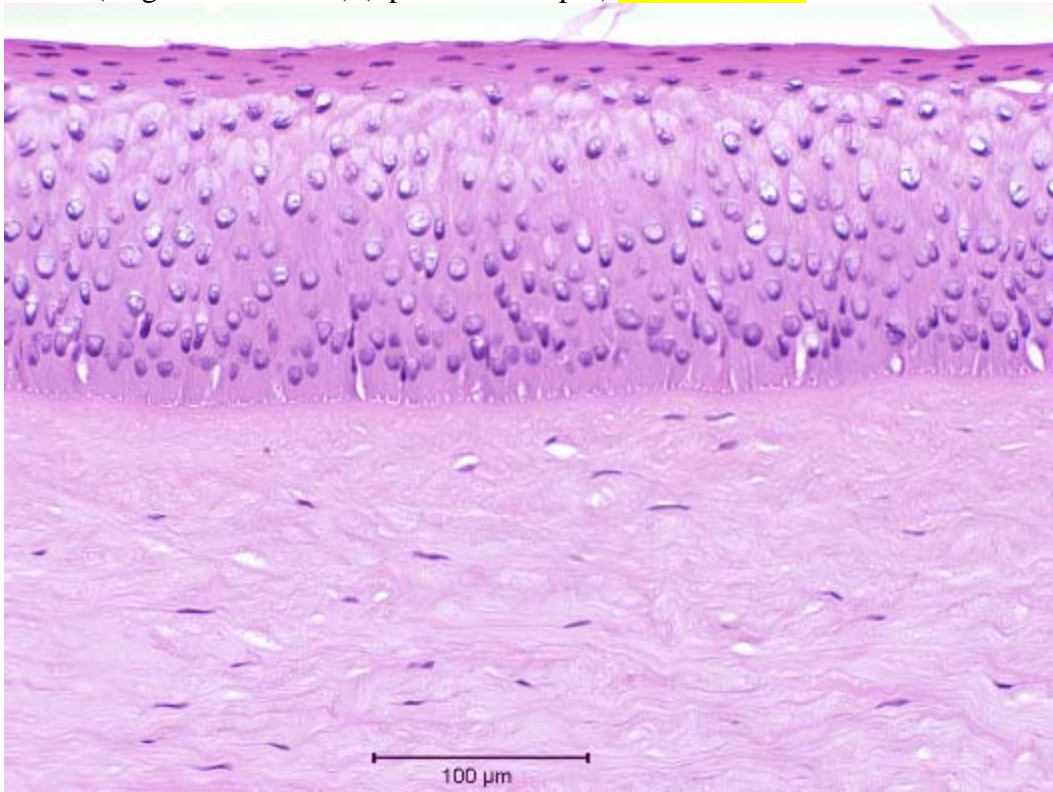


Figure 11. BCOP ETOH alone: 3-minute exposure, 2-hour post-exposure

(A) Epithelium – Marked cellular damage and separation between the basal cells and basal lamina (magnification 230x) (Epithelial Group E) [File 082903-35](#)



(B) Stroma – Moderate collagen matrix vacuolization to mid depth and moderate increase in keratinocytes with nuclear pyknosis in the upper 25% of the stroma (magnification 430x)
(Stromal Group B) [File 082903-37](#)

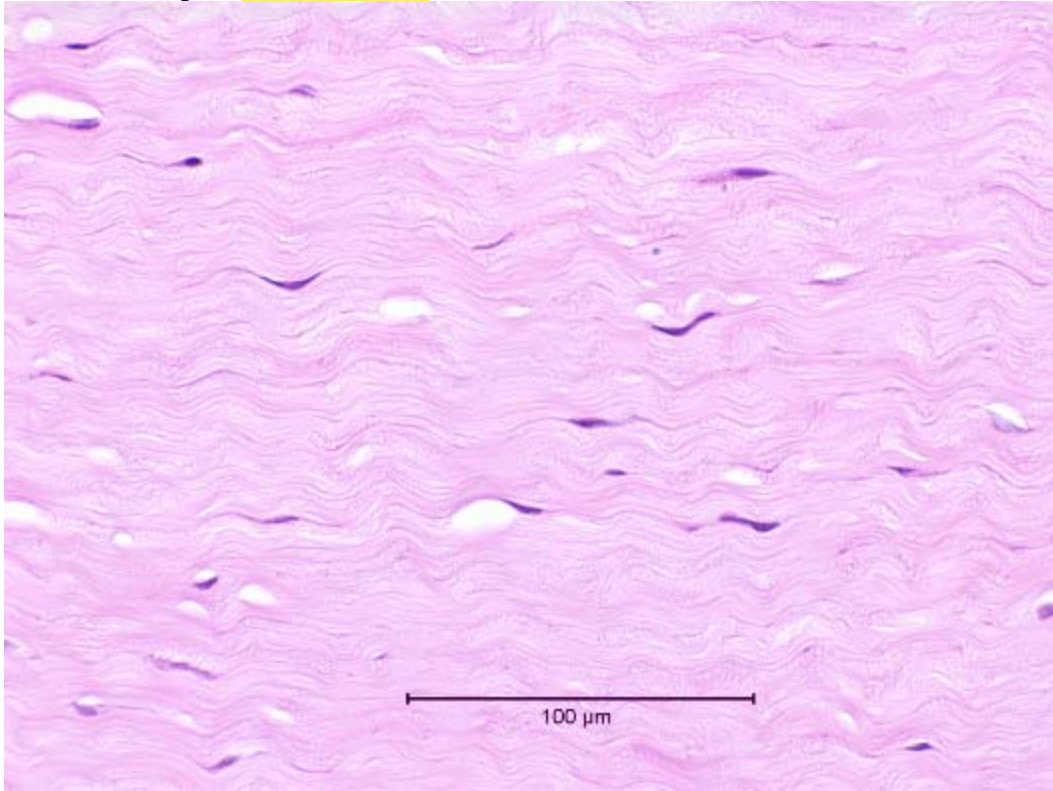
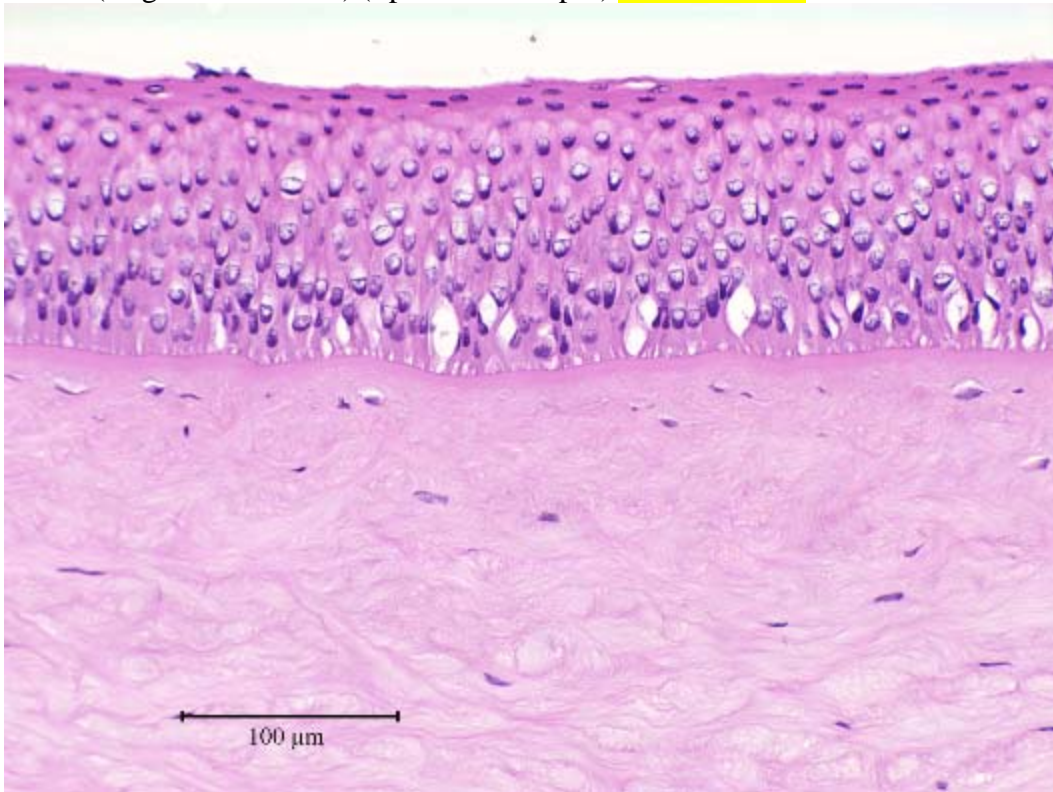
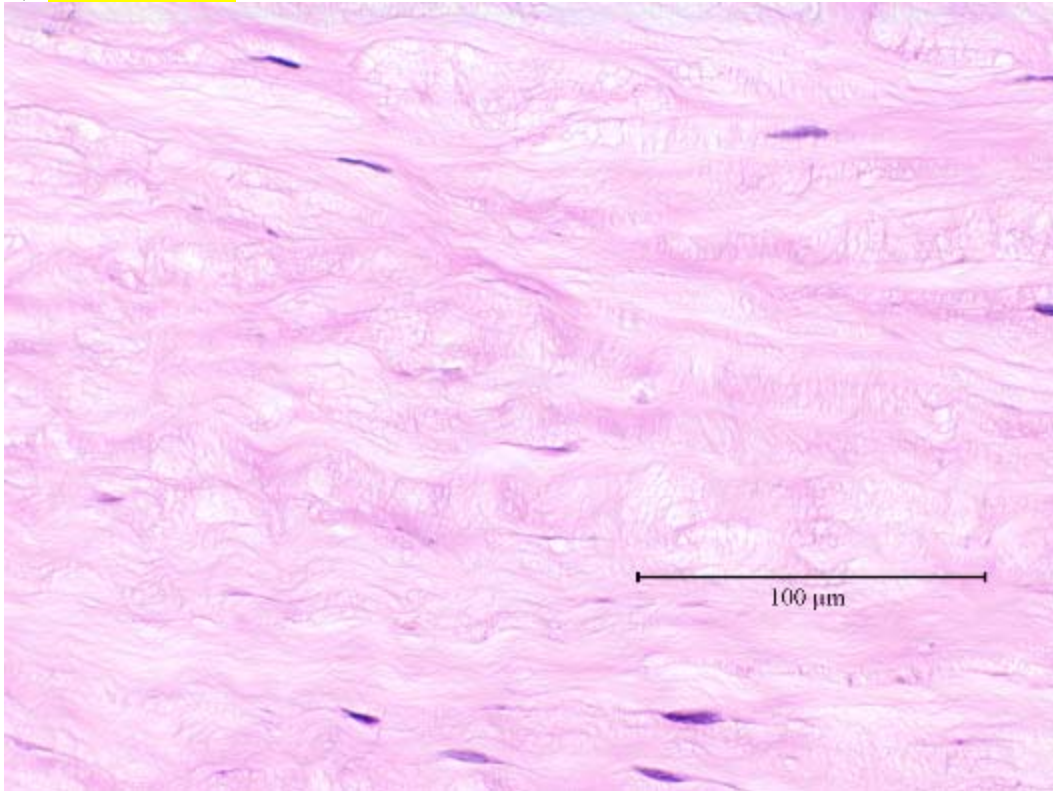


Figure 12. BCOP ETOH alone: 3-minute exposure, 4-hour post-exposure

(A) Epithelium - Marked cellular damage and separation between the basal cells and basal lamina (magnification 230x) (Epithelial Group E) [File 091503-43](#)



(B) Stroma – Marked collagen matrix vacuolization and a decrease in viable keratocytes extended to 30% depth. Marked keratocyte nuclear enlargement cytoplasmic eosinophilia was present at mid depth but is not shown in this micrograph (magnification 430x) (Stromal Group E) [File 091503-45](#)



FORMULAS

Test Material #	Group	Raw Material	Percentage
1	Fragrance	Benzyl acetate	25
		linalool	25
		Dihydroxymyrcenol	25
		Verdox	25
2	Ethanol	Ethanol	100
3	Dowanol DPM	Dowanol DPM	100
4	Isopar M	Isopar M	100
5	Dipropylene glycol	Dipropylene glycol	100
6	Carbitol	Carbitol	100
7	Benzyl benzoate	Benzyl benzoate	100
8	Ethanol + Fragrance	Ethanol	20
		Benzyl acetate	20
		linalool	20
		Dihydroxymyrcenol	20
		Verdox	20
9	Dowanol DPM + Fragrance	Dowanol DPM	20
		Benzyl acetate	20
		linalool	20
		Dihydroxymyrcenol	20
		Verdox	20
10	Isopar M + Fragrance	Isopar M	20
		Benzyl acetate	20
		linalool	20
		Dihydroxymyrcenol	20
		Verdox	20
11	Dipropylene glycol + Fragrance	Dipropylene glycol	20
		Benzyl acetate	20
		linalool	20
		Dihydroxymyrcenol	20
		Verdox	20
12	Carbitol + Fragrance	Carbitol	20
		Benzyl acetate	20
		linalool	20
		Dihydroxymyrcenol	20
		Verdox	20

FORMULAS

Test Material #	Group	Raw Material	Percentage
13	Benzyl benzoate + Fragrance	Benzyl benzoate	20
		Benzyl acetate	20
		linalool	20
		Dihydroxymyrcenol	20
		Verdox	20

Appendix G2

**Dataset Received from S.C. Johnson & Son, Inc. in Support of
Cuellar et al. (2002) Poster Presentation**

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A FAMILY COMPANY

S.C. Johnson & Son, Inc.
Worldwide Consumer Products, RD & E
Global Safety Assessment and Regulatory Affairs, Product Toxicology
MS 139 1525 Howe Street, Racine WI 53403

September 3, 2004

Christina Inhof, MSPH
Senior Project Coordinator/Technical Writer ILS, Inc.
NICEATM
P.O. Box 12233
NIEHS MD EC-17
Research Triangle Park, NC 27709

Christina,

Hi! How are you? I am happy to be submitting the data on benchmark and fragrance formulations, which were partially discussed in the poster citation listed below:

Cuellar, N., Merrill, J.C., Clear, M.L., Mun G., and Harbell J.W. 2002. The application of benchmarks for the evaluation of the potential ocular irritancy of aerosol fragrances. *The Toxicologist* 66(1-S): 243-244.

Included with this submission are the following documents:

1. Cover letter
2. Data spreadsheet
3. Fragrance graphs
4. Coded formula spreadsheet

Study Protocols:

Standard Draize protocol was used for 4 of the in-vivo studies. The EPA aerosol protocol was used for test material #3. Standard BCOP protocol was used for the in-vitro work at IIVS. BCOP exposure times were 3 and 10 minutes with post exposure of 2 hours.

Formula Spreadsheet:

The formulas listed in this spreadsheet are coded similarly to past submissions. For benchmarks, test material number is the unique sample number whereas the group description is referenced in the poster as type of benchmark. Test material #3 and #4 (Alcohol-based benchmark) is not listed in the poster. For fragrance formulas, test material denotes the category (formula) whereas the group describes the formula form (i.e aerosol vs membrane (gel)). Fragrances formulas are referenced in the poster. For both benchmarks and formulations, raw materials are listed followed by their percentages.

Poster:

Benchmark poster not included. John Harbell previously sent it to you.

Graphs:

Graphs plot the BCOP total score per each unique fragrance formulation. Graphs include reference benchmarks (see formula spreadsheet) and the ethanol control. The bars show one standard deviation from the mean value for each benchmark and the ethanol. Please note that the ethanol values displayed on the 3-minute exposure graphs are for a 3-minute exposure to ethanol (not the 10-minute exposure ethanol that was performed as the positive control). There are 9 tabs in this spreadsheet. Graphs are labeled per form ((2 for aerosol and 2 for membrane (gel)) and exposure time (3 or 10 minutes) in tabs 1-8. The first two graphs refer to the aerosol formulas and the second two graphs refer to the membrane. Each graph includes the corresponding raw data in the next tab. There are 44 aerosol formulas depicted in the aerosol graphs and 36 membrane formulas depicted in the membrane graphs. The final tab describes the basic statistics on the ethanol control and each benchmark by exposure time.

Data Worksheet:

The data worksheet consists of 4 tabs at the bottom of the page. We are including all tabs to clearly demonstrate how we analyzed the data into the GHS and EPA categories in the summary spreadsheet shown in tab #4.

Summary spreadsheet:

The summary spreadsheet is sorted by test material. The test material number refers to the benchmark formula or ethanol listed in the formula spreadsheet. GHS and EPA categories are in the next 8 columns in yellow. The last 2 columns consist of the mean BCOP total scores (3 and 10 minute) in blue. EPA and GHS criteria are summarized in this spreadsheet.

Data was analyzed per formula. Raw data scores from the first three days and days to clear per each of 6 rabbits were randomly put into combinations of three and categorized accordingly based on EPA or GHS criteria. This analysis resulted in a total of 20 combinations per formula. Each combination was listed in the appropriate GHS or EPA category. Scoring assumptions are also listed in this spreadsheet based on protocol differences.

Protocol used for the BCOP assay was the same for all benchmarks and ethanol formulas. In-vivo studies were conducted using the standard Draize protocol with the exception of the ethanol/fragrance benchmark. The ethanol/fragrance benchmark utilized the EPA aerosol dosing Draize protocol.

The ethanol/fragrance benchmark is used to evaluate specific aerosol formulations. This benchmark shows that even though the formulation would be irritating in the standard Draize Assay, the product is provided in a form that restricts exposure to the aerosol route by limiting exposure via a metered dose. The metered dosing approach demonstrates that new formulations would not exceed the irritation potential of the benchmark.

As shown in the graphs and the summary table, the BCOP is able to rank irritation of a variety of formulations in comparison to the benchmarks. Severe irritants can be identified using this methodology. The fragrance level in the formula does impact the irritation potential of the formula.

September 2, 2004

These data demonstrate the importance of assessing all new formulations relative to an appropriate fixed benchmark.

If you have any questions or comments on this data set, please feel free to contact either Judith Swanson or myself at the following:

Nicole Cuellar
(262) 260-6916
ncuellar@scj.com

Judith Swanson
(262) 260-2688
jeswanso@scj.com

Sincere regards,

A handwritten signature in cursive script that reads "Nicole Cuellar".

Nicole Cuellar
Sr. Research Toxicologist

In Vivo Data - S.C. Johnson Submission Dated September 3, 2004

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	F38948	#1	24	1	2	1	2	2	2	27	EPA
			48	1	1	0	2	1	0	11	14
			72	1	1	0	0	1	0	7	GHS
			7 days	0	0	0	2	0	0	4	14
			14 days	0	0	0	0	0	0	0	
			21 days							0	
GHS Tissue	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS
	F38948	#1	27	1.0	1.3	0.3	1.3	1.3	0.7	14	14
Summary block used analysis of the twenty combinations	ANIMAL ID										
	1	#1	27	1.0	1.3	0.3	1.3	1.3	0.7	14	14
	2	#1	34	0.7	1.3	0.3	2.3	1.3	0.7	14	14
	3	#1	37	0.7	2.0	0.3	2.0	1.3	0.7	7	14
	4	#1	35	1.0	2.3	1.0	2.0	1.3	0.3	7	14
	5	#1	39	1.0	2.7	1.0	2.7	1.3	2.0	14	14
6	#1	30	1.0	1.7	1.0	2.7	1.3	0.3	14	14	
	Dose Vol	0.1									

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	R2266	#2	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days								0	2
			14 days								0	
			21 days								0	
GHS Tissue	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS	
	R2266	#2	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
Summary block used analysis of the twenty combinations	ANIMAL ID											
	1	#2	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	2	#2	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	3	#2	4	0.0	0.0	0.0	0.7	0.3	0.0	0	3	
	4	#2	2	0.0	0.0	0.0	0.7	0.0	0.0	0	3	
	5	#2	2	0.0	0.0	0.0	0.7	0.0	0.0	0	3	
6	#2	4	0.0	0.0	0.0	0.7	0.7	0.0	0	3		
	Dose Vol	0.1										

In Vivo Data - S.C. Johnson Submission Dated September 3, 2004

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	F38949	#1	24	1	3	1	3	2	2	34	EPA
			48	1	1	0	2	1	0	11	14
			72	0	0	0	2	1	0	6	GHS
			7 days	1	1	0	1	0	0	7	14
			14 days	0	0	0	0	0	0	0	0
			21 days							0	0
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	F38949	#1	34	0.666667	1.333333	0.333333	2.333333333	1.333333333	0.666666667	14	14
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combin- ation block #1	1,2,3	0.833333	0.333333	2.166667	1.333333	14	14	Combin- ation block #2	1,3,4	1	0.666667
	GHS Rating	4	4	2	4	14	14		GHS Rating	2	4
	1,2,4	1	0.666667	2.166667	1.333333	14	14		1,3,5	1	0.666667
	GHS Rating	2	4	2	4	14	14		GHS Rating	2	4
	1,2,5	1	0.666667	2.5	1.333333	14	14		1,3,6	1	0.666667
	GHS Rating	2	4	2	4	14	14		GHS Rating	2	4
	1,2,6	1	0.666667	2.5	1.333333	14	14		1,4,5	1	1
GHS Rating	2	4	2	4	14	14	GHS Rating	2	4		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	R2317	#2	24	0	0	0	1	0	0	2	EPA
			48	0	0	0	0	0	0	0	0
			72							0	GHS
			7 days							0	2
			14 days							0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	R2317	#2	2	0	0	0	0.5	0	0	0	2
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combin- ation block #1	1,2,3	0	0	0.583333	0.166667	0	3	Combin- ation block #2	1,3,4	0	0
	GHS Rating	4	4	4	4	0	3		GHS Rating	4	4
	1,2,4	0	0	0.583333	0	0	3		1,3,5	0	0
	GHS Rating	4	4	4	4	0	3		GHS Rating	4	4
	1,2,5	0	0	0.583333	0	0	3		1,3,6	0	0
	GHS Rating	4	4	4	4	0	3		GHS Rating	4	4
	1,2,6	0	0	0.583333	0.333333	0	3		1,4,5	0	0
GHS Rating	4	4	4	4	0	3	GHS Rating	4	4		

In Vivo Data - S.C. Johnson Submission Dated September 3, 2004

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	F38951	#1	24	1	4	1	2	2	1	35	EPA
			48	1	2	1	2	1	0	21	7
			72	1	1	1	2	1	0	16	GHS
			7 days	0	0	0	1	0	0	2	14
			14 days	0	0	0	0	0	0	0	0
			21 days	0	0	0	0	0	0	0	0
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS
	F38951	#1	35	1	2.333333	1	2	1.333333333	0.333333333	7	14
	Combinatio Opacity			Iris	Redness	Chemosis	DIC EPA	DIC GHS	Combinations	Opacity	Iris
Combina- tion block #4	2,3,6	0.8	0.7	2.5	1.3	14	14	Combina- tion block #5	3,4,5	1.0	1.0
	GHS Rating	4	4	2	4	14	14	GHS Rating	2	4	
	2,4,5	1.0	1.0	2.5	1.3	14	14	3,4,6	1.0	1.0	
	GHS Rating	2	4	2	4	14	14	GHS Rating	2	4	
	2,4,6	1.0	1.0	2.5	1.3	14	14	3,5,6	1.0	1.0	
	GHS Rating	2	4	2	4	14	14	GHS Rating	2	4	
	2,5,6	1.0	1.0	2.7	1.3	14	14	4,5,6	1.0	1.0	
GHS Rating	2	4	2	4	14	14	GHS Rating	2	2		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS
0.1	R2299	#2	24	0	0	0	1	0	0	2	EPA
			48	0	0	0	1	0	0	2	0
			72	0	0	0	0	0	0	0	GHS
			7 days	0	0	0	0	0	0	0	3
			14 days	0	0	0	0	0	0	0	0
			21 days	0	0	0	0	0	0	0	0
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS
	R2299	#2	2	0	0	0	0.66666667	0	0	0	3
	Combinatio Opacity			Iris	Redness	Chemosis	DIC EPA	DIC GHS	Combinations	Opacity	Iris
Combina- tion block #4	2,3,6	0.0	0.0	0.7	0.5	0	3	Combina- tion block #5	3,4,5	0.0	0.0
	GHS Rating	4	4	4	4	0	3	GHS Rating	4	4	
	2,4,5	0.0	0.0	0.7	0.0	0	3	3,4,6	0.0	0.0	
	GHS Rating	4	4	4	4	0	3	GHS Rating	4	4	
	2,4,6	0.0	0.0	0.7	0.3	0	3	3,5,6	0.0	0.0	
	GHS Rating	4	4	4	4	0	3	GHS Rating	4	4	
	2,5,6	0.0	0.0	0.7	0.3	0	3	4,5,6	0.0	0.0	
GHS Rating	4	4	4	4	0	3	GHS Rating	4	4		

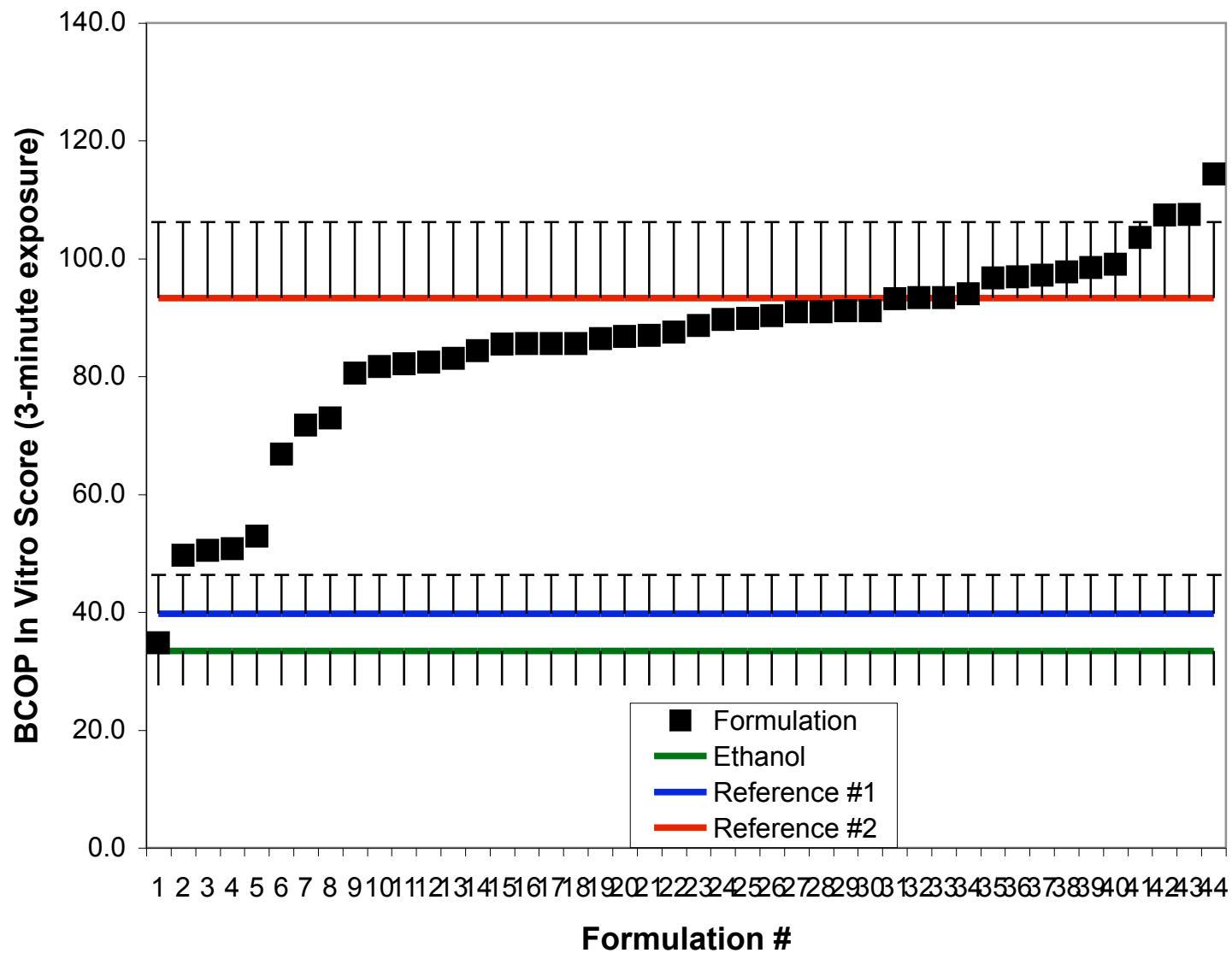
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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F38952	#1	24	1	4	1	2	2	3	39	EPA	
			48	1	3	1	3	1	2	32	14	
			72	1	1	1	3	1	1	20	GHS	
			7 days	1	1	0	1	1	0	9	14	
			14 days	0	0	0	0	0	0	0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS	
	F38952	#1	39	1	2.666667	1	2.6666667	1.333333333	2	14	14	
Redness	Chemosis	DIC EPA	DIC GHS									
2.3	1.3	14	14				Summary	1,2,3	2	14		
2	4	14	14				#1	1,2,4	2	14		
2.3	1.3	14	14					1,2,5	2	14		
2	4	14	14					1,2,6	2	14		
2.7	1.3	14	14					1,3,4	2	14		
2	4	14	14					1,3,5	2	14		
2.7	1.3	14	14					1,3,6	2	14		
2	4	14	14					1,4,5	2	14		
2.7	1.3	14	14					1,4,6	2	14		
2	4	14	14					1,5,6	2	14		
									2	14		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	R2275	#2	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	1	0	0	2	0	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DIC EPA	DIC GHS	
	R2275	#2	2	0	0	0	0.6666667	0	0	0	3	
Redness	Chemosis	DIC EPA	DIC GHS									
0.7	0.2	0	3				Summary	1,2,3	4	3		
4	4	0	3				#2	1,2,4	4	3		
0.7	0.5	0	3					1,2,5	4	3		
4	4	0	3					1,2,6	4	3		
0.7	0.5	0	3					1,3,4	4	3		
4	4	0	3					1,3,5	4	3		
0.7	0.3	0	3					1,3,6	4	3		
4	4	0	3					1,4,5	4	3		
								1,4,6	4	3		
								1,5,6	4	3		

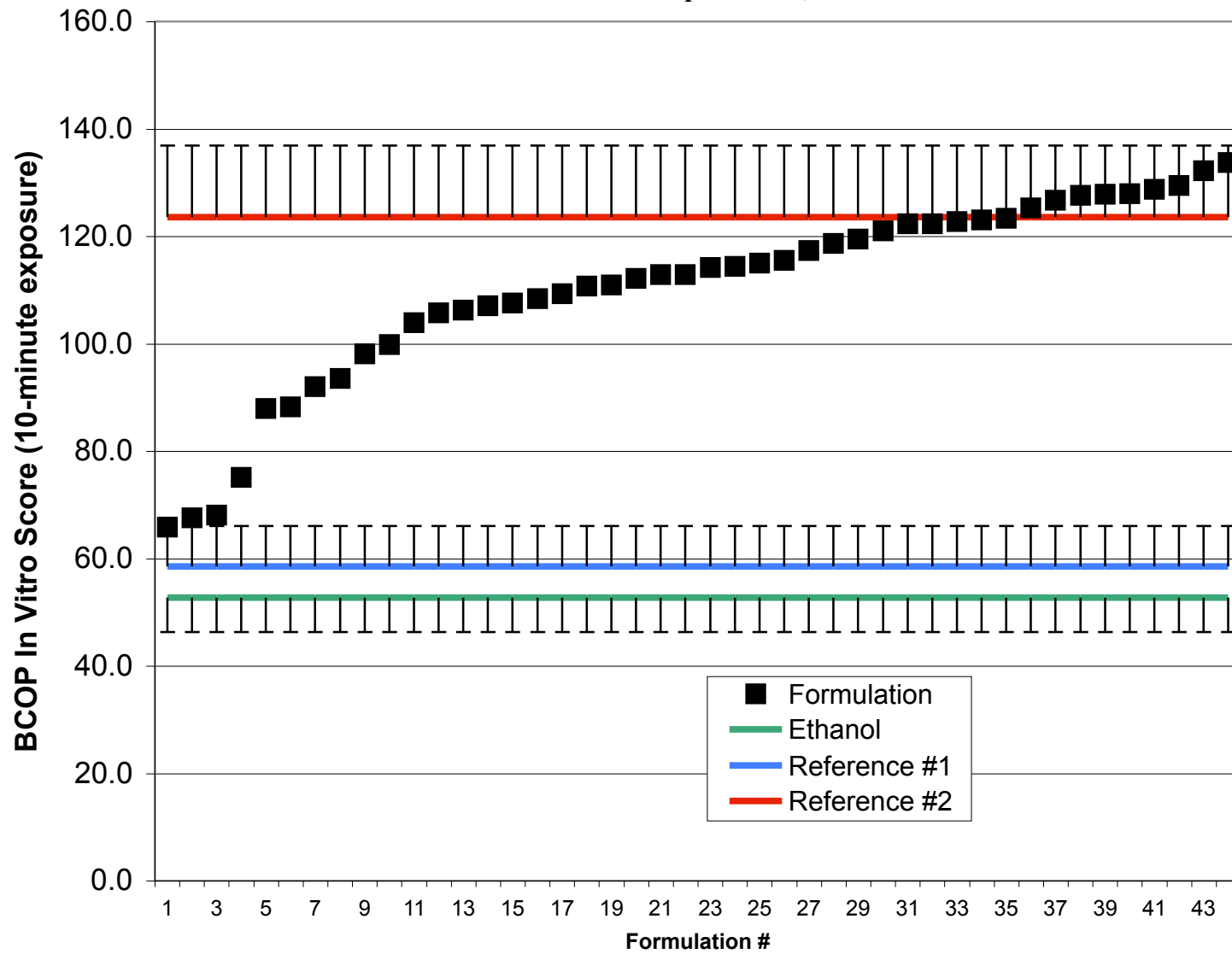
In Vivo Data - S.C. Johnson Submission Dated September 3, 2004

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F38953	#1	24	1	3	1	2	2	1	30	EPA	
			48	1	1	1	3	1	0	18	14	
			72	1	1	1	3	1	0	18	GHS	
			7 days	0	0	0	2	1	0	6	14	
			14 days	0	0	0	0	0	0	0	0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	F38953	#1	30	1	1.666667	1	2.66666667	1.333333333	0.333333333	14	14	
14		2,3,4		2	14							
14		2,3,5		2	14							
14		2,3,6		2	14							
14		2,4,5		2	14							
14		2,4,6		2	14							
14		2,5,6		2	14							
14		3,4,5		2	14							
14		3,4,6		2	14							
14		3,5,6		2	14							
14		4,5,6		2	14							
	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	R2267	#2	24	0	0	0	1	1	0	4	EPA	
			48	0	0	0	1	1	0	4	0	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	3
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	R2267	#2	4	0	0	0	0.66666667	0.66666667	0	0	3	
0		2,3,4		4	3							
0		2,3,5		4	3							
0		2,3,6		4	3							
0		2,4,5		4	3							
0		2,4,6		4	3							
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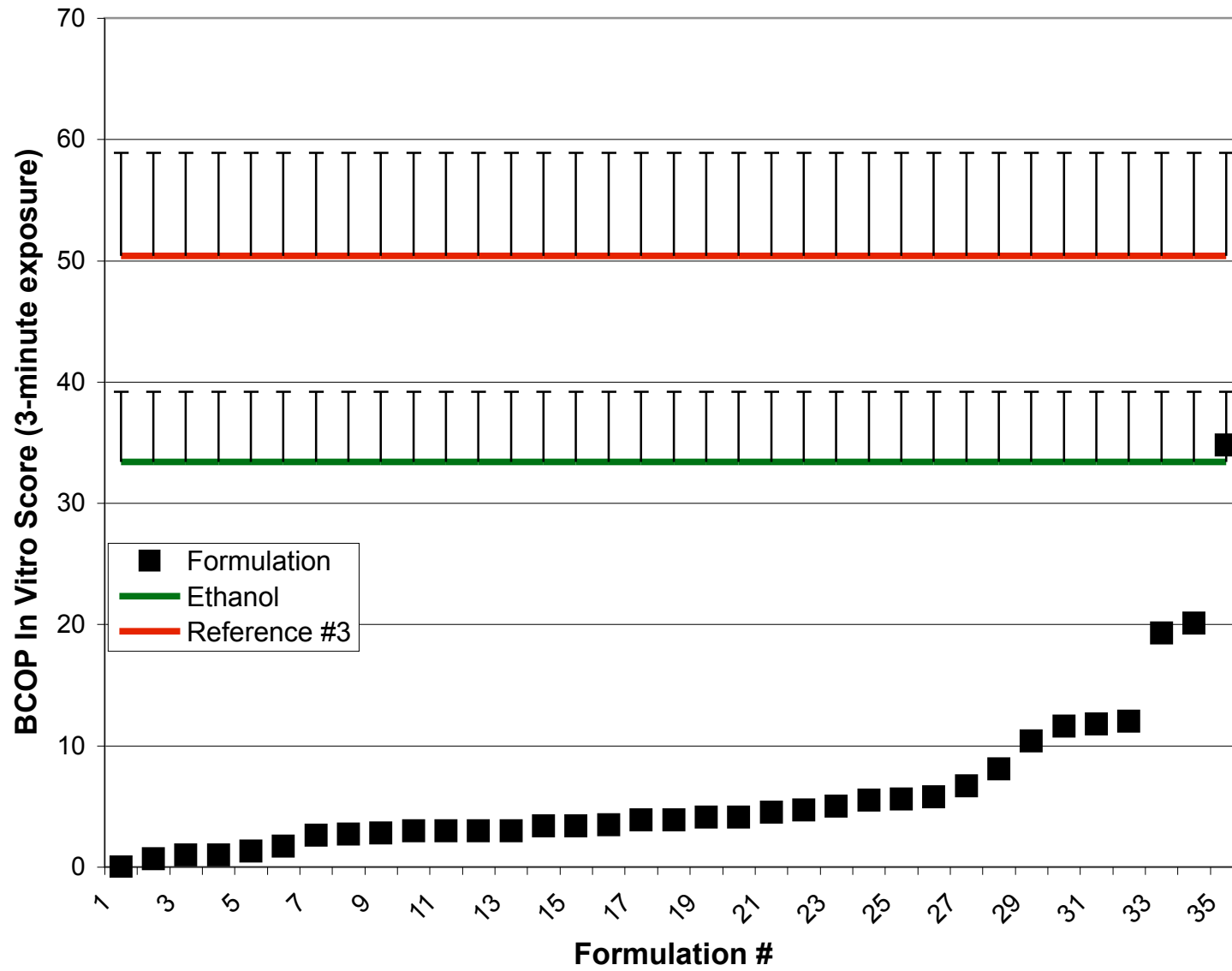
Fragrance Graphs for
SC Johnson Submission
Dated September 3, 2004



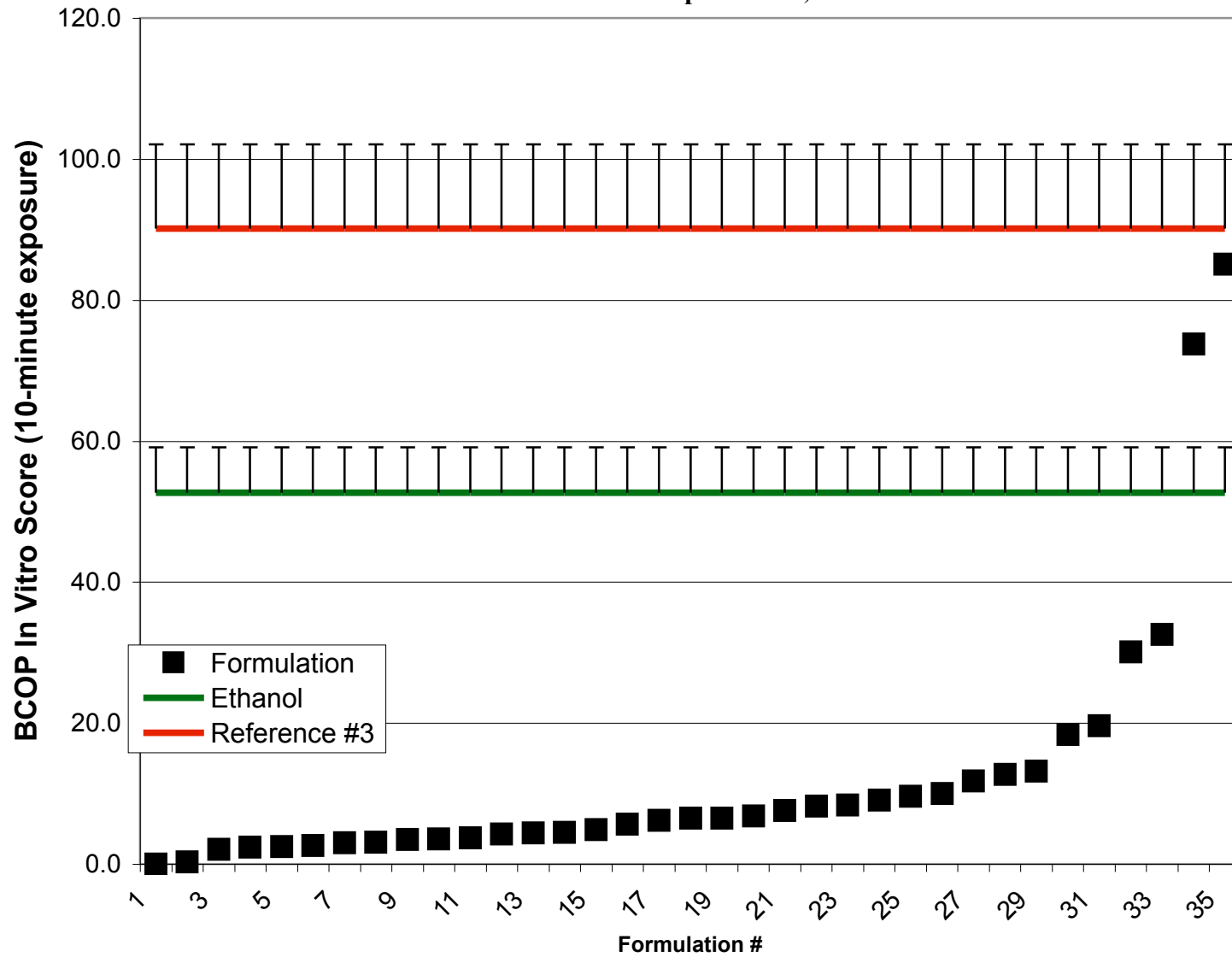
**Fragrance Graphs for
SC Johnson Submission
Dated September 3, 2004**



**Fragrance Graphs for
SC Johnson Submission
Dated September 3, 2004**



**Fragrance Graphs for
SC Johnson Submission
Dated September 3, 2004**



**BCOP Data for SC Johnson Submission
Dated September 3, 2004**

Ethanol	3-minute exposure			
		Opacity	OD490	In Vitro Score
	Mean	21.1	0.820	33.4
	STD	2.9	0.238	5.8
	CV	13.7%	29.0%	17.5%
	n=7			
Ethanol	10-minute exposure (normal positive control)			
		Opacity	OD490	In Vitro Score
	Mean	31.2	1.422	52.7
	STD	4.8	0.345	6.4
	CV	15.3%	24.3%	12.1%
	n = 632			
	Oct 1997 to the present			
Reference #1	Alcohol-based benchmark		Used as the first benchmark formulation	
	3-minute exposure		for the aerosol formulations	
		Opacity	OD490	IV Score
	Mean	20.6	1.270	39.7
	STD	3.5	0.308	6.6
	CV	16.8%	24.2%	16.7%
	n=21			
	10-minute exposure			
		Opacity	OD490	IV Score
	Mean	28.6	2.001	58.5
	STD	4.1	0.415	7.6
	CV	14.3%	20.7%	13.0%
	n=43			
Reference #2	Ethanol Fragrance benchmark			
	3-minute exposure			
		Opacity	OD490	IV Score
	Mean	53.7	2.6	93.3
	STD	8.5	0.5	12.9
	CV	15.8%	20.0%	13.8%
	n=32			
	10-minute exposure			
		Opacity	OD490	IV Score
	Mean	81.5	2.805	123.6
	STD	11.9	0.520	13.3
	CV	14.6%	18.5%	10.8%
	n=32			
Reference #3	Fragrance benchmark (no ethanol)			
	3-minute exposure			
		Opacity	OD490	IV Score
	Mean	39.9	0.693	50.4
	STD	6.0	0.238	8.5
	CV	14.9%	34.3%	16.8%
	n=84			
	10-minute exposure			
		Opacity	OD490	IV Score
	Mean	61.0	1.941	90.1
	STD	7.9	0.459	12.0
	CV	12.9%	23.7%	13.3%
	n=90			

FORMULAS

Test Material #	Group	Raw Material	Percentage
1	Fragrance Benchmark (Reference #3)	Fragrance Thickener	95-100 0-5
2	Ethanol/ Fragrance Benchmark (Reference #2)	Ethanol Fragrance	70-75 25-30
3, 4	Alcohol-based Benchmark (Reference #1)	Alcohol Active Dimethicone	85-90 10-15 1-5
5	Ethanol	Fragrance Ethanol	< 1 100
Fragrance Formulas	Membrane Formula	Fragrance Thickener	95-100 0-5
Fragrance Formulas	Aerosol Formula-1 ¹	Alcohol Fragrance	70-75 25-30
Fragrance Formulas	Aerosol Formula-2	Alcohol Fragrance	80-85 15-20
Fragrance Formulas	Aerosol Formula-3	Alcohol Fragrance	90-95 5-10

¹Most aerosol formulas fall within this category

Appendix G3

**Dataset Received from S.C. Johnson & Son, Inc. in Support of
Gran et al. (2003) Poster Presentation**

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A FAMILY COMPANY

S.C. Johnson & Son, Inc.
Worldwide Consumer Products, RD & E
Global Safety Assessment and Regulatory Affairs, Product Toxicology
MS 139 1525 Howe Street, Racine WI 53403

October 13, 2004

Christina Inhof, MSPH
Senior Project Coordinator/Technical Writer ILS, Inc.
NICEATM
P.O. Box 12233
NIEHS MD EC-17
Research Triangle Park, NC 27709

Christina,

Hi! How are you? I am happy to be submitting data on sodium percarbonate, which was discussed in the poster citation listed below:

Gran B.P., Swanson J.E., Merrill J.C., and Harbell J.W. 2003. Evaluating the irritancy potential of sodium percarbonate: A case study using the bovine corneal opacity and permeability (BCOP) assay. *The Toxicologist*, Abstract Number 1066, Volume 72, Number S-1, March 2003.

Included with this submission are the following documents:

1. Cover letter
2. Poster text
3. Histology slides
4. Coded formula spreadsheet

Study Protocols:

The standard Draize protocol was used by the supplier for the *in vivo* studies. We have been granted permission to share this data on sodium percarbonate for the purpose of this review. Due to the powdered form of the raw material, a bulk density determination was made to determine the weight equivalent of a 100 uL dose. Because significant irritation was observed in the acute dermal study, anesthetic was applied to the rabbit eyes five minutes prior to dosing in the primary eye irritation study.

The standard BCOP protocol for solid test articles was not used for the *in vitro* work at IIVS. Test articles were tested as 50% (w/w) slurry suspensions in sterile, deionized water. Treated corneas were incubated for 10 and 30 minutes with post-exposure incubation

periods of 4- and 20-24 hours. The details of the protocol are provided in the poster text. Concurrent positive and negative controls were performed with each assay. Negative control corneas were prepared for each post-exposure incubation time.

Formula Spreadsheet:

The formulas listed in this spreadsheet are coded similarly to formulas listed in the poster. Test material number is the unique sample number and the group name denotes formula description. Raw materials are listed followed by their percentages in each formula.

Poster:

The poster offprint is not included. John Harbell sent it to you previously.

Poster Text:

A word document consisting of poster text and tables is included in this submission for ease of reading. This document highlights where the histology slides should be inserted for ease of understanding.

Histology Slides:

Histology slides should be referenced on page 8.

Data Worksheet:

Since the rabbit study was terminated at 96 hours because of the severe nature of the responses, we must assume that the *in vivo* response fits Category 1 (both GHS and EPA). The 96-hours readings are listed in the table below:

Animal	Opacity	Area	Iris	Redness	Chemosis	Discharge
1	3	1	1	3	2	2
2	3	4	a	3	3	0
3	3	1	a	3	3	2
4	1	1	0	3	2	0
5	3	4	a	3	4	3
6	2	4	1	3	3	1

a – Iris could not be scored because of severe corneal opacity

Summary:

The standard BCOP protocol for solids was not utilized in this investigation of sodium percarbonate. The standard protocol, developed for pharmaceutical intermediates that are relatively insoluble, calls for using a 20% suspension with a 4-hour exposure time. Based on past experience with the BCOP assay, the eye irritancy potential of more aqueous-soluble

solids such as laundry powders using the standard solids protocol is vastly overpredictive of the outcome resulting from accidental human exposure. Furthermore, experience has shown that reactive/oxidizing chemistries (such as bleach, percarbonates and peroxides) have a delayed toxicity response in the assay necessitating increased post-exposure observation time.

The question the investigators faced in this case study of sodium percarbonate was what protocol parameters were needed to model the bolus exposure for an extended period that occurs in the Draize eye irritation protocol as well as what might be expected to be a realistic maximum exposure for humans. The following parameters were chosen: A 50% suspension of the solid with a 30-minute exposure time to model the *in vivo* exposure and 10-minute exposure time to model maximum accidental human exposure. While post-exposure time in the BCOP is typically 2 hours, times of 4 and 20-24 hours were chosen.

Utilizing the protocol considerations discussed above, the BCOP assay was able to adequately predict the irritancy potential of two different concentrations of sodium percarbonate for both a realistic human exposure scenario and an *in vivo* exposure scenario. Reduction of sodium percarbonate concentration predictably reduced the irritancy potential of the end-use formulation. Histology as a third endpoint in the BCOP assay was critical in evaluating the depth and degree of injury.

If you have any questions or comments on this data set, please feel free to contact either Judith Swanson or myself at the following:

Nicole Cuellar
(262) 260-6916
ncuellar@scj.com

Judith Swanson
(262) 260-2688
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Sincere regards,



Nicole Cuellar
Sr. Research Toxicologist

POSTER TEXT FOR S.C. JOHNSON SUBMISSION DATED OCTOBER 13, 2004**TITLE**

EVALUATING THE IRRITANCY POTENTIAL OF SODIUM PERCARBONATE: A CASE STUDY USING THE BOVINE CORNEAL OPACITY AND PERMEABILITY (BCOP) ASSAY.

B.P. Gran¹, J.E. Swanson¹, J.C. Merrill² and J.W. Harbell²

¹S.C. Johnson & Son, Inc. Racine, WI; ²Institute for In Vitro Sciences, Inc., Gaithersburg, MD.

ABSTRACT

Sodium percarbonate ($2\text{Na}_2\text{CO}_3 \cdot 3\text{H}_2\text{O}_2$) is a component in cleaning products but the neat powder has the potential to be highly irritating to the ocular tissue of rabbits (EPA Category I). This injury results from the chemical's reactivity and dosing method that may trap the powder against the eye. In the BCOP assay, experience has now shown that oxidizing/reactive materials often require a longer post-exposure time to fully manifest cytopathic changes. When testing reactive chemistries, the post-exposure incubation times are increased from 2 hours to 4 and 24 hours. Exposure times of 10, 20, 30 and 60 minutes were used in this study. Sodium percarbonate and percarbonate-based formulations were evaluated as 50% suspensions in water. Abattoir-derived corneas were received, mounted, exposed to test materials, and opacity, permeability and histological endpoints measured as previously reported Curren et al.(2000). Opacity and permeability scores increased with increasing exposure times and concentration of percarbonate. After the 10-minute exposure to percarbonate alone, the 4-hour post-exposure corneas showed focal epithelial layer changes that progressed to a loss of epithelium after 24 hours. Stromal damage included collagen matrix vacuolization and loss of basophilic components in the keratocyte cytoplasm. Exposures of 20 minutes or greater led to rapid destruction of both the epithelial and stromal cells and marked collagen matrix swelling. Tissue lesions declined rapidly with decreasing percarbonate concentration. Thus, the marked ocular damage induced by neat percarbonate in the rabbit, could also be reproduced in the modified BCOP. These data suggest that the modified BCOP assay can be effectively used to evaluate the safety of percarbonate-based formulations and lead to appropriate labeling and packaging decisions.

INTRODUCTION

The sodium percarbonate molecule owes its current popularity in cleaning products to its capability to be a powerful oxygen generator when combined with water. This crystalline solid is a highly reactive molecule that has been shown to be very irritating to rabbit eye tissue. When rabbits were exposed in the standard EPA Guideline eye irritation assay, corneal epithelial peeling, iridial involvement and severe conjunctival irritation occurred. (supplier data)

An initial investigation of the eye irritation potential of sodium percarbonate using the standard BCOP Assay protocol resulted in a relatively benign profile, a strikingly different result from the *in vivo* study.

This case study of sodium percarbonate presents an effort to understand how a non-animal assay, the BCOP Assay, can be utilized to realistically predict human eye irritancy potential of reactive molecules. The BCOP Assay was chosen for this work as it allows exact control over the exposure times and provides several measures of tissue damage. Exposure times were chosen to encompass the range of effective exposures that might occur in the rabbit. This enabled us to identify the exposure time in the BCOP Assay that resulted in a comparable level of injury to that seen in the rabbit study. Corneal injury was evaluated using the standard BCOP endpoints, opacity and permeability, as well as histological examination.

MATERIALS AND METHODSError! Bookmark not defined.

Bovine Eyes

The BCOP assay was performed following the methods of Sina et al. (1995). Bovine eyes were obtained from a local abattoir as a by-product from freshly slaughtered animals. The eyes were grossly examined for damage and those exhibiting defects were discarded. The corneas were excised such that a 2 to 3 mm rim of sclera was present around the cornea. The corneas were mounted in the holders and the two chambers filled with Minimum Essential Medium Eagle (MEM) without phenol red, supplemented with 1% fetal bovine serum (complete MEM). The corneal holders were incubated at $32 \pm 1^\circ\text{C}$ for a minimum of 1 hour.

Bovine Corneal Opacity and Permeability Assay

After a minimum of 1 hour of incubation, the medium replaced in both chambers and the opacity was determined for each cornea using a Spectro Designs OP-KIT opacitometer. Three corneas, whose opacity readings were close to the median opacity for all the corneas, were selected as the negative control corneas. The medium was then removed from the anterior chamber and replaced with the test article, positive control, or negative control.

Method for Testing Liquid or Surfactant Materials

The test articles were tested as 50% (w/w) slurry suspension in sterile, deionized water. An aliquot of 750 μl of the test article, positive control, or negative control was introduced into the anterior chamber while slightly rotating the holder to ensure uniform distribution over the cornea. A total of three corneas per treatment group were incubated in the presence of each test article at $32 \pm 1^\circ\text{C}$ for 10, 20, or 30 minutes with a post-exposure incubation period of 4, 20, or 24 hours. The negative control was tested, in groups of 3 corneas each, to match the short and long post-exposure incubation periods. The positive control was tested in three corneas at $32 \pm 1^\circ\text{C}$ for 10 minutes with a post-exposure incubation period of two hours. After the test or control article exposure, the epithelial side of the corneas was washed at least three times with complete MEM to ensure total removal of the test or control articles. The anterior chamber was refilled with fresh complete MEM and an opacity measurement was performed. After the post-exposure incubation period, a second measure of opacity was obtained. The corneas designated for the post-exposure incubation periods of 2 or 4 hours did not require refeeding with fresh medium prior to the second measure of opacity. The corneas designated for the over night post-exposure incubation periods were refeed with fresh medium approximately every 6 hours and immediately prior to the second measure of opacity.

After the final opacity measurement was performed, the medium was removed from both chambers of the holder. The posterior chamber was refilled with complete MEM, and 1 ml of a 4 mg/ml fluorescein solution was added to the anterior chamber. The corneas were then incubated in a horizontal position (anterior side up) for approximately 90 minutes at $32 \pm 1^\circ\text{C}$. After the incubation, an aliquot of 360 μl from each chamber was placed into the designated well on a 96-well plate. The optical density at 490 nm (OD_{490}) was determined using a Molecular Devices *V*max kinetic microplate reader.

Opacity Measurement: The change in opacity for each cornea was calculated by subtracting the pre-treatment opacity readings from the final opacity readings. The corrected opacity value of each cornea was calculated by subtracting the average change in opacity of the time-matched negative control corneas from that of each treated cornea. The mean opacity values of each treatment group were then calculated.

Permeability Measurement: The corrected OD₄₉₀ was calculated by subtracting the mean OD₄₉₀ of the time-matched negative control corneas from the OD₄₉₀ value of each treated cornea. The mean OD₄₉₀ values of each treatment group were then calculated.

Histology

The corneas were placed in individual, prelabelled cassettes and fixed for at least 24 hours in 10% buffered formalin. The fixed corneas were transferred to Pathology Associates - A Charles River Company (Frederick, MD) for embedding, sectioning and staining. Each slide was then stained with hematoxylin and eosin. Slides were returned to the Institute for In Vitro Sciences, Inc. for evaluation. Cornea sections were examined for the presence of changes in the epithelial, stromal, and endothelial areas of the tissue. Treated tissues were compared to concurrent negative and positive control tissues. Photomicrographs and thickness measurements were prepared using a Spot Insight (Spot Diagnostic Instruments) digital camera and associated software.

Primary Eye Irritation Study of FB Sodium Percarbonate in Rabbits (1982 EPA Guidelines 81-4)

The primary eye irritation study of sodium percarbonate in six albino rabbits [Hra: (NZW)SPF] was conducted in 1989 according to the 1982 EPA Guidelines for Acute Eye Irritation (81-4). The study was also in accordance with GLP standards of 1983 since the in-life portion of the study was completed before the effective date of the revised standards (9/18/89). A bulk density determination was made to determine the weight equivalent of a 100 µl dose. Due to irritation observed in the acute dermal study, anesthetic was applied to the eyes five minutes prior to dosing. The weight equivalent of 100 µl was placed in the conjunctival sac of rabbit and the eyelids were gently held together for one second. The contralateral eye served as the untreated control. Observations for ocular irritation were made at 1, 24, 48, 72 and 96 hours after treatment. The study was terminated at 96 hours after consultation with Sponsor due to severity of irritation observed. Acute irritation seemed to peak at 48 hours after instillation. (Study information provided by supplier under confidentiality agreement.)

RESULTS

The BCOP Assay was chosen as a non-whole animal tool for evaluating the potential eye irritancy of sodium percarbonate because it allowed exact control over exposure and observation times, and provided several measures of tissue damage. All assays were performed using a 50% slurry of the percarbonate salt in water to model a concentrated solution of the powder when tearing occurs following accidental exposure.

Exposure times were chosen to encompass the range of what might be a realistic worst possible case in accidental human exposure to an exposure time that would approximate the level of injury found in the *in vivo* study. Corneal injury was evaluated initially using opacity and permeability endpoints, the standard BCOP Assay measures of irritation. Since the full manifestation of oxidative damage to cells may be delayed for some hours after exposure with some materials, several post-exposure periods were selected to compare the manifestation of damage over time. Table 1 shows the impact of exposure times and post-exposure observations on the quantitative BCOP endpoints and the effects of reducing the concentration of sodium percarbonate in formulation at two exposure times..

Table 1. BCOP Opacity and Permeability Scores from Sodium Percarbonate Exposure: Impact of Exposure and Post-Exposure Time

Test Material	Exposure Time	Post-Exposure Incubation Time	Opacity	Permeability	In Vitro Score
1. Sodium Percarbonate (500 mg/ml suspension) pH 10.5	10 minutes	4 hours	8.3	0.123	10.2
	30 minutes	4 hours	14.0	2.598	53.0
	60 minutes	4 hours	19.8	4.344	85.0
	10 minutes	24 hours	16.0	0.636	25.5
	30 minutes	24 hours	27.7	1.392	48.5
	60 minutes	24 hours	27.3	1.333	47.3
2. Sodium Percarbonate (500 mg/ml suspension)	10 minutes	20 hours	11.0	0.025	11.4
	20 minutes	20 hours	14.0	2.810	56.1
3. Sodium Percarbonate* (300 mg/ml suspension)	10 minutes	20 hours	6.0	0.015	6.2
	20 minutes	20 hours	13.3	0.366	18.8

*Formulation with 60% sodium percarbonate

Additionally, the corneas were sectioned, stained and examined microscopically for depth of injury and histological markers of irritancy for this oxidative material. Table 2 summarizes morphological changes seen in the corneas for different exposure times at both short-and long-term post-exposure times.

Table 2. Morphological Changes in Corneas Treated with Sodium Percarbonate: Impact of Exposure and Post-Exposure Time

Test Article Exposure time	Post Exposure time			Post Exposure time		
	4 hours			20 to 24		
	Epithelium	Stromal Collagen	Keratocytes	Epithelium	Stromal Collagen	Keratocytes
10 min	Surface cells lost but deeper layers remained. Marked focal lesions observed	Increased stromal thickness and moderate CMV* to 40% depth	Moderate increase in cytoplasmic eosinophilia to 40% depth	Surface cells lost and upper wing cells were pyknotic. Deeper cells lost in some fields	Increased stromal thickness and moderate CMV >50% depth	Marked cytoplasmic eosinophilia to 40% depth
20 min**				Epithelium completely lost	Severe CMV throughout the stroma	Few viable cells remained
30 min	Surface cells lost, remaining cells in place but damaged	Marked increase in stromal thickness and CMV past 50% depth	Marked nuclear pyknosis and cytoplasmic eosinophilia – full depth	Epithelium completely lost	Severe CMV throughout the stroma	Few if any viable cells remained
60 min	Epithelium present but not viable	Marked increase in stromal thickness, gas pockets visible	Marked nuclear pyknosis and cytoplasmic eosinophilia – full depth	Epithelium completely lost	Severe CMV throughout the stroma	Few if any viable cells remained

* CMV = Collagen Matrix Vacuolization

** 20-hour post-exposure time

See attached FIGURES for specific histology slides.

The following Figures illustrate the qualitative changes in corneal tissue that are summarized in Table 2.

- Figures 1 and 2, A, B, & C show normal untreated corneal tissue to afford a basis for comparison with the tissues that have been exposed to percarbonate slurries.
- Figures 3-7, A, B & C show injury to corneal structures at different time periods.
- Figures 8, A, B & C shows the effects of a reduced concentration end-use formulation compared to full-strength percarbonate in Figures 4, A, B & C.

DISCUSSION

- ❑ With reactive molecules like sodium percarbonate, reliance on the traditional 2-hour post exposure incubation in the BCOP assay can be misleading. The delayed manifestation of toxicity requires an increased post-exposure incubation time (see Table 1).
- ❑ The opacity and permeability endpoints may underestimate the toxicity where the epithelium remains physically intact. The focal lesions do not lead to an appreciable increase in permeability scores (see for example Table 1, 10-minute exposures).
- ❑ The pattern of lesions in the corneal epithelium suggests that focal lesions develop which breach the epithelial barrier and allow subsequent penetration into the stroma. This pattern of damage is different from what is observed with exposure to surfactants or solvents where the lesions tend to be more uniformly progressive across the epithelial surface of the cornea.
- ❑ Loss of the corneal epithelium leads to extensive fluorescein permeability while the corneal stroma is in the process of swelling (Table 1, 30- and 60-minute exposures at 4 hours post-exposure). However, once the corneal stroma has swollen, the relative fluorescein permeability decreases (Table 1, 30- and 60-minute exposures at 24 hours post-exposure). Note the stromal thickness in Figures 5C and 6C.
- ❑ The degree and depth of injury to the stromal keratocytes has been shown to be predictive of the degree and duration of ocular injury in vivo (Maurer et al., 2002). Histological evaluation of the bovine corneas, treated in vitro, provides data on keratocyte damage. This damage may not be fully reflected in the opacity and permeability measurements.
- ❑ The Draize Test protocol leads to an overestimation of the irritancy of powders. The effects resulting from the Draize methodology greatly exceed what could realistically be expected from accidental human exposure.. The differences in exposure include: the quantity and location of material instilled, the occlusion and pressure of the crystalline material against the cornea, mechanical abrasion and a different tearing response. (see Bruner's discussion of ocular irritation in Frazier's In Vitro Toxicity Testing, pp.160-161, Wilkie and Wyman's chapter in Hobson's Dermal and Ocular Toxicology, p.487. and Maurer et al., 2002)

CONCLUSION

- Testing reactive molecules, such as sodium percarbonate, requires a modification of the BCOP protocol to fully evaluate the potential for delayed effects on corneal tissue.
- Because important changes may come at the cellular rather than tissue level (see Jester et al. [1998] and Maurer et al. [2001]), histology evaluation is critical as a third end-point in the BCOP Assay for this type of molecule. These combined endpoints allow for the determination of depth and degree of injury that is required to predict irritation potential (see Maurer et al [2002]).
- In the BCOP assay, exposures of greater than 10 minutes to a 50% suspension of sodium percarbonate are required to achieve tissue damage consistent with the damage reported for the rabbit eyes in the Draize test. These data suggest that trapping of the powder against the cornea in the conjunctival sac may appreciably impact its toxicity in the rabbit.
- Reduction of sodium percarbonate concentration greatly reduced the irritancy potential of the test formulation, even in the more exaggerated 20-minute exposure.

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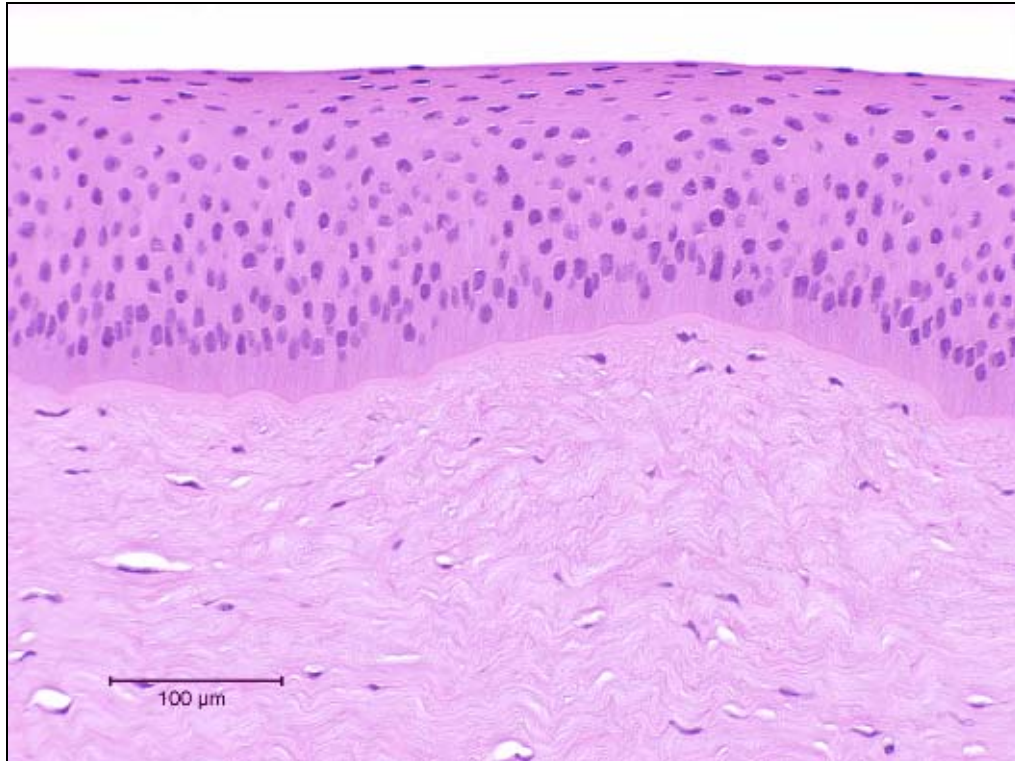
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Swanson, J.E. and Harbell, J.W. (2000) Evaluating the eye irritancy potential of ethanolic test materials with the bovine corneal opacity and permeability assay. *The Toxicologist* 54(1):188-189.

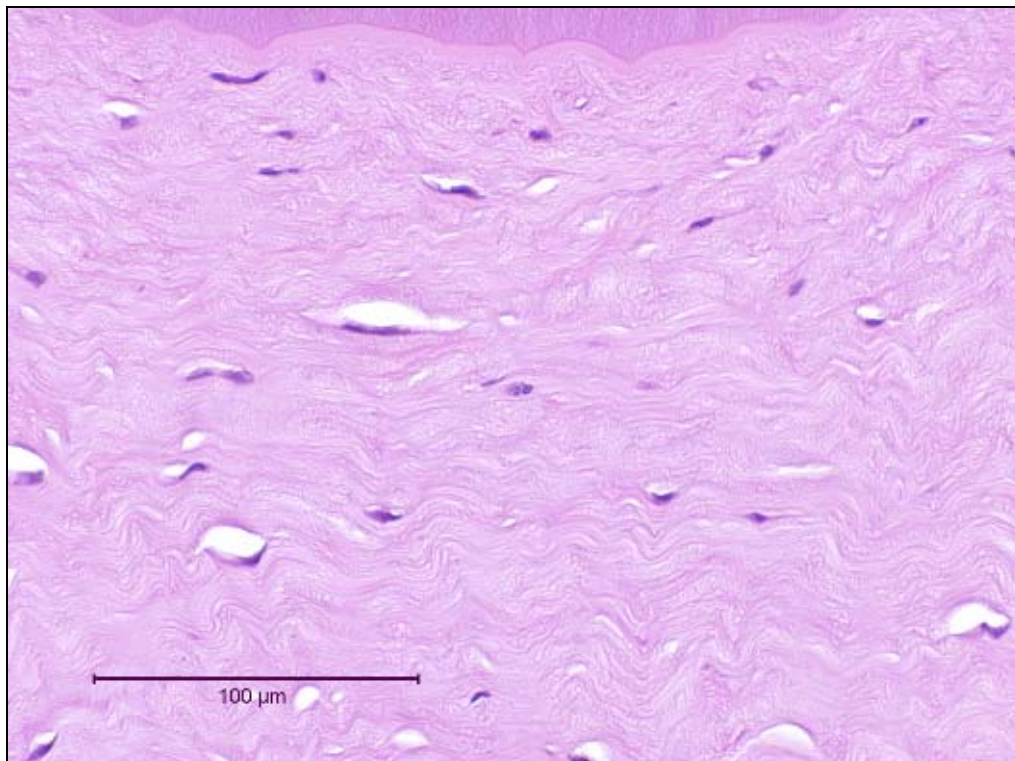
J.E. Swanson, B.T. White, B.P. Gran, J.C. Merrill and J.W. Harbell; 42nd Annual SOT, Poster #1068.

Figure 1. Negative Control, 4-hour post-exposure

(A) Epithelium (magnification 230x)



(B) Stroma directly below the Bowman's Layer (magnification 430x)



(C) Full thickness (magnification 45x)

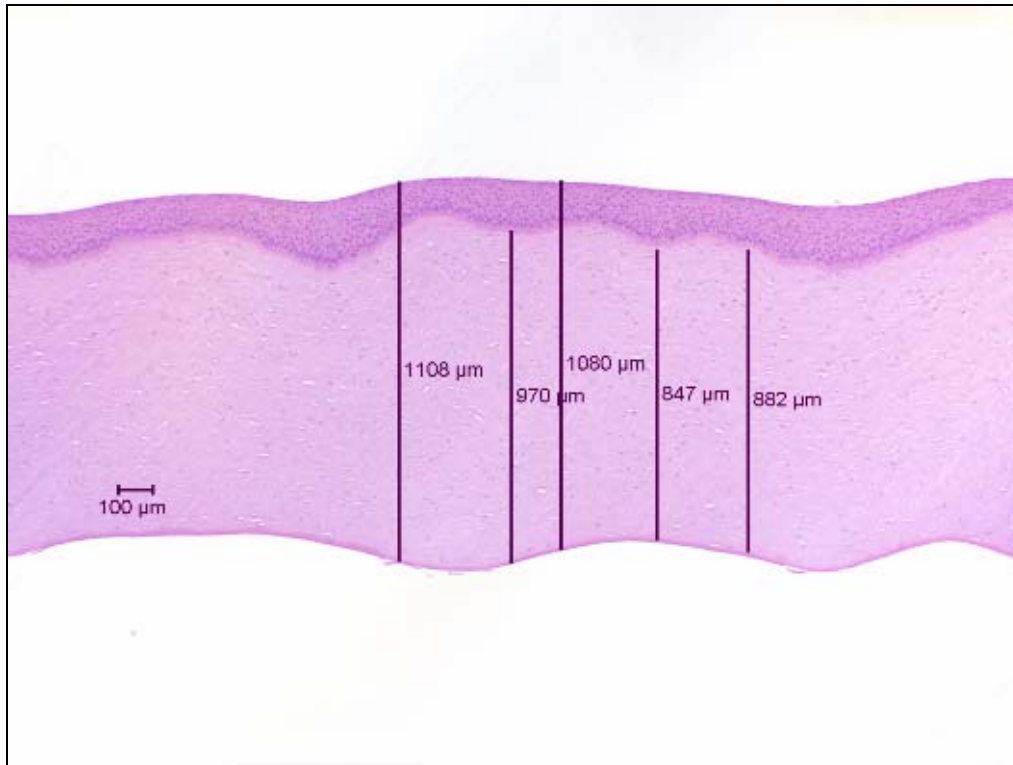
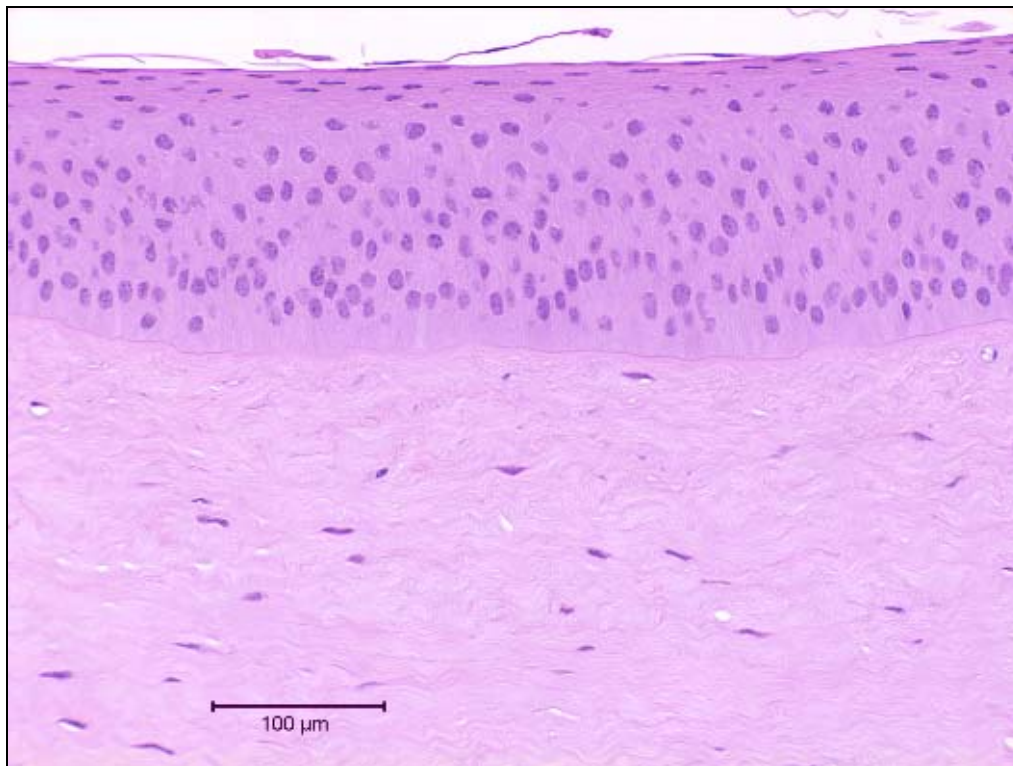
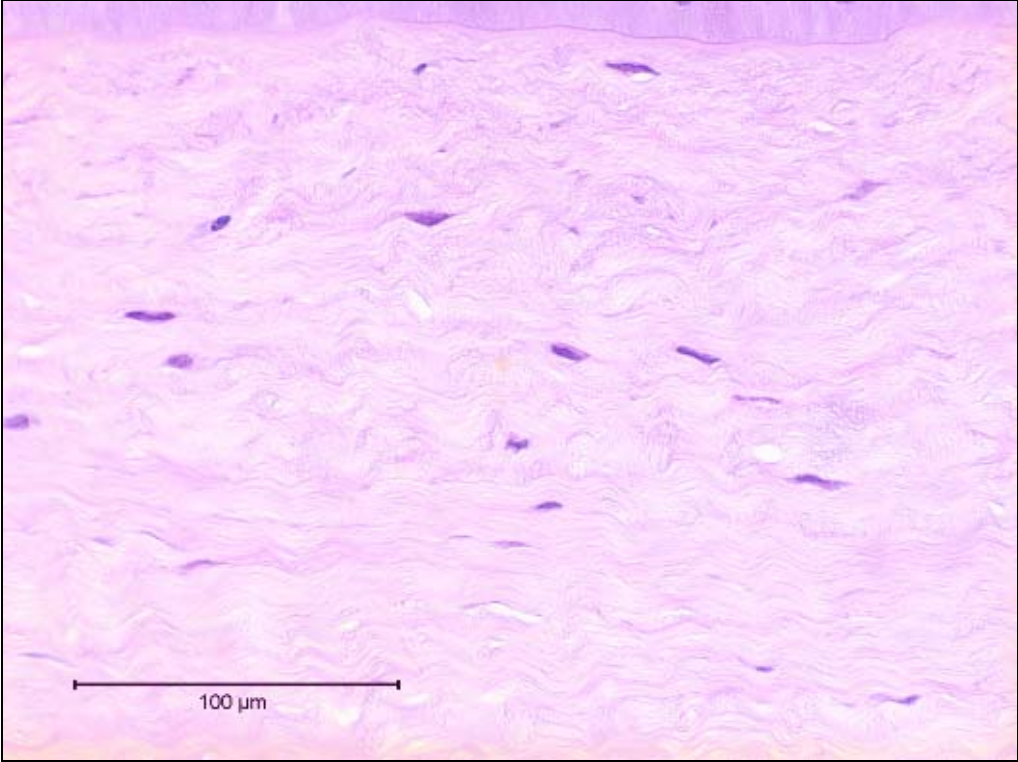


Figure 2. Negative Control, 20-hour post-exposure
(A) Epithelium (magnification 230x)



(B) Stroma directly below the Bowman's Layer (magnification 430x)



(C) Full thickness (magnification 45x)

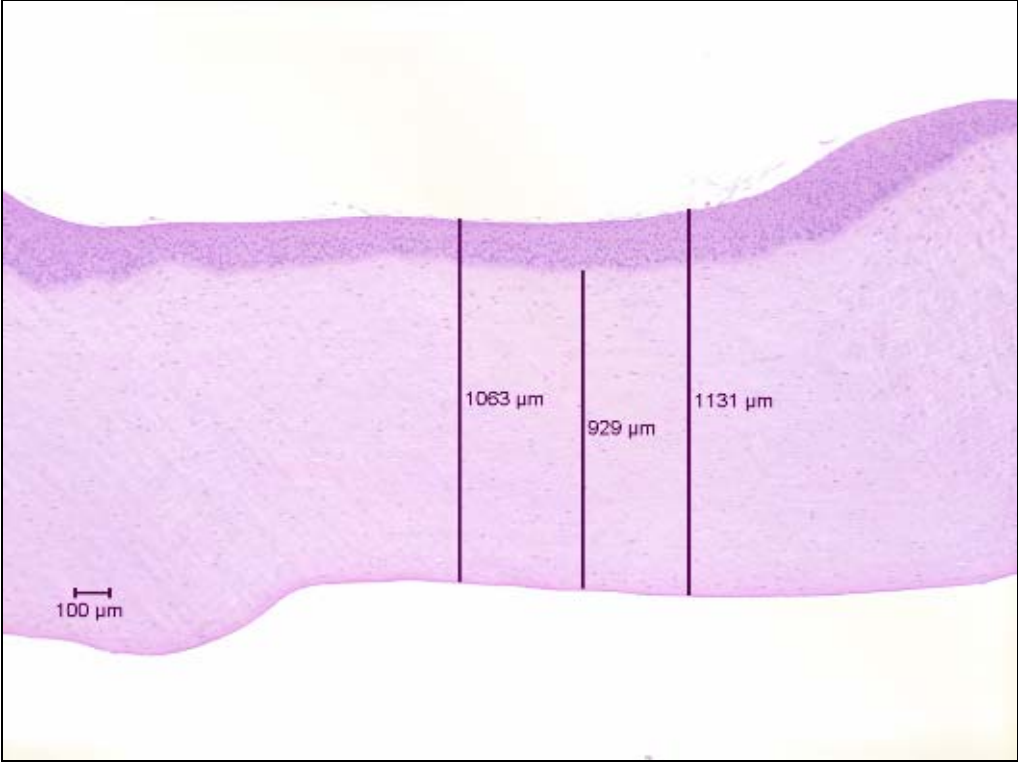
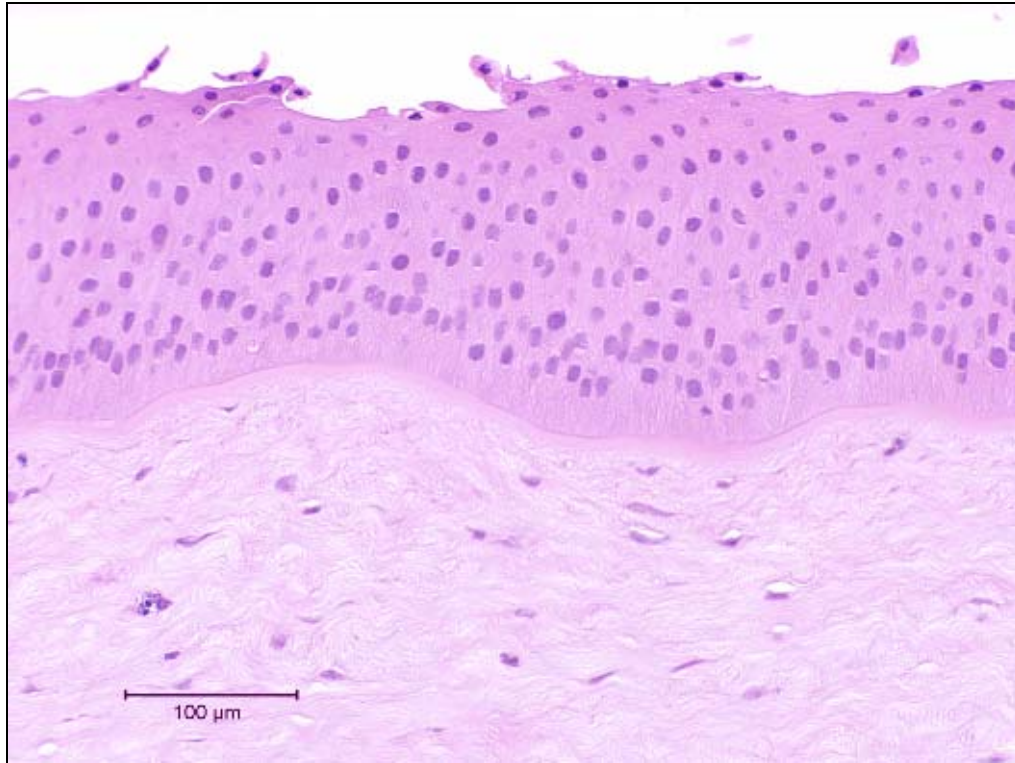
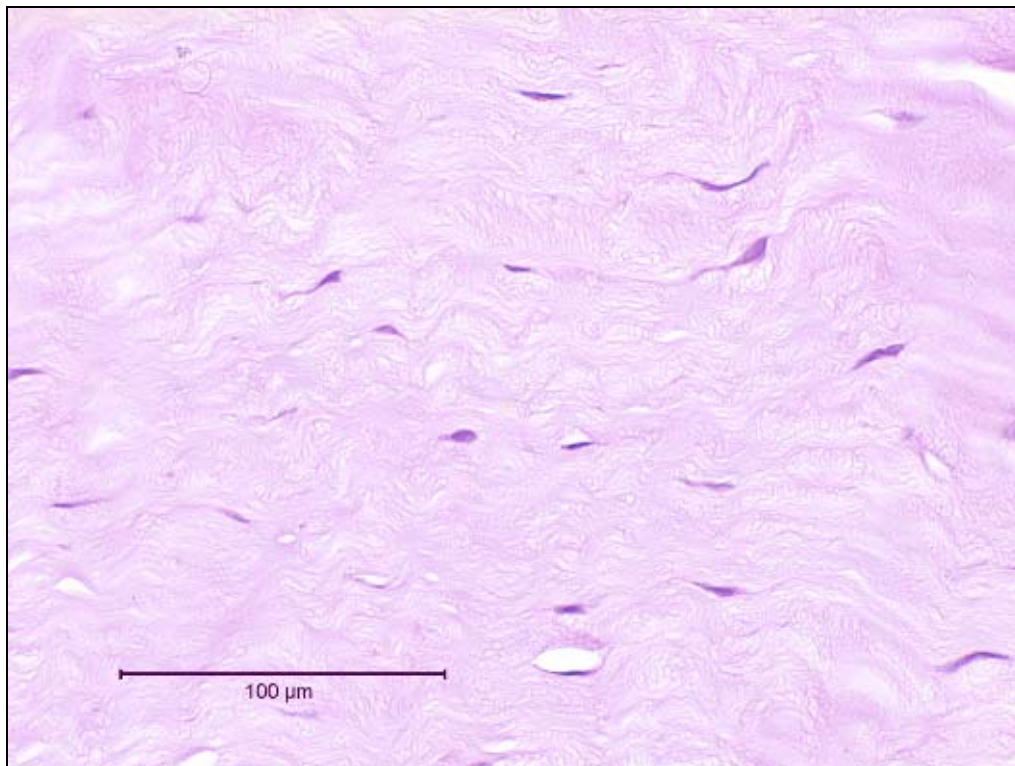


Figure 3. Sodium Percarbonate 50% (w/v) suspension, 10-minute exposure, 4-hour post-exposure
(A) Epithelium (magnification 230x)



(B) Stroma at mid-depth (magnification 230x)



(C) Full thickness (magnification 45x)

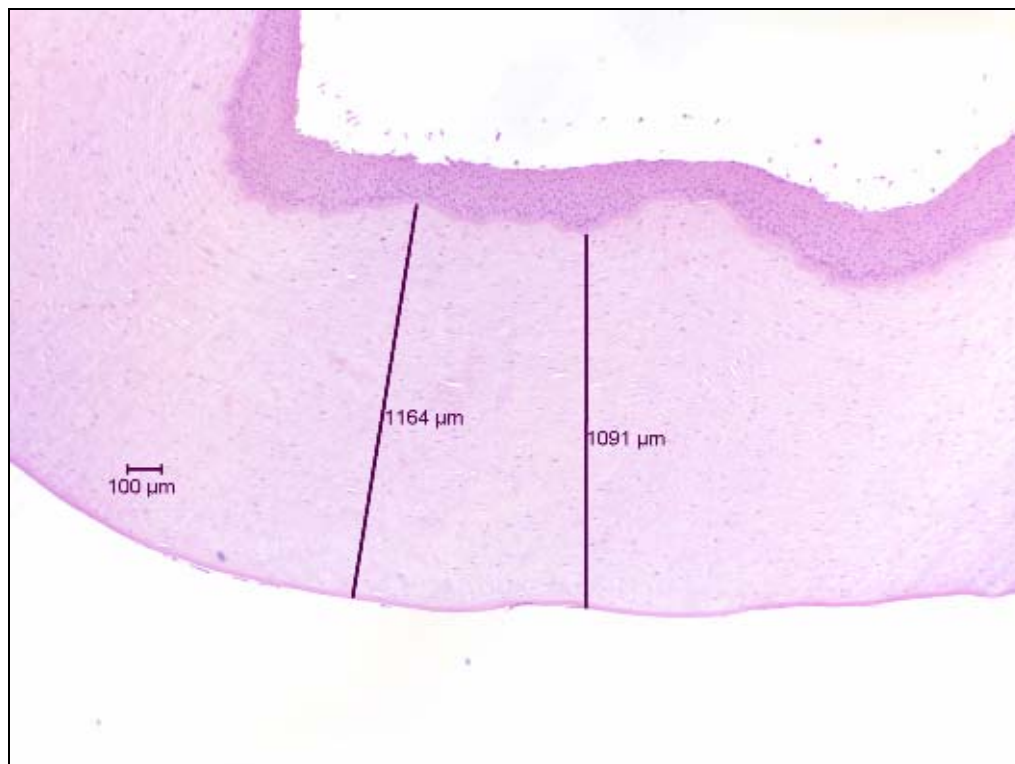
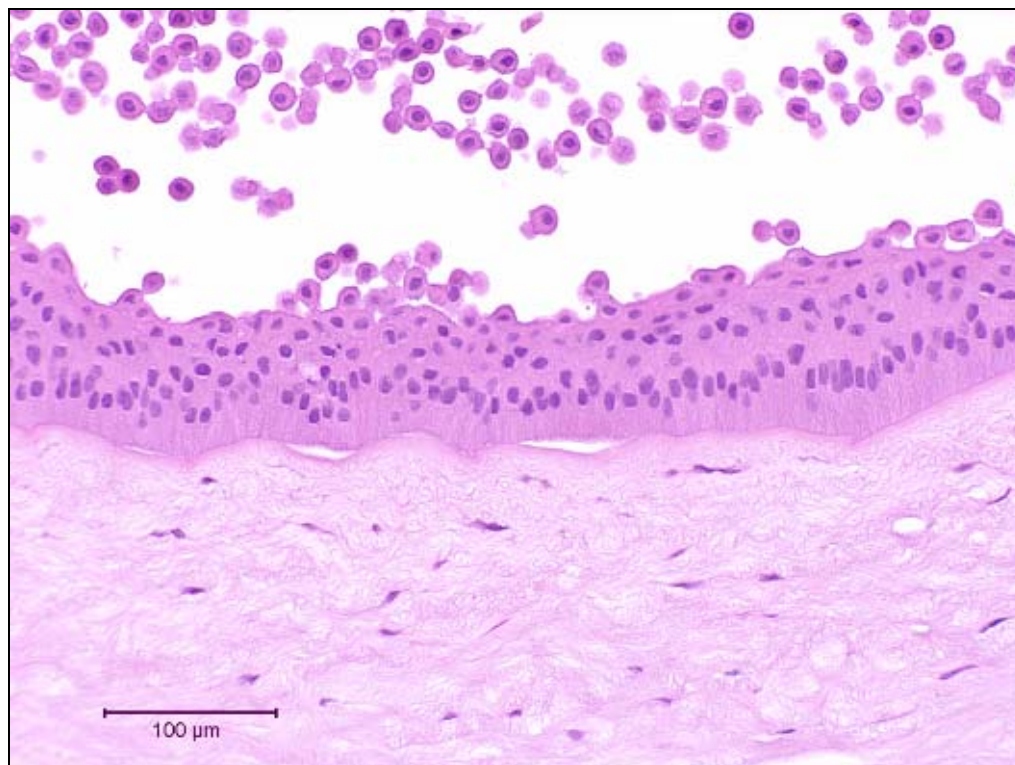
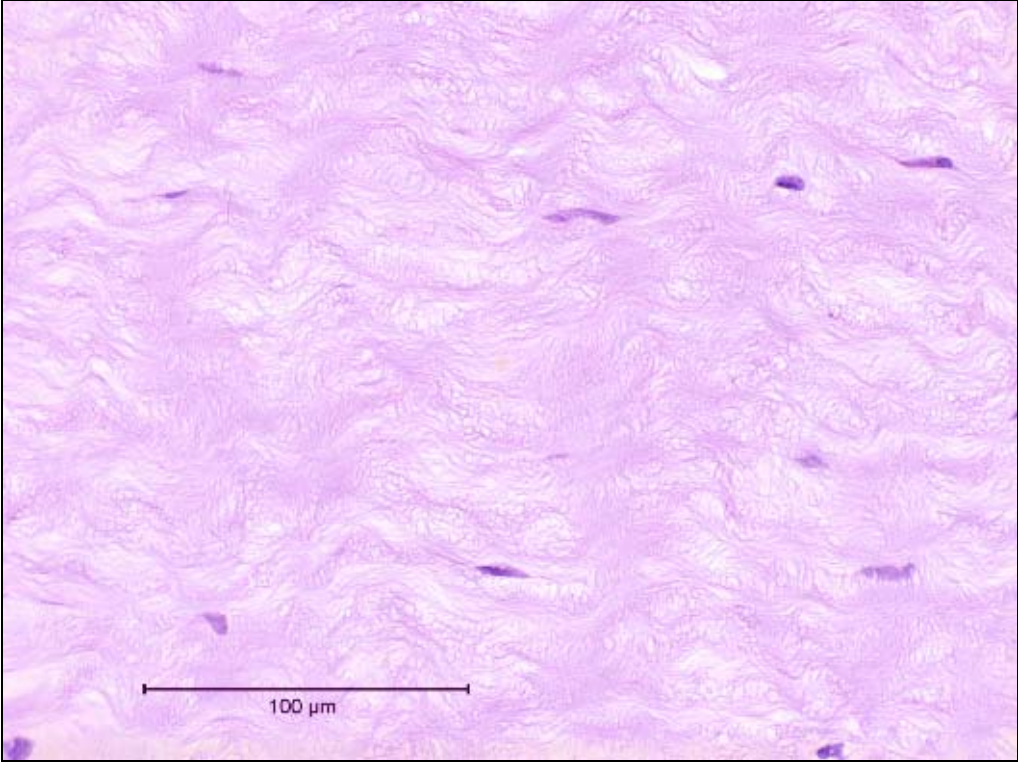


Figure 4. Sodium Percarbonate 50% (w/v) suspension, 10-minute exposure, 24-hour post-exposure (A) Epithelium showing marked cell loss (magnification 230x)



(B) Stroma at mid depth showing increased collagen matrix vacuolization (magnification 230x)



(C) Full thickness (magnification 45x)

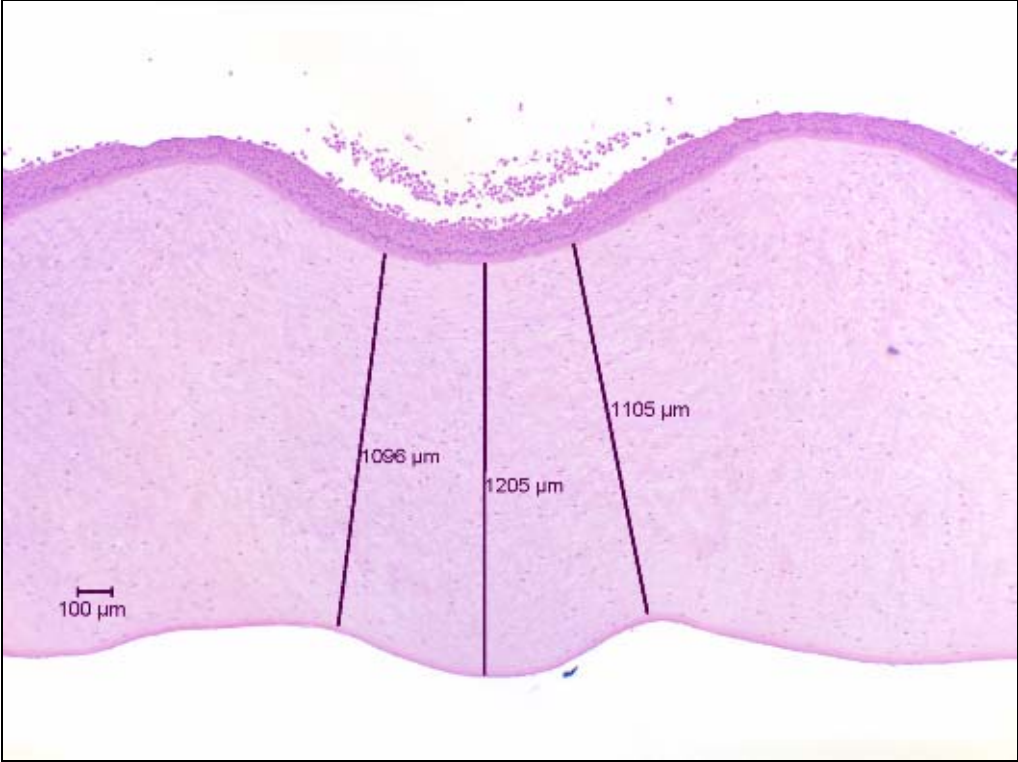
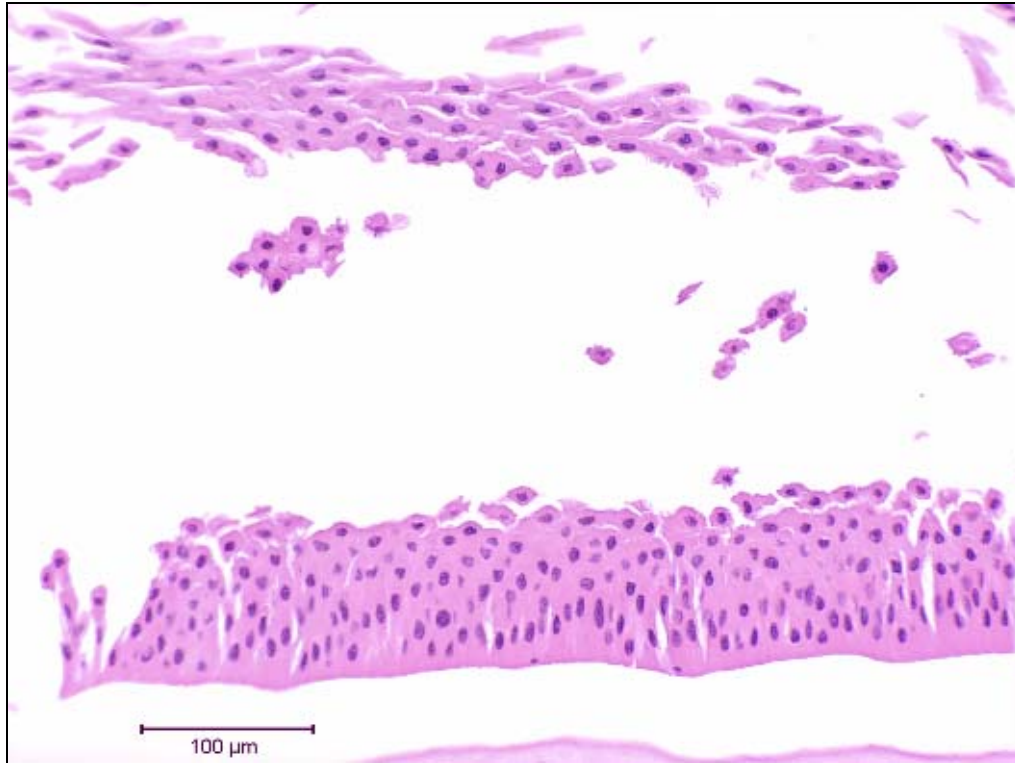
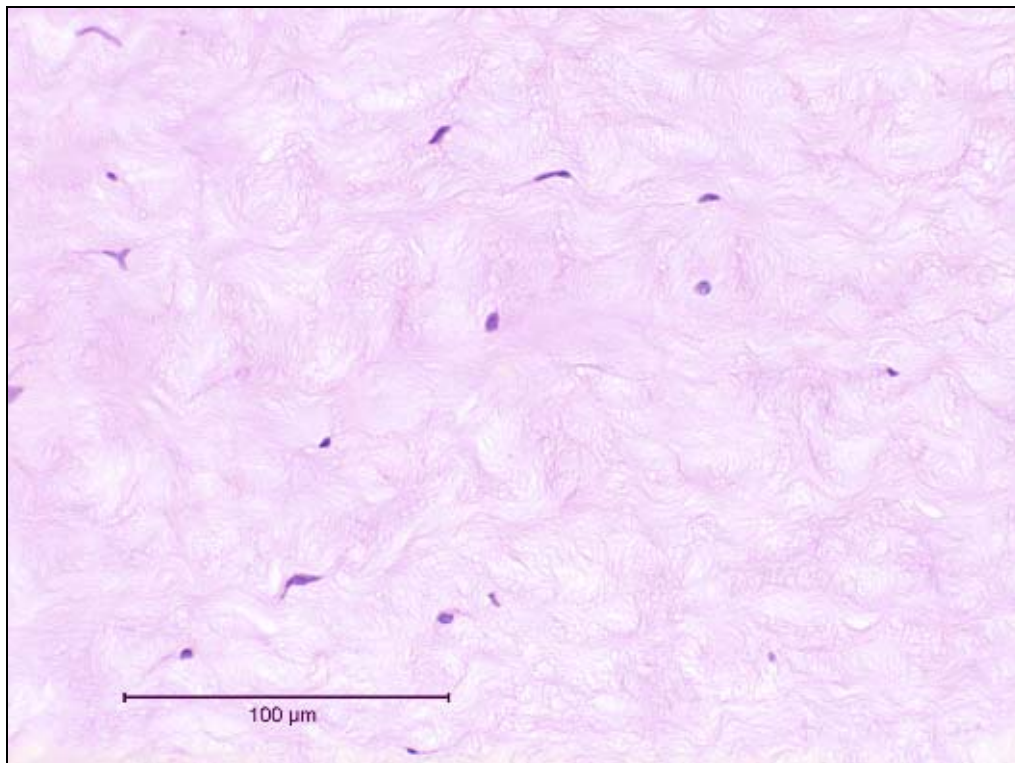


Figure 5. Sodium Percarbonate, 50% (w/v) suspension, 30-minute exposure, 4-hour post-exposure
(A) Epithelium separated from the basal lamina (magnification 230x)



(B) Stroma at mid depth showing marked nuclear pyknosis (magnification 430x)



(C) Full thickness (magnification 45x)

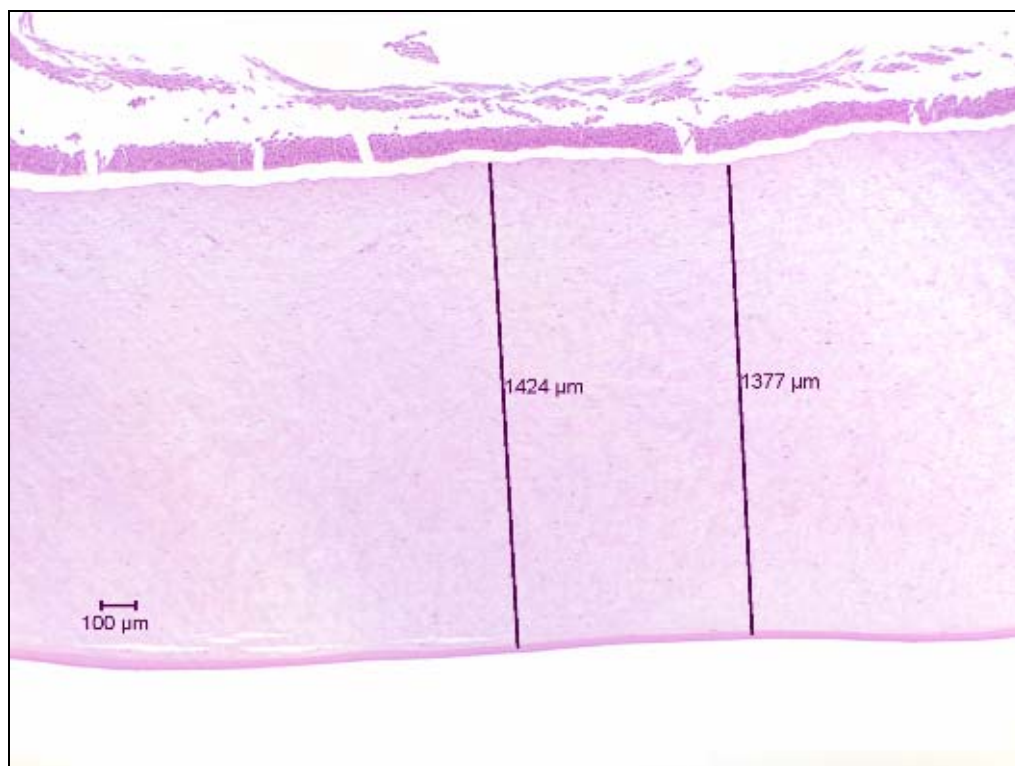
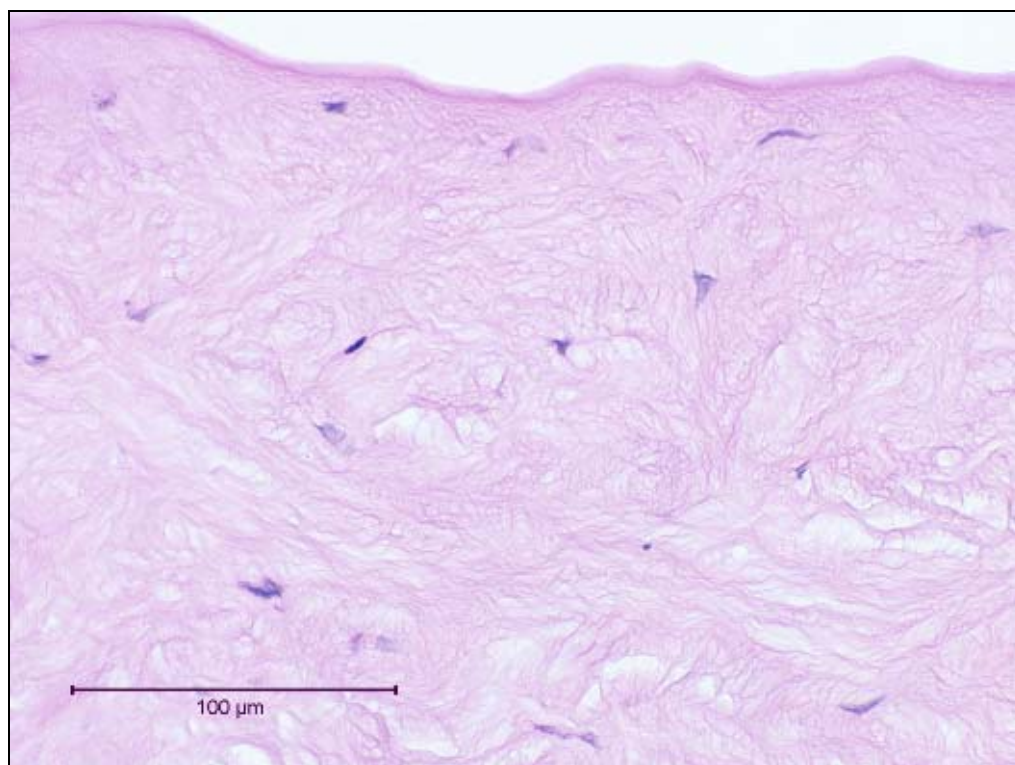
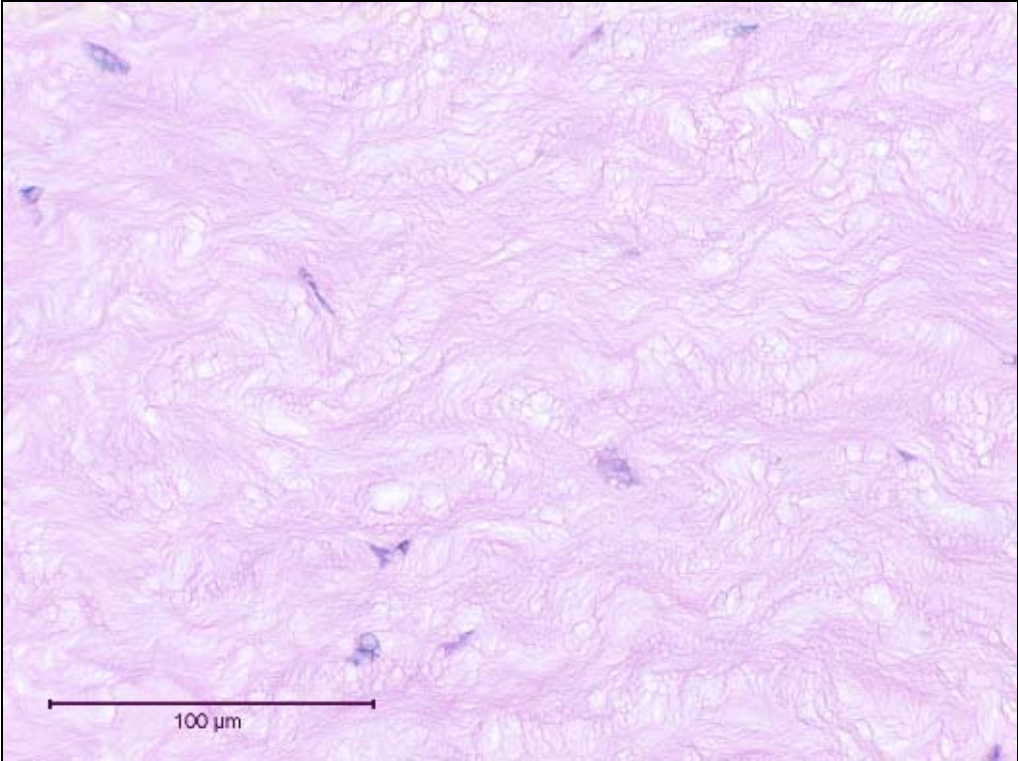


Figure 6. Sodium Percarbonate, 50% (w/v) suspension, 30-minute exposure, 24-hour post-exposure (A) Epithelium (lost) (magnification 430x)



(B) Stroma at mid depth showing marked collagen matrix vacuolization and dead keratocytes (magnification 430x)



(C) Full thickness (magnification 45x)

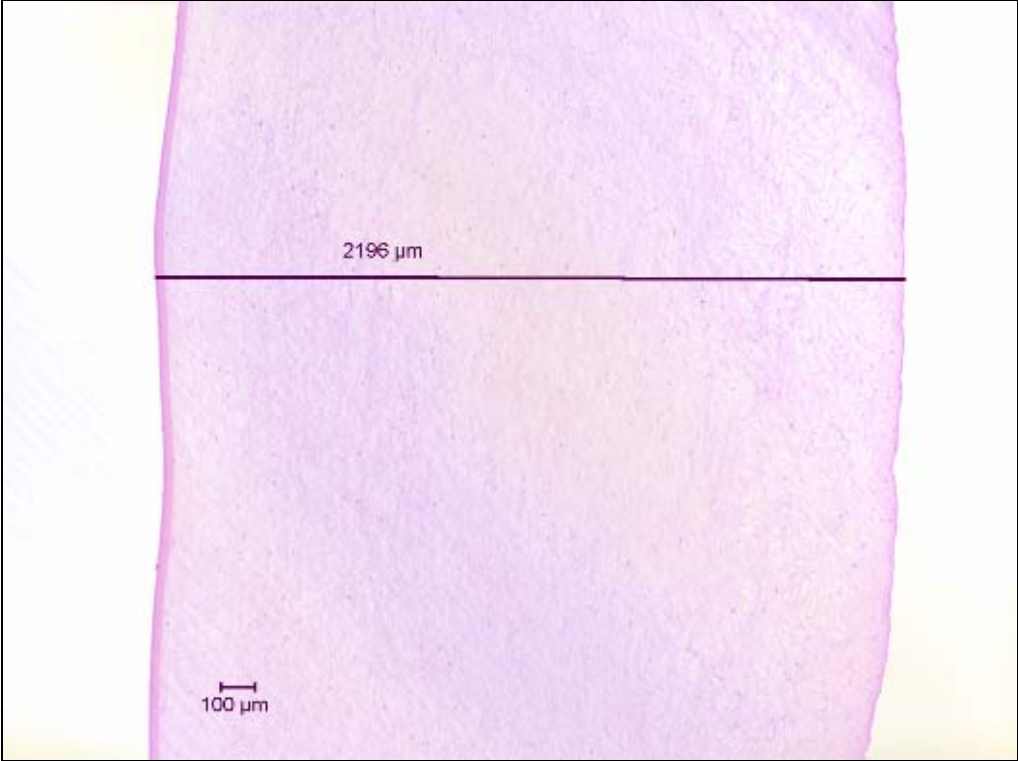
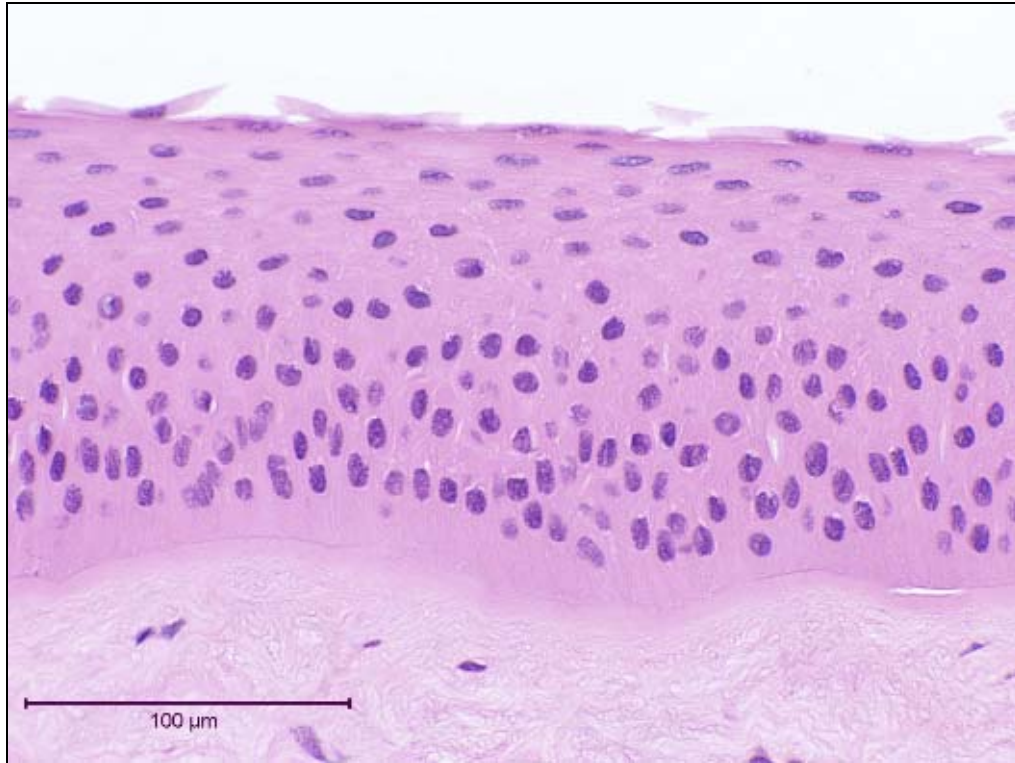
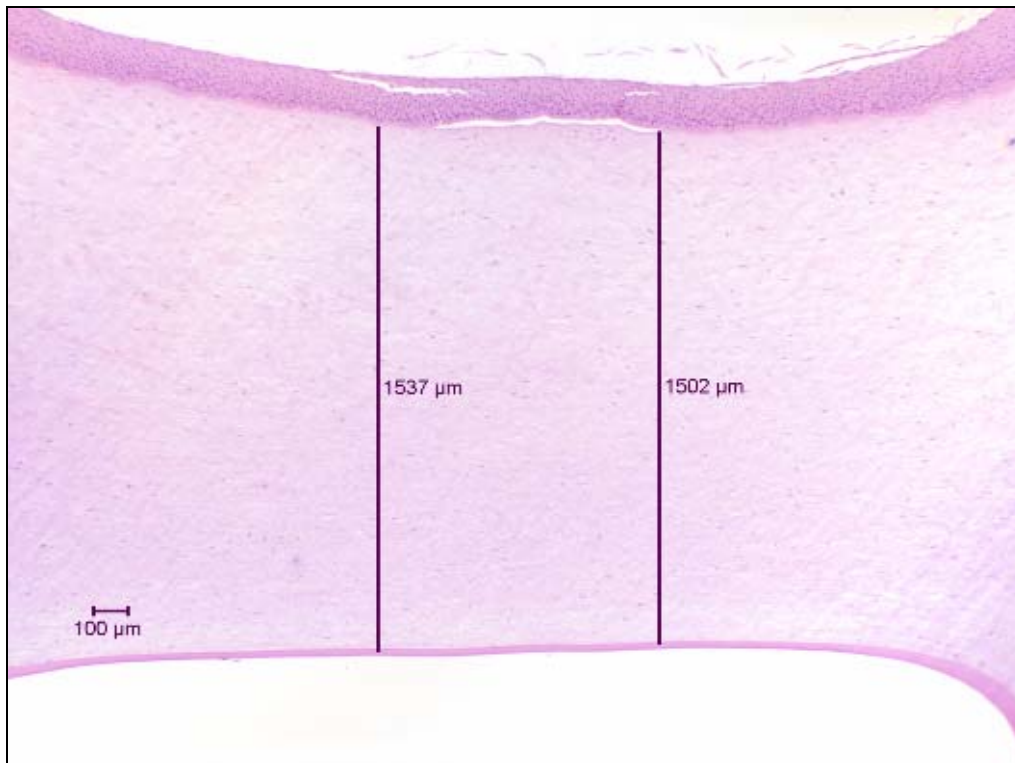


Figure 7. Sodium Percarbonate, 50% (w/v) suspension, 60-minute exposure, 4-hour post-exposure
(A) Epithelium (nonviable) (magnification 430x)



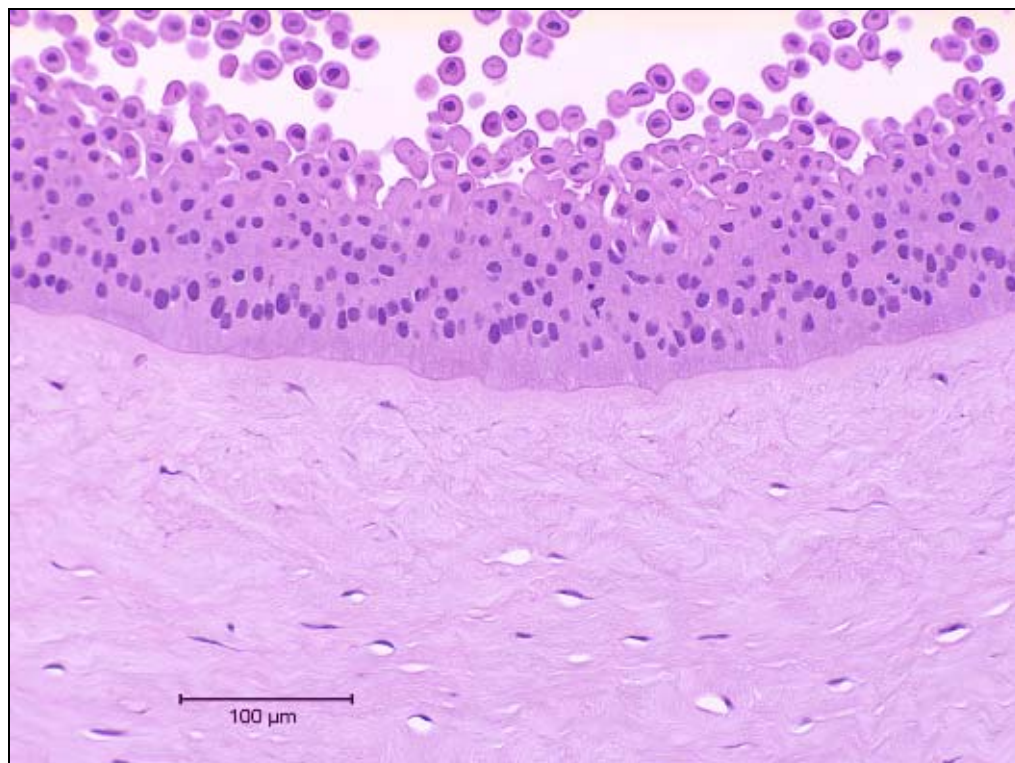
(C) Full thickness (magnification 45x)



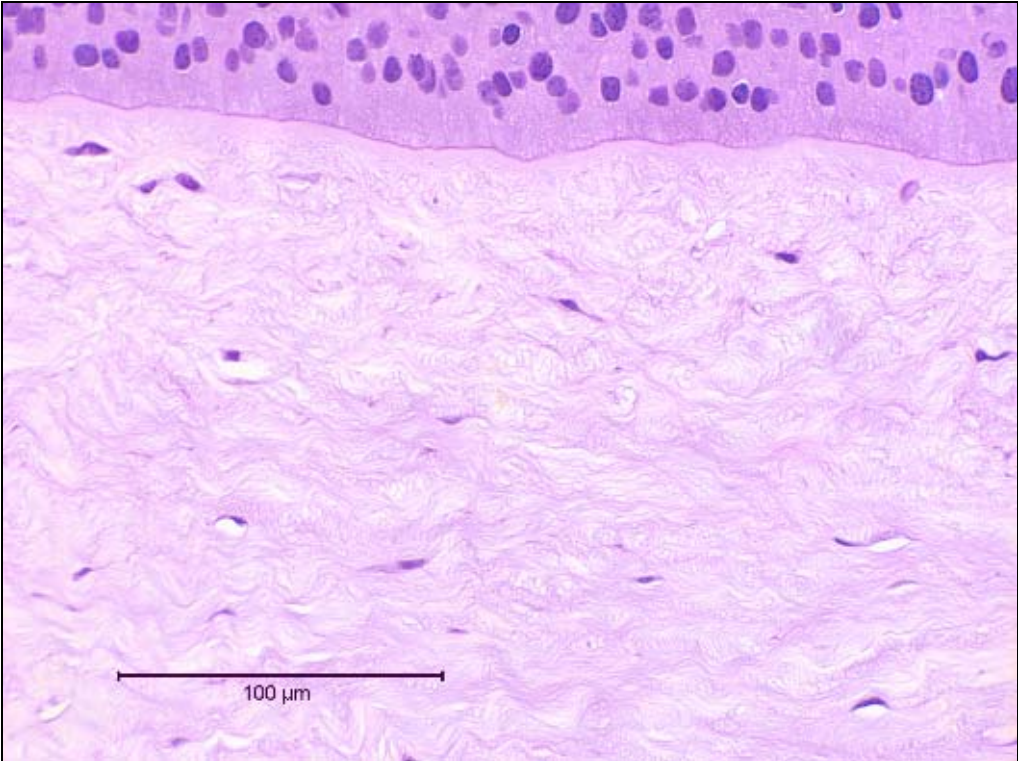
(C) Full thickness showing collagen delamination (magnification 45x)



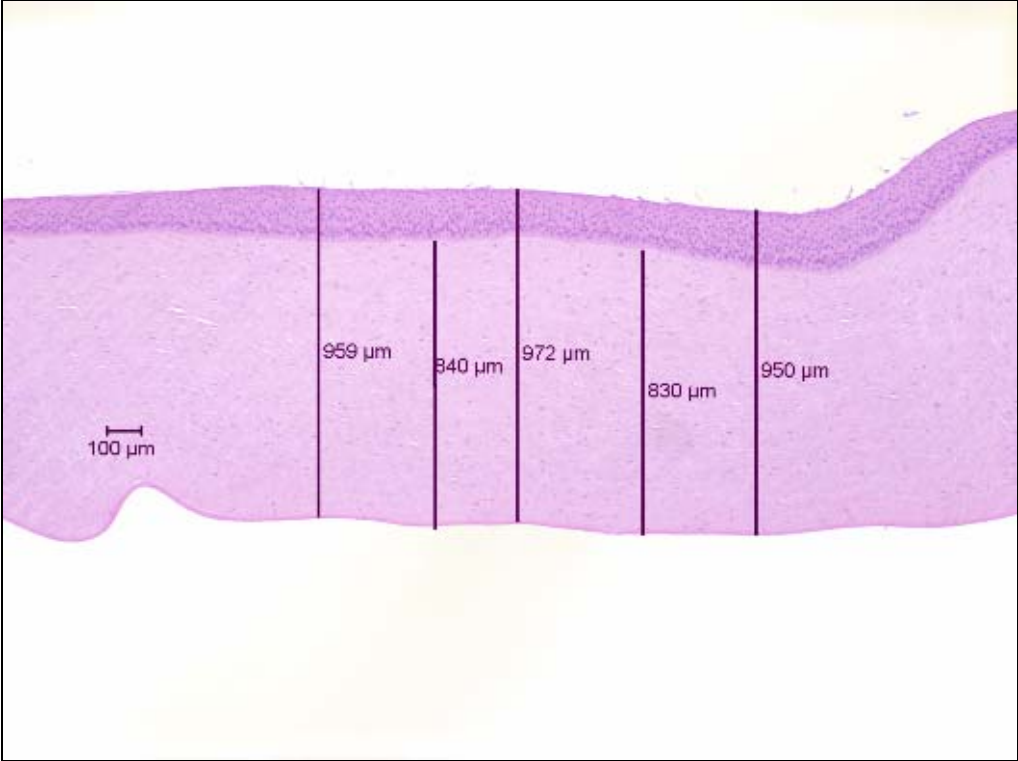
Figure 8. Sodium Percarbonate (60% in formulation), 50% (w/v) suspension, 10-minute exposure, 20-hour post-exposure
(A) Epithelium (magnification 230x)



(B) Stroma directly below Bowman's Layer showing the slight increase in collagen matrix vacuolization (magnification 430x)



(C) Full thickness (magnification 45x)



FORMULAS

Test Material #	Group	Raw Material	Percentage
1	Sodium Percarbonate	Reactive Chemical	
	(CAS #15630-89-4)	Mixture	40-45
	Sodium carbonate (CAS	Reactive Chemical	
	#497-19-8	Mixture	5-10
		Water	45-50
2	Sodium Percarbonate	Reactive Chemical	
	(CAS #15630-89-4)	Mixture	40-45
	Sodium carbonate (CAS	Reactive Chemical	
	#497-19-8	Mixture	5-10
		Water	45-50
3	Sodium Percarbonate	Reactive Chemical	
	(CAS #15630-89-4)	Mixture	25-30
	Sodium carbonate (CAS	Reactive Chemical	
	#497-19-8	Mixture	20-25
		Water	45-50

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Appendix G4

**Dataset Received from L'OREAL Advanced Research for an In-House
Porcine Corneal Opacity and Permeability Assay**

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Preliminary comments :

L'OREAL Advanced Research understood very early the usefulness of isolated cornea assay as a predictive tool for ocular irritancy. Due to constraints of supply and use of bovine eyes, we decided to use porcine corneas.

We have developed an in-house PCOP protocol to provide adequate safety data for cosmetic ingredients. Our PCOP protocol is basically that previously described by P. Gautheron, with some changes linked to species.

For liquid form and water-soluble materials we obtained a prediction model based on only one endpoint (O.D. 30) allowing to distinguish non irritating compounds ($MAS \leq 15$ if $O.D. 30 < 0.35$) from irritating compounds ($MAS > 15$ if $O.D. 30 \geq 0.35$).

Using this two classes scheme, 49 of the 50 raw ingredients tested in our PCOP assay were accurately classified. Only one was over-predicted. Agreement between *in vivo* and *in vitro* classification was high (concordance 98% -Kappa = 0.96, $p < 0.01$).

Predicted class (<i>in vitro</i>)	Observed class (<i>in vivo</i>)	
	Mild irritant MAS ≤ 15	Moderate/ Irritant / Severe MAS > 15
Mild irritant MAS ≤ 15	25	0
Moderate/ Irritant / Severe MAS > 15	1	24

As MAS were available for 43 of the materials, a linear regression was carried out to predict the Draize Maximum Average Score (MAS).

An equation PM was obtained to predict MAS value, but despite satisfactory statistical coefficients - $R^2 Y = 0.84$, concordance = 90 % - this algorithm is not recommended. Data analysis showed that 95% confidence interval was wide and there was too much uncertainty of the MAS prediction for it to be used.

We used the Draize test classification scheme according to French regulations applied to cosmetics (J. O. R. F. June 1992.) as follows :

MAS value	Class
≤ 15	mild irritant
>15 and ≤ 30	moderate irritant
> 30 and ≤ 50	irritant
> 50	severe irritant

Table 1 summarized our PCOP results obtained on 50 liquid and water-soluble compounds, selected on the basis of preexisting *in vivo* data - including 32 surfactants, 7 polymers, 5 solvents, 4 active ingredients and 2 dyes.

All compounds were tested *in vitro* at the same concentration as *in vivo*.

Some of them, including references, were tested in both PCOP and BCOP - See Table II and III for details.

Taking into account those results PCOP seems to be more suitable to predict class irritation than BCOP. Future work need to be done to complete this comparison.

Abbreviations used :

PCOP = Porcine cornea permeability and opacity assay;

BCOP = Bovine cornea permeability and opacity assay;

MAS = maximum average score;

OP₁₀ or OP₃₀ = opacity induced by a 10-min or 30 min- exposure of corneas, respectively;

O.D.₁₀ or O.D.₃₀ = optical density measured after a 10-min or 30 min- exposure of corneas, respectively;

PM = prediction model.

Table 1: PCOP results obtained on 50 liquid and water-soluble compounds

N° product	Concentration tested	PCOP Data				Predicted data		In vivo data (historical)	
		OP ₁₀	O.D. ₁₀	OP ₃₀	O.D. ₃₀	PCOP class	MAS (Class deducted)	MAS	class
1	0.5%	4	- 0.043	0.3	0.084	Mild	10.2 (Mild)	0.7	Mild
2	10%	-0.3	- 0.006	6.3	0.008	Mild	8.3 (Mild)	2.3	Mild
3	20%	-1	- 0.003	0.4	0.003	Mild	8.2 (Mild)	3.7	Mild
4	10%	6.7	0.041	53.9	0.092	Mild	10.4 (Mild)	4.0	Mild
5	5%	7.7	0.042	12.7	0.028	Mild	8.8 (Mild)	4.7	Mild
6	10%	-0.7	- 0.001	2.7	0.096	Mild	10.5 (Mild)	5.3	Mild
7	10%	-1.3	- 0.004	5.7	0.044	Mild	9.2 (Mild)	5.7	Mild
8	100%	1.7	0.014	1.3	0.066	Mild	9.8 (Mild)	8.5	Mild
9	100%	2.6	0.036	-2.7	- 0.034	Mild	7.2 (Mild)	9.8	Mild
10	3.1%	0.3	- 0.009	-0.3	- 0.008	Mild	7.9 (Mild)	10.7	Mild
11	100%	-5.6	- 0.002	-4.0	0.003	Mild	8.2 (Mild)	10.7	Mild
12	100%	3.3	- 0.002	2.0	0.013	Mild	8.4 (Mild)	10.8	Mild
13	100%	4.3	- 0.002	39.0	0.133	Mild	11.5 (Mild)	11.0	Mild
14	100%	5	- 0.004	-2.3	- 0.003	Mild	8.0 (Mild)	11.3	Mild
15	10%	0.3	- 0.017	2.8	0.021	Mild	8.6 Mild)	11.3	Mild
16	5%	5.6	0.421	19.0	1.040	Irrg.	29.4 (Mod.)	12.0	Mild
17	100%	1	0.007	4.7	0.028	Mild	8.8 (Mild)	12.0	Mild
18	100%	3	- 0.001	12.3	- 0.007	Mild	7.9 (Mild)	12.3	Mild
19	6.7%	4.7	0.212	15.0	0.296	Mild	15.3 (Mod.)	12.7	Mild
20	100%	7.3	0.056	21.2	0.014	Mild	8.4 (Mild)	12.8	Mild

N° product	Concentration tested	PCOP Data				Predicted data		In vivo data (historical)	
		OP ₁₀	O.D. ₁₀	OP ₃₀	O.D. ₃₀	PCOP class	MAS (Class deducted)	MAS	class
21	2%	3.3	0.042	5.0	0.056	Mild	9.5 (Mild)	13.0	Mild
22	100%	9.3	0.049	17.0	0.089	Mild	Not AppL	NA	Mild
23	100%	2	0.053	7.3	- 0.007	Mild	Not AppL	NA	Mild
24	100%	-2.4	0.012	-1.0	0.003	Mild	Not AppL	NA	Mild
25	10%	0.3	0.003	2.7	0.014	Mild	Not AppL	NA	Mild
26	100%	20.7	0.118	67.1	0.367	Irrg.	16.9 (Mod.)	16.0	Mod.
27	6%	16	1.641	14.0	2.060	Irrg.	38.7 (Irr. to Sev.)	30.6	Irr.
28	10%	6.3	0.516	40.5	2.081	Irrg.	38.8 (Irr. to Sev.)	31.0	Irr.
29	0.5%	23	0.739	25.5	0.451	Irrg.	18.8 (mod.)	31.0	Irr.
30	10%	31.3	0.876	38.7	1.268	Irrg.	32.5 (Irr. to Sev.)	31.3	Irr.
31	10%	7.3	0.343	7.7	2.202	Irrg.	39.2 (Irr. to Sev.)	31.7	Irr.
32	10%	24.7	0.979	17.3	0.918	Irrg.	27.8 (Irr. to Sev.)	31.7	Irr.
33	10%	13.7	1.041	3.0	1.764	Irrg.	37.2 (Irr. to Sev.)	32.7	Irr.
34	10%	20	0.868	46.0	1.488	Irrg.	34.9 (Irr. to Sev.)	33.7	Irr.
35	6%	14	0.659	32.5	1.896	Irrg.	37 (Irr. to Sev.)	34.7	Irr.
36	6%	35.3	0.919	30.3	1.548	Irrg.	35.5 (Irr. to Sev.)	35.3	Irr.
37	10%	13	0.613	11.7	1.123	Irrg.	30.6 (Mod.)	35.7	Irr.
38	10%	16.7	1.917	22.3	2.132	Irrg.	38.9 (Irr. to Sev.)	37.4	Irr.
39	10%	14.3	0.750	16.7	2.016	Irrg.	38.6 (Irr. to Sev.)	39.3	Irr.
40	10%	9.3	2.433	22.3	1.738	Irrg.	37 (Irr. to Sev.)	40.3	Irr.
41	10%	8.3	0.668	23.0	1.667	Irrg.	36.5 (Irr. to Sev.)	40.7	Irr.
42	10%	1.3	0.308	38.3	1.714	Irrg.	36.8 (Mod.)	43.0	Irr.
43	10%	11.3	0.786	18.0	2.094	Irrg.	38.9 (Irr. to Sev.)	45.0	Irr.
44	10%	29	1.568	33.3	1.978	Irrg.	38.4	46.0	Irr.

N° product	Concentration tested	PCOP Data				Predicted data		In vivo data (historical)	
		OP ₁₀	O.D. ₁₀	OP ₃₀	O.D. ₃₀	PCOP class	MAS (Class deducted)	MAS	class
							(Irr. to Sev.)		
45	10%	23	1.288	19.7	2.174	Irrg.	39.1 (Irr. to Sev.)	47.2	Irr.
46	10%	17.3	0.995	8.0	1.538	Irrg.	Not AppL	63.7	Sev.
47	10%	21.3	1.618	11.3	1.679	Irrg.	Not AppL	63.7	Sev
48	10%	16.7	0.495	27.3	0.878	Irrg.	Not AppL	NA	Irr.
49	10%	6.7	0.232	18.0	1.112	Irrg.	Not AppL	NA	Irr.
50	10%	10.7	0.639	48.3	0.997	Irrg.	Not AppL	NA	Irr.

OP₁₀. OP₃₀. O.D.₁₀ O.D.₃₀: Each data represents mean corrected value of three corneas.

NA: not available.

Not AppL: Not applicable

Predicted class is determined by the PM: $O.D._{30} < 0.35 \Rightarrow$ predict nonirritating (MAS ≤ 15 - mild irritant) - $O.D._{30} \geq$

$0.35 \Rightarrow$ predict irritating (Irrg.) corresponding to MAS > 15 , covering three French Draize classes - moderate, irritant, severe.

Predicted MAS is calculated using this algorithm $= 8.08 + 26.16 \times O.D._{30} - 5.47 \times O.D._{30}^2$, with deduction of Draize class in brackets. Evaluation of this PM was based on three classes – Mild irritant (MAS ≤ 15), Moderate irritant

($15 < MAS \leq 30$), irritant to severe (MAS > 30). Data analysis showed that 95% confidence interval was wide. There is too much uncertainty of the MAS prediction for it to be used.

Table II - References tested in PCOP and BCOP with historical data (N = 8)

N° PRODUCT	CONC	In vivo data (historical)		PCOP data					BCOP data						
		MAS	In vivo Class	OP ₁₀	O.D. ₁₀	OP ₃₀	O.D. ₃₀	Predicted class	OP ₁₀	O.D. ₁₀	Score 10	OP ₃₀	O.D. ₃₀	Score 30	Predicted Class
Propylene glycol (n°20)	100%	12.8	Mild	7.3	0.056	21.2	0.014	Mild	NA	NA	NA	11,7	0.001	1.8	1
Sodium dodecyl sulfate (n°38)	10%	37.4	Irr.	16.7	1.917	22.3	2.132	Irrg	NA	NA	NA	1.5	0.424	18	2
Triton X100 (n°40)	10%	40.3	Irr.	9.3	2.433	22.3	1.738	Irrg	3.2	2.717	43.9	2.1	5.197	79.5	3
Vaseline oil	100%	NI	Mild	-0.3	0.008	-1	-0.03	Mild	NA	NA	NA	NA	0.005	4.0	1
Tween 20 (n° 7)	10%	5.7	Mild	-1.3	0.004	5.7	0.044	Mild	0.3	0.003	0.3	1.8	0.001	1.8	1
<i>Ethanol</i>	100%	37 (at 1h)	Irr.	40	1.260	58.2	0.676	Irrg	26.9	2.912	70.6	NA	NA	NA	3
Ethanol	50%	NA	NA	8.3	0.036	18	0.075	Mild	NA	NA	22.9	NA	1.117	31.3	3
Ethanol	10%	NA	NA	-2.3	0.014	0.3	-0.016	Mild	NA	NA	NA	NA	0.021	0.5	1
Lactic Acid	10%	31.2	Irr.	78	0.928	271	1.552	Irrg	15.2	0.029	15.6	75.2	0.439	81.7	3
Hexadecyl trimethyl ammonium bromide (CTAB)	0.5%	NA	NA	42.3	0.562	53.0	1.270	Irrg	NA	NA	43.3	48.2	5.112	124.9	3

Numbers in brackets refer to table I.

NA: not available.

TABLE III: Results obtained on compounds tested in both PCOP and BCOP (N = 15)

N°	CONC TESTED	In vivo data (historical)		PCOP data					BCOP data						
		MAS	Classe	OP ₁₀	O.D. ₁₀	OP ₃₀	O.D. ₃₀	Predicted Class	OP ₁₀	O.D. ₁₀	Score 10	OP ₃₀	O.D. ₃₀	Score 30	Predicted Class
8	100%	8,5	Mild	1,7	0,014	1,3	0,066	Mild	NA	NA	NA	0,8	-0,006	0,7	1
13	100%	11,0	Mild	4,3	-0,002	39,0	0,133	Mild	4,4	0,040	5,0	24,7	0,958	39,1	2 or 3
18	100%	12,3	Mild	3,0	-0,001	12,3	-0,007	Mild	NA	NA	NA	5,8	0,057	6,6	1
20	100%	12,8	Mild	7,3	0,056	21,2	0,014	Mild	NA	NA	NA	11,7	0,424	18,0	2
26	100%	16,0	Mod.	20,7	0,118	67,1	0,367	Irrg	71,5	0,971	86,1	58,6	2,346	93,8	3
A	10%	30,3	Irrg	47,3	1,256	186,0	0,796	Irrg	12,1	1,505	34,7	51,3	4,107	112,9	3
30	10%	31,3	Irrg	31,3	0,876	38,7	1,268	Irrg	56,8	1,786	83,6	98,8	2,327	133,7	3
31	10%	31,7	Irrg	7,3	0,343	7,7	2,202	Irrg	2,5	1,058	18,4	3,0	3,238	51,6	2 or 3
32	10%	31,7	Irrg	24,7	0,979	17,3	0,918	Irrg	3,7	1,977	33,4	3,5	5,231	82,0	3
33	10%	32,7	Irrg	13,7	1,041	3,0	1,764	Irrg	0,3	0,860	13,2	2,7	4,439	69,8	3
39	10%	39,3	Irrg	14,3	0,750	16,7	2,016	Irrg	0,4	0,721	11,2	3,9	1,043	16,9	2
42	10%	43,0	Irrg	1,3	0,308	38,3	1,714	Irrg	5,7	1,082	22,0	6,1	5,392	86,9	3
43	10%	45,0	Irrg	11,3	0,786	18,0	2,094	Irrg	3,6	1,077	19,8	3,6	3,921	62,4	3
45	10%	47,2	Irrg	23,0	1,288	19,7	2,174	Irrg	5,1	3,098	51,6	2,3	5,040	77,9	3
46	10%	63,7	Irrg	17,3	0,995	8,0	1,538	Irrg	4,9	1,812	32,1	2,4	3,854	60,2	3

Product numbers refer to table I .

Our BCOP protocol is a variation on the original protocol developed by P. GAUTHERON .

Corneal score = OP + (15 x O.D.). Classification depends on corneal scores at 30 minutes completed with results at 10 minutes :

Score at 30 min	Class
≤ 10	Class 1 : mild irritant
10 - 25	Class 2 : moderate irritant if score 10 mn ≤ 10 Class 2 or 3 if $10 < \text{score } 10 \text{ mn} \leq 25$ Class 3 : irritant to strong irritant if score 10 mn >25
25 - 55	Class 2 or 3 if score 10 mn ≤ 10 Class 3 : irritant to strong irritant if score 10 mn >10
>55	Class 3 : irritant to strong irritant

Appendix G5

Supporting Analyses Received from IIVS for Gettings et al. (1996) Study

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IIVS Submission - In Vivo Data and Analysis for the Gettings et al. (1996) Study

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	1	HZA	24	1	4	1	2	1	1	33	EPA
			48	1	3	0	2	1	0	21	7
			72	1	1	0	2	1	1	13	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
GHS Tissue											
	1	HZA	33	1.0	2.7	0.3	2.0	1.0	0.7	7	7
Summary block used analysis of the twenty combinations											
	ANIMAL ID										
	1	HZA	33	1.0	2.7	0.3	2.0	1.0	0.7	7	7
	2	HZA	27	1.0	1.3	0.7	2.3	1.3	1.3	22	22
	3	HZA	34	1.0	1.7	1.0	2.7	1.7	1.3	7	7
	4	HZA	37	1.0	3.0	1.0	2.0	1.7	1.3	14	14
	5	HZA	35	1.0	2.3	0.7	2.3	1.3	0.3	22	22
	6	HZA	39	1.0	3.0	0.7	2.7	1.7	1.7	21	21
Dose Vol		0.1									

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	1	HZB*	24	1	1	1	2	1	0	16	EPA
			48	1	1	0	2	1	1	13	3
			72	0	0	0	0	0	0	0	GHS
			7 days							0	3
			14 days							0	
			21 days							0	
GHS Tissue											
	1	HZB*	16	0.7	0.7	0.3	1.3	0.7	0.3	3	3
Summary block used analysis of the twenty combinations											
	ANIMAL ID										
	1	HZB*	16	0.7	0.7	0.3	1.3	0.7	0.3	3	3
	2	HZB*	4	0.0	0.0	0.0	1.0	0.0	0.0	2	2
	3	HZB*	11	1.0	1.0	0.0	1.3	1.0	0.0	7	7
	4	HZB*	27	0.7	1.0	0.3	1.7	1.0	0.7	3	7
	5	HZB*	35	1.0	2.3	1.0	2.0	1.3	1.0	7	7
	6	HZB*	0	0.3	0.3	0.3	1.7	1.0	0.0	3	7
Dose Vol		0.1									

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZA	24	1	2	1	2	2	2	27	EPA	
			48	1	1	1	3	1	2	22	22	
			72	1	1	0	2	1	0	11	GHS	
			7 days	1	1	0	2	1	1	13	22	
			14 days	1	1	0	2	2	1	15		
			21 days	1	1	0	2	1	0	11		
	2	HZA	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	2	HZA		27	1	1.333333	0.666667	2.333333333	1.333333333	1.333333333	22	22
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	1	0.833333	2.5	1.5	22	22	Combina- tion block #2	1,3,4	1	1	
	GHS Rating	2	4	2	4	22	22	GHS Rating	2	4	4	
	1,2,4	1	0.833333	2.166667	1.5	22	22	1,3,5	1	0.833333		
	GHS Rating	2	4	2	4	22	22	GHS Rating	2	4	4	
	1,2,5	1	0.666667	2.333333	1.333333	22	22	1,3,6	1	0.833333		
	GHS Rating	2	4	2	4	22	22	GHS Rating	2	4	4	
	1,2,6	1	0.666667	2.5	1.5	22	22	1,4,5	1	0.833333		
GHS Rating	2	4	2	4	22	22	GHS Rating	2	4	4		

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZB*	24	0	0	0	2	0	0	4	EPA	
			48	0	0	0	0	0	0	0	2	
			72							0	GHS	
			7 days							0	2	
			14 days							0		
			21 days							0		
	2	HZB*	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	2	HZB*		4	0	0	0	1	0	0	2	2
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0.833333	0.166667	1.333333	0.833333	7	7	Combina- tion block #2	1,3,4	0.833333	0.333333	
	GHS Rating	4	4	4	4	7	7	GHS Rating	4	4	4	
	1,2,4	0.666667	0.333333	1.5	0.833333	3	7	1,3,5	1	0.666667		
	GHS Rating	4	4	4	4	3	7	GHS Rating	2	4	4	
	1,2,5	0.833333	0.666667	1.666667	1	7	7	1,3,6	0.833333	0.333333		
	GHS Rating	4	4	4	4	7	7	GHS Rating	4	4	4	
	1,2,6	0.5	0.333333	1.5	0.833333	3	7	1,4,5	0.833333	0.666667		
GHS Rating	4	4	4	4	3	7	GHS Rating	4	4	4		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA		REDNESS	CHEMOSIS	DISCHARGE		
0.1	3	HZA	24	1	3	1	3	2	2	34	EPA
			48	1	1	1	3	1	2	22	7
			72	1	1	1	2	2	0	18	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZA	34	1	1.666667	1	2.666666667	1.66666667	1.333333333	7	7
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
2.333333	1.666667	14	14	Combina- tion block #3	1,4,6 GHS Rating	1.0	0.8	2.3	1.7	21	21
2	4	14	14		1,5,6 GHS Rating	2	4	2	4	21	21
2.5	1.5	22	22		2,3,4 GHS Rating	1.0	0.7	2.5	1.5	22	22
2	4	22	22		2,3,5 GHS Rating	2	4	2	4	22	22
2.666667	1.666667	21	21		2,3,5 GHS Rating	1.0	1.0	2.5	1.7	22	22
2	4	21	21		2,3,5 GHS Rating	2	2	2	4	22	22
2.166667	1.5	22	22		2,3,5 GHS Rating	1.0	0.8	2.5	1.5	22	22
2	4	22	22		2,3,5 GHS Rating	2	4	2	4	22	22

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA		REDNESS	CHEMOSIS	DISCHARGE		
0.1	3	HZB*	24	1	1	0	2	1	0	11	EPA
			48	1	1	0	1	1	0	9	7
			72	1	1	0	1	1	0	9	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZB*	11	1	1	0	1.333333333	1	0	7	7
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
1.5	1	7	7	Combina- tion block #3	1,4,6 GHS Rating	0.7	0.3	1.7	1.0	3	7
4	4	7	7		1,5,6 GHS Rating	4	4	4	4	3	7
1.666667	1.166667	7	7		2,3,4 GHS Rating	0.8	0.7	1.8	1.2	7	7
4	4	7	7		2,3,5 GHS Rating	4	4	4	4	7	7
1.5	1	7	7		2,3,5 GHS Rating	0.8	0.2	1.5	1.0	7	7
4	4	7	7		2,3,5 GHS Rating	4	4	4	4	7	7
1.833333	1.166667	7	7		2,3,5 GHS Rating	1.0	0.5	1.7	1.2	7	7
4	4	7	7		2,3,5 GHS Rating	2	4	4	4	7	7

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	4	HZA	24	1	4	1	2	2	2	37	EPA
			48	1	3	1	2	1	0	26	14
			72	1	2	1	2	2	2	27	GHS
			7 days	1	1	0	1	1	0	9	14
			14 days	0	0	0	0	0	0	0	
			21 days							0	
	4	HZA	37	1	3	1	2	1.666666667	1.333333333	14	14
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combina- tion block #4	2,3,6	1.0	0.8	2.7	1.7	22	22	Combina- tion block #5	3,4,5	1.0	1.0
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	2
	2,4,5	1.0	0.8	2.3	1.5	22	22		3,4,6	1.0	1.0
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	2
	2,4,6	1.0	0.8	2.5	1.7	22	22		3,5,6	1.0	0.8
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	4
	2,5,6	1.0	0.7	2.5	1.5	22	22		4,5,6	1.0	0.8
GHS Rating	2	4	2	4	22	22	GHS Rating	2	4		

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	4	HZB*	24	1	2	1	2	2	2	27	EPA
			48	1	1	0	2	1	0	11	3
			72	0	0	0	1	0	0	2	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	4	HZB*	27	0.666667	1	0.333333	1.66666667	1	0.666666667	3	7
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combina- tion block #4	2,3,6	0.7	0.2	1.5	1.0	7	7	Combina- tion block #5	3,4,5	1.0	0.7
	GHS Rating	4	4	4	4	7	7		GHS Rating	2	4
	2,4,5	0.8	0.7	1.8	1.2	7	7		3,4,6	0.8	0.3
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4
	2,4,6	0.5	0.3	1.7	1.0	3	7		3,5,6	1.0	0.7
	GHS Rating	4	4	4	4	3	7		GHS Rating	2	4
	2,5,6	0.7	0.7	1.8	1.2	7	7		4,5,6	0.8	0.7
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZA	24	1	4	1	3	2	0	35	EPA	
			48	1	2	1	2	1	1	23	22	
			72	1	1	0	2	1	0	11	GHS	
			7 days	1	1	0	0	0	0	5	22	
			14 days	1	1	0	0	0	0	5		
			21 days	1	1	0	0	0	0	5		
	5	HZA	35	1	2.333333	0.666667	2.333333333	1.333333333	0.333333333	22	22	
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	2	22		
2.5	1.7	22	22				HZA	1,2,4	2	22		
2	4	22	22					1,2,5	2	22		
2.7	1.7	21	21					1,2,6	2	22		
2	4	21	21					1,3,4	2	14		
2.7	1.7	22	22					1,3,5	2	22		
2	4	22	22					1,3,6	2	21		
2.5	1.7	22	22					1,4,5	2	22		
2	4	22	22					1,4,6	2	21		
								1,5,6	2	22		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZB*	24	1	4	1	2	2	1	35	EPA	
			48	1	1	1	2	1	1	18	7	
			72	1	2	1	2	1	1	23	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	5	HZB*	35	1	2.333333	1	2	1.333333333	1	7	7	
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	4	7		
1.8	1.2	7	7				HZB*	1,2,4	4	7		
4	4	7	7					1,2,5	4	7		
1.7	1.0	7	7					1,2,6	4	7		
4	4	7	7					1,3,4	4	7		
1.8	1.2	7	7					1,3,5	2	7		
4	4	7	7					1,3,6	4	7		
1.8	1.2	7	7					1,4,5	4	7		
4	4	7	7					1,4,6	4	7		
								1,5,6	4	7		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZA	24	1	4	1	3	2	2	39	EPA
			48	1	3	1	3	2	2	34	21
			72	1	2	0	2	1	1	18	GHS
			7 days	1	1	0	1	1	1	11	21
			14 days	1	1	0	1	0	0	7	
			21 days	0	0	0	0	0	0	0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	6	HZA	39	1	3	0.666667	2.66666667	1.666666667	1.666666667	21	21
22		2,3,4	2	22		22					
22		2,3,5	2	22		22					
22		2,3,6	2	22		22					
22		2,4,5	2	22		22					
14		2,4,6	2	22		22					
22		2,5,6	2	22		22					
21		3,4,5	2	22		22					
22		3,4,6	2	21		21					
21		3,5,6	2	22		22					
22		4,5,6	2	22		22					
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZB*	24	1	1	1	2	2	0	0	EPA
			48	0	0	0	2	1	0	0	3
			72	0	0	0	1	0	0	0	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days								0
			21 days								0
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	6	HZB*	0	0.333333	0.333333	0.333333	1.66666667	1	0	3	7
7		2,3,4	4	7		7					
3		2,3,5	2	7		7					
7		2,3,6	4	7		7					
3		2,4,5	4	7		7					
7		2,4,6	4	7		3					
7		2,5,6	4	7		7					
7		3,4,5	2	7		7					
7		3,4,6	4	7		7					
3		3,5,6	2	7		7					
7		4,5,6	4	7		7					

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZC*	24	0	0	0	2	1	2	10	EPA	
			48	0	0	0	1	0	0	2	3	
			72	0	0	0	0	0	0	0	GHS	
			7 days							0	3	
			14 days							0		
			21 days							0		
GHS Tissue		1 HZC*	10	0.0	0.0	0.0	1.0	0.3	0.7	3	3	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZC*	10	0.0	0.0	0.0	1.0	0.3	0.7	3	3	
	2	HZC*	32	1.0	1.7	0.3	2.0	1.3	0.7	7	7	
	3	HZC*	35	1.0	2.3	1.0	2.0	1.3	1.3	7	7	
	4	HZC*	6	0.0	0.0	0.0	1.7	0.3	0.0	3	7	
	5	HZC*	35	1.0	2.7	0.7	2.0	1.3	0.7	7	7	
	6	HZC*	11	0.7	0.7	0.0	1.0	0.3	0.0	3	3	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F41401	HZD*	24	1	1	0	3	2	3	21	EPA	
			48	1	1	0	2	1	0	11	7	
			72	1	1	0	1	1	0	9	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
GHS Tissue		F41401 HZD*	21	1.0	1.0	0.0	2.0	1.3	1.0	7	7	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	F41401	HZD*	21	1.0	1.0	0.0	2.0	1.3	1.0	7	7	
	2	HZD*	15	0.7	0.7	0.0	1.7	0.7	1.0	3	7	
	3	HZD*	19	0.3	0.3	0.0	1.7	1.0	1.0	3	7	
	4	HZD*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	F41356	HZD*	11	0.7	0.7	0.0	1.0	0.3	0.0	3	3	
	F41386	HZD*	13	0.5	0.5	0.0	1.0	0.5	0.5	2	2	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	2	HZC*	24	1	3	1	2	2	2	32	EPA
			48	1	1	0	2	1	0	11	7
			72	1	1	0	2	1	0	11	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	2	HZC*	32	1	1.666667	0.333333	2	1.333333333	0.666666667	7	7
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	1	0.666667	2	1.333333	7	7	Combina- tion block #2	1,3,4	0.5	0.5
	GHS Rating	2	4	2	4	7	7		GHS Rating	4	4
	1,2,4	0.5	0.166667	1.833333	0.833333	7	7		1,3,5	1	0.833333
	GHS Rating	4	4	4	4	7	7		GHS Rating	2	4
	1,2,5	1	0.5	2	1.333333	7	7		1,3,6	0.833333	0.5
	GHS Rating	2	4	2	4	7	7		GHS Rating	4	4
	1,2,6	0.833333	0.166667	1.5	0.833333	7	7		1,4,5	0.5	0.333333
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4		
	2	HZD*	15	0.666667	0.666667	0	1.666666667	0.666666667	1	3	7
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	0.833333	0	1.833333	1.166667	7	7	Combina- tion block #2	1,3,4	0.666667	0
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4
	1,2,4	0.833333	0	1.833333	1	7	7		1,3,5	0.833333	0
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4
	1,2,5	0.833333	0	1.833333	1	7	7		1,3,6	0.75	0
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4
	1,2,6	0.833333	0	1.833333	1	7	7		1,4,5	0.833333	0
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZC*	24	1	4	1	2	1	2	35	EPA	
			48	1	2	1	2	1	0	21	7	
			72	1	1	1	2	2	2	22	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZC*	35	1	2.333333	1	2	1.33333333	1.33333333	7	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.833333	0.833333	7	7	Combina- tion block #3	1,4,6	0.3	0.0	1.3	0.3	3	7	
4	4	7	7		GHS Rating	4	4	4	4	3	7	
2	1.333333	7	7		1,5,6	0.8	0.3	1.5	0.8	7	7	
2	4	7	7		GHS Rating	4	4	4	4	7	7	
1.5	0.833333	7	7		2,3,4	1.0	0.7	2.0	1.3	7	7	
4	4	7	7		GHS Rating	2	4	2	4	7	7	
1.833333	0.833333	7	7		2,3,5	1.0	0.8	2.0	1.3	7	7	
4	4	7	7		GHS Rating	2	4	2	4	7	7	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZD*	24	1	1	0	2	2	3	19	EPA	
			48	0	0	0	2	1	0	6	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZD*	19	0.333333	0.333333	0	1.66666667	1	1	3	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.833333	1.166667	7	7	Combina- tion block #3	1,4,6	0.8	0.0	1.5	0.9	7	7	
4	4	7	7		GHS Rating	4	4	4	4	7	7	
1.833333	1.166667	7	7		1,5,6	0.8	0.0	1.5	0.9	7	7	
4	4	7	7		GHS Rating	4	4	4	4	7	7	
1.833333	1.166667	7	7		2,3,4	0.5	0.0	1.7	0.8	3	7	
4	4	7	7		GHS Rating	4	4	4	4	3	7	
1.5	0.833333	7	7		2,3,5	0.7	0.0	1.7	0.8	3	7	
4	4	7	7		GHS Rating	4	4	4	4	3	7	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZC*	24	0	0	0	2	1	0	6	EPA	
			48	0	0	0	2	0	0	4	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	4	HZC*	6	0	0	0	1.66666667	0.33333333	0	3	7	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	1.0	0.7	2.0	1.3	7	7	7	Combina- tion block #5	3,4,5	1.0	0.8
	GHS Rating	2	4	2	4	7	7	7		GHS Rating	2	4
	2,4,5	1.0	0.5	2.0	1.3	7	7	7		3,4,6	0.8	0.5
	GHS Rating	2	4	2	4	7	7	7		GHS Rating	4	4
	2,4,6	0.8	0.2	1.8	0.8	7	7	7		3,5,6	1.0	0.8
	GHS Rating	4	4	4	4	7	7	7		GHS Rating	2	4
	2,5,6	1.0	0.5	2.0	1.3	7	7	7		4,5,6	0.8	0.3
GHS Rating	2	4	2	4	7	7	7	GHS Rating	4	4		
	4	HZD*	2	0	0	0	0.5	0	0	0	2	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	0.6	0.0	1.7	0.8	3	7	7	Combina- tion block #5	3,4,5	0.5	0.0
	GHS Rating	4	4	4	4	3	7	7		GHS Rating	4	4
	2,4,5	0.7	0.0	1.3	0.5	3	7	7		3,4,6	0.4	0.0
	GHS Rating	4	4	4	4	3	7	7		GHS Rating	4	4
	2,4,6	0.6	0.0	1.3	0.6	3	7	7		3,5,6	0.6	0.0
	GHS Rating	4	4	4	4	3	7	7		GHS Rating	4	4
	2,5,6	0.7	0.0	1.3	0.6	3	7	7		4,5,6	0.6	0.0
GHS Rating	4	4	4	4	3	7	7	GHS Rating	4	4		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZC*	24	1	4	1	2	2	1	35	EPA	
			48	1	3	1	2	1	1	28	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZC*	35	1	2.666667	0.666667	2	1.333333333	0.666666667	7	7	
Redness	Chemosis	DtC EPA	DtC GHS					Summary				
2.0	1.3	7	7					HZC*	1,2,3	2	7	
2	4	7	7						1,2,4	4	7	
1.8	0.8	7	7						1,2,5	2	7	
4	4	7	7						1,2,6	4	7	
2.0	1.3	7	7						1,3,4	4	7	
2	4	7	7						1,3,5	2	7	
1.8	0.8	7	7						1,3,6	4	7	
4	4	7	7						1,4,5	4	7	
									1,4,6	4	7	
									1,5,6	4	7	
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F41356	HZD*	24	1	1	0	2	1	0	11	EPA	
			48	1	1	0	1	0	0	7	3	
			72	0	0	0	0	0	0	0	GHS	
			7 days							0	3	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	F41356	HZD*	11	0.666667	0.666667	0	1	0.333333333	0	3	3	
Redness	Chemosis	DtC EPA	DtC GHS					Summary				
1.3	0.7	3	7					HZD*	1,2,3	4	7	
4	4	3	7						1,2,4	4	7	
1.3	0.8	3	7						1,2,5	4	7	
4	4	3	7						1,2,6	4	7	
1.3	0.8	3	7						1,3,4	4	7	
4	4	3	7						1,3,5	4	7	
1.0	0.4	3	3						1,3,6	4	7	
4	4	3	3						1,4,5	4	7	
									1,4,6	4	7	
									1,5,6	4	7	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	6	HZC*	24	1	1	0	2	1	0	11	EPA		
			48	1	1	0	1	0	0	7	3		
			72	0	0	0	0	0	0	0	GHS		
			7 days							0	3		
			14 days							0			
			21 days							0			
			ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
			6	HZC*	11	0.666667	0.666667	0	1	0.3333333333	0	3	3
			7	2,3,4	2	7		7					
			7	2,3,5	2	7		7					
7	2,3,6	2	7		7								
7	2,4,5	2	7		7								
7	2,4,6	4	7		7								
7	2,5,6	2	7		7								
7	3,4,5	2	7		7								
7	3,4,6	4	7		7								
3	3,5,6	2	7		7								
7	4,5,6	4	7		7								
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR		
0.1	F41386	HZD*	24	1	1			0	2			1	1
			48	0	0	0	0	0	0	0	2		
			72							0	GHS		
			7 days							0	2		
			14 days							0			
			21 days							0			
			ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
			F41386	HZD*	13	0.5	0.5	0	1	0.5	0.5	2	2
			7	2,3,4	4	7		3					
			7	2,3,5	4	7		3					
7	2,3,6	4	7		3								
7	2,4,5	4	7		3								
7	2,4,6	4	7		3								
7	2,5,6	4	7		3								
7	3,4,5	4	7		3								
7	3,4,6	4	7		3								
7	3,5,6	4	7		3								
7	4,5,6	4	3		3								

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZE	24	0	0	0	1	1	0	0	4	EPA
			48	0	0	0	1	0	0	0	2	2
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
GHS Tissue		1 HZE	4	0.0	0.0	0.0	0.7	0.3	0.0	2	3	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZE	4	0.0	0.0	0.0	0.7	0.3	0.0	2	3	
	2	HZE	20	0.3	0.3	0.3	1.3	0.7	0.3	3	3	
	3	HZE	29	1.0	1.3	0.3	2.0	1.7	1.7	7	7	
	4	HZE	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	5	HZE	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	6	HZE	32	1.0	2.7	0.3	2.0	1.7	1.0	22	22	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZF	24	1	3	1	2	2	2	32	EPA	
			48	1	2	1	3	2	2	29	14	
			72	1	1	1	3	2	1	22	GHS	
			7 days	1	1	0	1	1	1	11	14	
			14 days	0	0	0	0	0	0	0		
			21 days							0		
GHS Tissue		1 HZF	32	1.0	2.0	1.0	2.7	2.0	1.7	14	14	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZF	32	1.0	2.0	1.0	2.7	2.0	1.7	14	14	
	2	HZF	29	1.0	1.3	0.7	2.7	1.3	1.0	7	7	
	3	HZF	34	1.0	2.3	0.7	2.0	2.0	2.3	22	22	
	4	HZF	41	1.0	3.3	1.0	2.0	2.3	2.7	22	22	
	5	HZF	39	1.0	2.3	1.0	2.3	2.0	0.7	14	14	
	6	HZF	32	1.0	2.0	0.7	1.7	1.7	0.7	7	7	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	2	HZE	24	1	1	1	2	2	1	20	EPA
			48	0	0	0	2	0	0	4	3
			72	0	0	0	0	0	0	0	GHS
			7 days	0	0	0	0	0	0	0	3
			14 days								0
			21 days								0
	2	HZE	20	0.333333	0.333333	0.333333	1.333333333	0.666666667	0.333333333	3	3
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	0.666667	0.333333	1.666667	1.166667	7	7	Combina- tion block #2	1,3,4	0.5	0.166667
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4
	1,2,4	0.166667	0.166667	1	0.5	3	3		1,3,5	0.5	0.166667
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4
	1,2,5	0.166667	0.166667	1	0.5	3	3		1,3,6	1	0.333333
	GHS Rating	4	4	4	4	3	3		GHS Rating	2	4
	1,2,6	0.666667	0.333333	1.666667	1.166667	22	22		1,4,5	0	0
GHS Rating	4	4	4	4	22	22	GHS Rating	4	4		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	2	HZF	24	1	2	1	3	2	2	29	EPA
			48	1	1	1	3	1	1	20	7
			72	1	1	0	2	1	0	11	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days								0
			21 days								0
	2	HZF	29	1	1.333333	0.666667	2.666666667	1.333333333	1	7	7
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	1	0.833333	2.666667	2	22	22	Combina- tion block #2	1,3,4	1	1
	GHS Rating	2	4	2	2	22	22		GHS Rating	2	2
	1,2,4	1	1	2.666667	2.166667	22	22		1,3,5	1	1
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	2
	1,2,5	1	1	2.666667	2	14	14		1,3,6	1	0.833333
	GHS Rating	2	2	2	2	14	14		GHS Rating	2	4
	1,2,6	1	0.833333	2.666667	1.833333	14	14		1,4,5	1	1
GHS Rating	2	4	2	4	14	14	GHS Rating	2	2		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	3	HZE	24	1	2	1	2	2	3	29	EPA
			48	1	1	0	2	2	2	17	7
			72	1	1	0	2	1	0	11	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZE	29	1	1.333333	0.333333	2	1.66666667	1.66666667	7	7
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
1.333333	1	7	7	Combina- tion block #3	1,4,6	0.5	0.2	1.3	1.0	22	22
4	4	7	7		GHS Rating	4	4	4	4	22	22
1.333333	1	7	7		1,5,6	0.5	0.2	1.3	1.0	22	22
4	4	7	7		GHS Rating	4	4	4	4	22	22
2	1.666667	22	22		2,3,4	0.7	0.3	1.7	1.2	7	7
4	4	22	22		GHS Rating	4	4	4	4	7	7
0.583333	0.166667	2	3		2,3,5	0.7	0.3	1.7	1.2	7	7
4	4	2	3		GHS Rating	4	4	4	4	7	7

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	3	HZF	24	1	3	1	2	2	3	34	EPA
			48	1	3	1	2	2	2	32	22
			72	1	1	0	2	2	2	17	GHS
			7 days	1	1	0	3	2	3	21	22
			14 days	1	1	0	2	1	1	13	
			21 days	1	1	0	2	1	1	13	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZF	34	1	2.333333	0.666667	2	2	2.333333333	22	22
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
2.333333	2.166667	22	22	Combina- tion block #3	1,4,6	1.0	1.0	2.3	2.2	22	22
2	2	22	22		GHS Rating	2	2	2	2	22	22
2.5	2	22	22		1,5,6	1.0	1.0	2.5	2.0	14	14
2	2	22	22		GHS Rating	2	2	2	2	14	14
2.333333	2	22	22		2,3,4	1.0	0.8	2.3	2.2	22	22
2	2	22	22		GHS Rating	2	4	2	2	22	22
2.5	2.166667	22	22		2,3,5	1.0	0.8	2.5	2.0	22	22
2	2	22	22		GHS Rating	2	4	2	2	22	22

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZE	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	4	HZE	2	0	0	0	0.5	0	0	0	2	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combinatio block #4	2,3,6	1.0	0.3	2.0	1.7	22	22	Combinatio block #5	3,4,5	0.5	0.2	
	GHS Rating	4	4	2	4	22	22		GHS Rating	4	4	
	2,4,5	0.2	0.2	0.9	0.3	3	3		3,4,6	1.0	0.3	
	GHS Rating	4	4	4	4	3	3		GHS Rating	2	4	
	2,4,6	0.7	0.3	1.7	1.2	22	22		3,5,6	1.0	0.3	
	GHS Rating	4	4	4	4	22	22		GHS Rating	2	4	
	2,5,6	0.7	0.3	1.7	1.2	22	22		4,5,6	0.5	0.2	
GHS Rating	4	4	4	4	22	22	GHS Rating	4	4			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	4	HZF	24	1	4	1	2	3	3	41	EPA
			48	1	3	1	2	2	3	34	22
			72	1	3	1	2	2	2	32	GHS
			7 days	1	2	0	2	2	1	20	22
			14 days	1	2	0	2	2	2	22	
			21 days	2	1	0	2	2	1	20	
	4	HZF	41	1	3.333333	1	2	2.333333333	2.666666667	22	22
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	0.7	2.3	1.8	22	22	Combinatio block #5	3,4,5	1.0	1.0
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	2
	2,4,5	1.0	1.0	2.5	2.2	22	22		3,4,6	1.0	0.8
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	4
	2,4,6	1.0	0.8	2.3	2.0	22	22		3,5,6	1.0	0.8
	GHS Rating	2	4	2	2	22	22		GHS Rating	2	4
	2,5,6	1.0	0.8	2.5	1.8	14	14		4,5,6	1.0	1.0
GHS Rating	2	4	2	4	14	14	GHS Rating	2	2		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZE	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	5	HZE	2	0	0	0	0.5	0	0	0	2	
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	4	7		
1.3	0.8	7	7				HZE	1,2,4	4	3		
4	4	7	7					1,2,5	4	3		
2.0	1.7	22	22					1,2,6	4	22		
2	4	22	22					1,3,4	4	7		
2.0	1.7	22	22					1,3,5	4	7		
2	4	22	22					1,3,6	2	22		
1.3	0.8	22	22					1,4,5	4	3		
4	4	22	22					1,4,6	4	22		
								1,5,6	4	22		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZF	24	1	4	1	3	2	2	39	EPA	
			48	1	2	1	2	2	0	23	14	
			72	1	1	1	2	2	0	18	GHS	
			7 days	1	1	0	1	1	0	9	14	
			14 days	0	0	0	0	0	0	0		
			21 days							0		
	5	HZF	39	1	2.333333	1	2.33333333	2	0.666666667	14	14	
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	2	22		
2.2	2.2	22	22				HZF	1,2,4	2	22		
2	2	22	22					1,2,5	2	14		
2.0	2.2	22	22					1,2,6	2	14		
2	2	22	22					1,3,4	2	22		
2.2	2.0	22	22					1,3,5	2	22		
2	2	22	22					1,3,6	2	22		
2.2	2.2	22	22					1,4,5	2	22		
2	2	22	22					1,4,6	2	22		
								1,5,6	2	14		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZE	24	1	4	0	2	2	2	32	EPA	
			48	1	2	0	2	2	1	20	22	
			72	1	2	1	2	1	0	21	GHS	
			7 days	1	1	0	2	1	0	11	22	
			14 days	1	1	0	2	2	1	15		
			21 days	2	1	0	2	2	1	20		
	6	HZE	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZE	32	1	2.666667	0.333333	2	1.666666667	1	22	22	
7		2,3,4	4	7		7						
3		2,3,5	4	7		7						
3		2,3,6	2	22		22						
22		2,4,5	4	3		3						
7		2,4,6	4	22		22						
7		2,5,6	4	22		22						
22		3,4,5	4	7		7						
2		3,4,6	2	22		22						
22		3,5,6	2	22		22						
22		4,5,6	4	22		22						
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZF	24	1	3	1	2	2	2	32	EPA	
			48	1	2	1	2	2	0	23	7	
			72	1	1	0	1	1	0	9	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	6	HZF	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZF	32	1	2	0.666667	1.666666667	1.666666667	0.666666667	7	7	
22		2,3,4	2	22		22						
22		2,3,5	2	22		22						
14		2,3,6	2	22		22						
14		2,4,5	2	22		22						
22		2,4,6	2	22		22						
22		2,5,6	2	14		14						
22		3,4,5	2	22		22						
22		3,4,6	2	22		22						
22		3,5,6	2	22		22						
14		4,5,6	2	22		22						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZG*	24	1	1	0	2	0	0	0	9	EPA
			48	0	0	0	1	0	0	0	2	2
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
GHS Tissue		1 HZG*	9	0.3	0.3	0.0	1.0	0.0	0.0	0.0	2	3
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZG*	9	0.3	0.3	0.0	1.0	0.0	0.0	2	3	
	2	HZG*	18	0.3	0.3	0.3	1.0	0.3	0.3	3	3	
	3	HZG*	20	0.7	1.0	0.0	1.7	1.0	0.3	3	7	
	4	HZG*	18	0.7	0.7	0.3	1.7	0.3	0.3	3	7	
	5	HZG*	15	0.7	0.7	0.0	1.0	1.0	0.3	3	3	
	6	HZG*	11	0.3	0.3	0.0	1.7	0.7	0.0	7	7	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZH	24	0	0	0	0	0	0	0	0	EPA
			48	0	0	0	0	0	0	0	0	0
			72								0	GHS
			7 days								0	0
			14 days								0	
			21 days								0	
GHS Tissue		1 HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	2	HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	3	HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	4	HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	5	HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	6	HZH	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZG*	24	1	1	1	2	1	1	18	EPA	
			48	0	0	0	1	0	0	2	3	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	3
			14 days								0	
			21 days								0	
	2	HZG*	18	0.333333	0.333333	0.333333	1	0.333333333	0.333333333	3	3	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0.5	0.166667	1.333333	0.666667	3	7	Combina- tion block #2	1,3,4	0.666667	0.166667	
	GHS Rating	4	4	4	4	3	7	GHS Rating	4	4	4	
	1,2,4	0.5	0.333333	1.333333	0.333333	3	7	1,3,5	0.666667	0	0	
	GHS Rating	4	4	4	4	3	7	GHS Rating	4	4	4	
	1,2,5	0.5	0.166667	1	0.666667	3	3	1,3,6	0.5	0	0	
	GHS Rating	4	4	4	4	3	3	GHS Rating	4	4	4	
	1,2,6	0.333333	0.166667	1.333333	0.5	7	7	1,4,5	0.666667	0.166667	0.166667	
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4	4		

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZH	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	GHS	
			72								0	
			7 days								0	
			14 days								0	
			21 days								0	
	2	HZH	0	0	0	0	0	0	0	0	0	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0	0	0	0	0	0	Combina- tion block #2	1,3,4	0	0	
	GHS Rating	4	4	4	4	0	0	GHS Rating	4	4	4	
	1,2,4	0	0	0	0	0	0	1,3,5	0	0	0	
	GHS Rating	4	4	4	4	0	0	GHS Rating	4	4	4	
	1,2,5	0	0	0	0	0	0	1,3,6	0	0	0	
	GHS Rating	4	4	4	4	0	0	GHS Rating	4	4	4	
	1,2,6	0	0	0	0	0	0	1,4,5	0	0	0	
GHS Rating	4	4	4	4	0	0	GHS Rating	4	4	4		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZG*	24	1	2	0	2	2	1	20	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZG*	20	0.666667	1	0	1.666666667	1	0.333333333	3	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.666667	0.666667	3	7	Combinatio	1,4,6	0.5	0.2	1.7	0.5	7	7	
4	4	3	7	tion block	GHS Rating	4	4	4	4	7	7	
1.333333	1	3	7	#3	1,5,6	0.5	0.0	1.3	0.8	7	7	
4	4	3	7		GHS Rating	4	4	4	4	7	7	
1.666667	0.833333	7	7		2,3,4	0.7	0.3	1.7	0.7	3	7	
4	4	7	7		GHS Rating	4	4	4	4	3	7	
1.333333	0.666667	3	7		2,3,5	0.7	0.2	1.3	1.0	3	7	
4	4	3	7		GHS Rating	4	4	4	4	3	7	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZH	24	0	0	0	0	0	0	0	0	EPA
			48	0	0	0	0	0	0	0	0	0
			72							0		GHS
			7 days							0		0
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZH	0	0	0	0	0	0	0	0	0	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
0	0	0	0	Combinatio	1,4,6	0.0	0.0	0.0	0.0	0	0	
4	4	0	0	tion block	GHS Rating	4	4	4	4	0	0	
0	0	0	0	#3	1,5,6	0.0	0.0	0.0	0.0	0	0	
4	4	0	0		GHS Rating	4	4	4	4	0	0	
0	0	0	0		2,3,4	0.0	0.0	0.0	0.0	0	0	
4	4	0	0		GHS Rating	4	4	4	4	0	0	
0	0	0	0		2,3,5	0.0	0.0	0.0	0.0	0	0	
4	4	0	0		GHS Rating	4	4	4	4	0	0	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	4	HZG*	24	1	1	1	2	1	1	18	EPA
			48	1	1	0	2	0	0	9	3
			72	0	0	0	1	0	0	2	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days						0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	4	HZG*	18	0.666667	0.666667	0.333333	1.66666667	0.333333333	0.333333333	3	7
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combina- tion block #4	2,3,6	0.5	0.2	1.7	0.8	7	7	7	3,4,5	0.7	0.2
	GHS Rating	4	4	4	4	7	7	7	GHS Rating	4	4
	2,4,5	0.7	0.3	1.3	0.7	3	7	7	3,4,6	0.7	0.2
	GHS Rating	4	4	4	4	3	7	7	GHS Rating	4	4
	2,4,6	0.5	0.3	1.7	0.5	7	7	7	3,5,6	0.7	0.0
	GHS Rating	4	4	4	4	7	7	7	GHS Rating	4	4
	2,5,6	0.5	0.2	1.3	0.8	7	7	7	4,5,6	0.7	0.2
GHS Rating	4	4	4	4	7	7	7	GHS Rating	4	4	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	4	HZH	24	0	0	0	0	0	0	0	EPA
			48	0	0	0	0	0	0	0	0
			72							0	GHS
			7 days							0	0
			14 days							0	
			21 days						0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	4	HZH	0	0	0	0	0	0	0	0	0
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combina- tion block #4	2,3,6	0.0	0.0	0.0	0.0	0	0	0	3,4,5	0.0	0.0
	GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4
	2,4,5	0.0	0.0	0.0	0.0	0	0	0	3,4,6	0.0	0.0
	GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4
	2,4,6	0.0	0.0	0.0	0.0	0	0	0	3,5,6	0.0	0.0
	GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4
	2,5,6	0.0	0.0	0.0	0.0	0	0	0	4,5,6	0.0	0.0
GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE					
0.1	5	HZG*	24	1	1	0	2	2	1	15	EPA			
			48	1	1	0	1	1	0	9	3			
			72	0	0	0	0	0	0	0	GHS			
			7 days							0	3			
			14 days							0				
			21 days							0				
			ANIMAL ID		MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
			5		HZG*	15	0.666667	0.666667	0	1	1	0.333333333	3	3
Redness	Chemosis	DtC EPA	DtC GHS			Summary	1,2,3		4	7				
1.7	1.0	3	7			HZG*	1,2,4		4	7				
4	4	3	7				1,2,5		4	3				
1.7	0.8	7	7				1,2,6		4	7				
4	4	7	7				1,3,4		4	7				
1.7	1.0	7	7				1,3,5		4	7				
4	4	7	7				1,3,6		4	7				
1.7	0.8	7	7				1,4,5		4	7				
4	4	7	7				1,4,6		4	7				
							1,5,6		4	7				
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE					
0.1	5	HZH	24	0	0	0	0	0	0	0	0	EPA		
			48	0	0	0	0	0	0	0	0	0		
			72									0	GHS	
			7 days									0	0	
			14 days									0		
			21 days									0		
			ANIMAL ID		MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
			5		HZH	0	0	0	0	0	0	0	0	0
Redness	Chemosis	DtC EPA	DtC GHS			Summary	1,2,3		4	0				
0.0	0.0	0	0			HZH	1,2,4		4	0				
4	4	0	0				1,2,5		4	0				
0.0	0.0	0	0				1,2,6		4	0				
4	4	0	0				1,3,4		4	0				
0.0	0.0	0	0				1,3,5		4	0				
4	4	0	0				1,3,6		4	0				
0.0	0.0	0	0				1,4,5		4	0				
4	4	0	0				1,4,6		4	0				

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZG*	24	1	1	0	2	1	0	11	EPA	
			48	0	0	0	2	1	0	6	7	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZG*	11	0.333333	0.333333	0	1.66666667	0.666666667	0	7	7	
3		2,3,4	4	7		3						
3		2,3,5	4	7		3						
3		2,3,6	4	7		7						
7		2,4,5	4	7		3						
3		2,4,6	4	7		7						
3		2,5,6	4	7		7						
7		3,4,5	4	7		3						
3		3,4,6	4	7		7						
7		3,5,6	4	7		7						
7		4,5,6	4	7		7						
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZH	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	0
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZH	0	0	0	0	0	0	0	0	0	
0		2,3,4	4	0		0						
0		2,3,5	4	0		0						
0		2,3,6	4	0		0						
0		2,4,5	4	0		0						
0		2,4,6	4	0		0						
0		2,5,6	4	0		0						
0		3,4,5	4	0		0						
0		3,4,6	4	0		0						
0		3,5,6	4	0		0						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	F40840	HZI	24	1	4	1	3	2	2	39	EPA
			48	1	3	1	3	2	2	34	7
			72	1	1	1	3	2	2	24	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
GHS Tissue											
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	F40840	HZI	39	1.0	2.7	1.0	3.0	2.0	2.0	7	7
Summary block used analysis of the twenty combinations											
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	F40840	HZI	39	1.0	2.7	1.0	3.0	2.0	2.0	7	7
	F40855	HZI	36	1.0	2.3	1.0	3.0	2.0	2.3	14	14
	F40881	HZI	39	1.0	3.0	1.0	2.0	1.7	1.7	22	22
	F41365	HZI	43	1.0	3.0	0.7	2.3	2.3	3.0	22	22
	F41379	HZI	29	1.0	1.3	0.3	2.0	1.7	1.3	7	7
	F41405	HZI	39	1.0	3.7	1.0	2.3	2.0	1.7	0	0
	Dose Vol		0.1								

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	1	HZJ	24	0	0	0	0	0	0	0	EPA
			48	0	0	0	0	0	0	0	0
			72							0	GHS
			7 days							0	0
			14 days							0	
			21 days							0	
GHS Tissue											
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	1	HZJ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Summary block used analysis of the twenty combinations											
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	1	HZJ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
	2	HZJ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
	3	HZJ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
	4	HZJ	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2
	5	HZJ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
	6	HZJ	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2
	Dose Vol		0.1								

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	F40855	HZI	24	1	3	1	3	2	3	36	EPA
			48	1	2	1	3	2	2	29	14
			72	1	2	1	3	2	2	29	GHS
			7 days	1	1	0	2	1	0	11	14
			14 days	0	0	0	0	0	0	0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	F40855	HZI	36	1	2.333333	1	3	2	2.333333333	14	14
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	1	1	3	2	22	22	Combina- tion block #2	1,3,4	1	1
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	2
	1,2,4	1	1	3	2.166667	22	22		1,3,5	1	1
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	2
	1,2,5	1	1	3	2	14	14		1,3,6	1	1
	GHS Rating	2	2	2	2	14	14		GHS Rating	2	2
	1,2,6	1	1	3	2	14	14		1,4,5	1	0.833333
	GHS Rating	2	2	2	2	14	14		GHS Rating	2	4

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZJ	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	0
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	2	HZJ	0	0	0	0	0	0	0	0	0	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0	0	0	0	0	0	Combina- tion block #2	1,3,4	0	0	
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4	
	1,2,4	0	0	0.25	0	0	2		1,3,5	0	0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	1,2,5	0	0	0	0	0	0		1,3,6	0	0	
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4	
	1,2,6	0	0	0.25	0	0	2		1,4,5	0	0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA		REDNESS	CHEMOSIS	DISCHARGE		
0.1	F40881	HZI	24	1	4	1	2	2	3	39	EPA
			48	1	3	1	2	1	1	28	22
			72	1	2	1	2	2	1	25	GHS
			7 days	1	1	0	2	1	1	13	22
			14 days	1	1	0	1	1	0	9	
			21 days	1	1	0	1	1	0	9	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	F40881	HZI	39	1	3	1	2	1.66666667	1.66666667	22	22
Redness	Chemosis	DtC EPA	DtC GHS		Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS
2.666667	2.166667	22	22	Combina- tion block #3	1,4,6	1.0	1.0	2.7	2.2	22	22
2	2	22	22		GHS Rating	2	2	2	2	22	22
2.5	1.833333	22	22		1,5,6	1.0	1.0	2.7	2.0	7	7
2	4	22	22		GHS Rating	2	4	2	2	7	7
2.666667	2	22	22		2,3,4	1.0	1.0	2.7	2.2	22	22
2	2	22	22		GHS Rating	2	2	2	2	22	22
2.666667	2.166667	22	22		2,3,5	1.0	1.0	2.5	1.8	22	22
2	2	22	22	GHS Rating	2	2	2	4	22	22	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA		REDNESS	CHEMOSIS	DISCHARGE			
0.1	3	HZJ	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	0
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZJ	0	0	0	0	0	0	0	0	0	
Redness	Chemosis	DtC EPA	DtC GHS		Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
0.25	0	0	2	Combina- tion block #3	1,4,6	0.0	0.0	0.5	0.0	0	2	
4	4	0	2		GHS Rating	4	4	4	4	0	2	
0	0	0	0		1,5,6	0.0	0.0	0.3	0.0	0	2	
4	4	0	0		GHS Rating	4	4	4	4	0	2	
0.25	0	0	2		2,3,4	0.0	0.0	0.3	0.0	0	2	
4	4	0	2		GHS Rating	4	4	4	4	0	2	
0.25	0	0	2		2,3,5	0.0	0.0	0.0	0.0	0	0	
4	4	0	2	GHS Rating	4	4	4	4	0	0		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F41365	HZI	24	1	4	1	3	3	3	43	EPA	
			48	1	3	1	2	2	3	34	22	
			72	1	2	0	2	2	3	24	GHS	
			7 days	1	1	0	2	2	2	17	22	
			14 days	2	1	0	2	2	2	22		
			21 days	1	1	0	1	1	0	9		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	F41365	HZI	43	1	3	0.666667	2.33333333	2.33333333	3	22	22	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	1.0	2.7	2.0	22	22	Combinatio block #5	3,4,5	1.0	0.8	
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	4	
	2,4,5	1.0	0.8	2.7	2.2	22	22		3,4,6	1.0	1.0	
	GHS Rating	2	4	2	2	22	22		GHS Rating	2	2	
	2,4,6	1.0	1.0	2.7	2.2	22	22		3,5,6	1.0	1.0	
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	4	
	2,5,6	1.0	1.0	2.7	2.0	14	14		4,5,6	1.0	0.8	
GHS Rating	2	4	2	2	14	14	GHS Rating	2	4			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZJ	2	0	0	0	0.5	0	0	0	2	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	0.0	0.0	0.3	0.0	0	2	Combinatio block #5	3,4,5	0.0	0.0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	2,4,5	0.0	0.0	0.3	0.0	0	2		3,4,6	0.0	0.0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	2,4,6	0.0	0.0	0.5	0.0	0	2		3,5,6	0.0	0.0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	2,5,6	0.0	0.0	0.3	0.0	0	2		4,5,6	0.0	0.0	
GHS Rating	4	4	4	4	0	2	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE	DISCHARGE			
0.1	F41379	HZI	24	1	2	1	2	2	3	29	EPA		
			48	1	1	0	2	2	1	15	7		
			72	1	1	0	2	1	0	11	GHS		
			7 days	0	0	0	0	0	0	0	7		
			14 days								0		
			21 days								0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	F41379	HZI	29	1	1.333333	0.333333	2	1.666666667	1.333333333	7	7		
Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	2	22		
2.2	2.0	22	22					HZI	1,2,4	2	22		
2	2	22	22						1,2,5	2	14		
2.3	2.2	22	22						1,2,6	2	14		
2	2	22	22						1,3,4	2	22		
2.2	1.8	22	22						1,3,5	2	22		
2	4	22	22						1,3,6	2	22		
2.3	2.2	22	22						1,4,5	2	22		
2	2	22	22						1,4,6	2	22		
									1,5,6	2	7		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE	DISCHARGE			
0.1	5	HZJ	24	0	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	0	
			72									0	GHS
			7 days									0	0
			14 days									0	
			21 days									0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	5	HZJ	0	0	0	0	0	0	0	0	0		
Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	4	0		
0.3	0.0	0	2					HZJ	1,2,4	4	2		
4	4	0	2						1,2,5	4	0		
0.5	0.0	0	2						1,2,6	4	2		
4	4	0	2						1,3,4	4	2		
0.3	0.0	0	2						1,3,5	4	0		
4	4	0	2						1,3,6	4	2		
0.5	0.0	0	2						1,4,5	4	2		
4	4	0	2						1,4,6	4	2		
									1,5,6	4	2		

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0 Volume	4,5,6		4	0		0	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR	
	ANIMAL ID	TEST MATL		TIME	OPACITY		AREA	IRIS	REDNESS			CHEMOSIS
0.1	F41405	HZI	24	1	4	1	2	2	2	37	EPA	
			48	1	4	1	3	2	2	39		
			72	1	3	1	2	2	1	30	GHS	
			7 days	1	1	0	1	1	0	9		
			14 days	1	1	0	1	0	0	7		
			21 days	1	1	0	0	0	0	5		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	F41405	HZI	39	1	3.666667	1	2.33333333	2	1.666666667	0	0	
22		2,3,4	2	22		22						
22		2,3,5	2	22		22						
14		2,3,6	2	22		22						
14		2,4,5	2	22		22						
22		2,4,6	2	22		22						
22		2,5,6	2	14		14						
22		3,4,5	2	22		22						
22		3,4,6	2	22		22						
22		3,5,6	2	22		22						
7		4,5,6	2	22		22						
Volume	4,5,6		4	0		0	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR	
	ANIMAL ID	TEST MATL		TIME	OPACITY		AREA	IRIS	REDNESS			CHEMOSIS
0.1	6	HZJ	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZJ	2	0	0	0	0.5	0	0	0	2	
0		2,3,4	4	2		0						
0		2,3,5	4	0		0						
0		2,3,6	4	2		0						
0		2,4,5	4	2		0						
0		2,4,6	4	2		0						
0		2,5,6	4	2		0						
0		3,4,5	4	2		0						
0		3,4,6	4	2		0						
0		3,5,6	4	2		0						
0		4,5,6	4	2		0						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	1	HZK	24	1	4	1	3	2	3	41	EPA
			48	1	3	1	3	1	2	32	7
			72	1	2	1	2	1	3	27	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
GHS Tissue		1 HZK	41	1.0	3.0	1.0	2.7	1.3	2.7	7	7
		ANIMAL ID									
Summary block used analysis of the twenty combinations		1	41	1.0	3.0	1.0	2.7	1.3	2.7	7	7
		2	39	1.0	3.7	1.0	2.7	1.7	2.3	22	22
		3	41	1.0	2.7	1.0	2.3	2.3	2.7	22	22
		4	35	1.0	4.0	1.0	2.0	1.7	1.0	22	22
		5	41	1.0	4.0	1.0	2.3	2.0	2.3	22	22
		6	41	1.0	3.0	1.0	2.7	2.0	2.3	22	22
		Dose Vol	0.1								

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	1	HZL	24	1	3	1	2	1	3	32	EPA
			48	1	2	1	3	1	1	25	22
			72	1	1	1	2	1	0	16	GHS
			7 days	1	1	0	2	1	0	11	22
			14 days	1	1	0	1	1	0	9	
			21 days	1	1	0	1	0	0	7	
GHS Tissue		1 HZL	32	1.0	2.0	1.0	2.3	1.0	1.3	22	22
		ANIMAL ID									
Summary block used analysis of the twenty combinations		1	32	1.0	2.0	1.0	2.3	1.0	1.3	22	22
		2	27	1.0	1.3	0.3	2.0	1.3	1.3	7	7
		3	35	1.0	2.0	0.3	1.7	1.0	1.0	7	7
		4	41	1.0	2.7	0.7	2.7	1.7	1.0	7	7
		5	41	1.0	2.0	1.0	3.0	2.0	2.3	22	22
		6	37	1.0	3.0	1.0	2.3	1.7	1.7	0	22
		Dose Vol	0.1								

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZK	24	1	4	1	2	2	3	39	EPA	
			48	1	4	1	3	1	2	37	22	
			72	1	3	1	3	2	2	34	GHS	
			7 days	1	2	0	2	1	0	16	22	
			14 days	1	1	0	2	1	1	13		
			21 days	1	1	0	2	1	1	13		
	2	HZK	39	1	3.666667	1	2.666666667	1.666666667	2.333333333	22	22	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	1	1	2.666667	2	22	22	Combina- tion block #2	1,3,4	1	1	
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	2	
	1,2,4	1	1	2.666667	1.666667	22	22		1,3,5	1	1	
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2	
	1,2,5	1	1	2.666667	1.833333	22	22		1,3,6	1	1	
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2	
	1,2,6	1	1	2.666667	1.833333	22	22		1,4,5	1	1	
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2			
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZL	24	1	2	1	2	2	2	27	EPA	
			48	1	1	0	2	1	2	15	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	2	HZL	27	1	1.333333	0.333333	2	1.333333333	1.333333333	7	7	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	1	0.666667	2.166667	1.166667	22	22	Combina- tion block #2	1,3,4	1	0.833333	
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	4	
	1,2,4	1	0.833333	2.5	1.5	22	22		1,3,5	1	1	
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	4	
	1,2,5	1	1	2.666667	1.666667	22	22		1,3,6	1	1	
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	4	
	1,2,6	1	1	2.333333	1.5	22	22		1,4,5	1	1	
GHS Rating	2	4	2	4	22	22	GHS Rating	2	2			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	3	HZK	24	1	4	1	2	3	3	41	EPA
			48	1	2	1	3	2	2	29	22
			72	1	2	1	2	2	3	29	GHS
			7 days	1	2	0	3	2	1	22	22
			14 days	1	1	0	1	1	0	9	
			21 days	1	1	0	2	1	1	13	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZK	41	1	2.666667	1	2.333333333	2.33333333	2.666666667	22	22
Redness	Chemosis	DtC EPA	DtC GHS		Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS
2.5	2	22	22	Combinatio n block #3	1,4,6	1.0	1.0	2.7	1.8	22	22
2	2	22	22		GHS Rating	2	2	2	4	22	22
2.5	2.166667	22	22		1,5,6	1.0	1.0	2.7	2.0	22	22
2	2	22	22		GHS Rating	2	2	2	2	22	22
2.666667	2.166667	22	22		2,3,4	1.0	1.0	2.5	2.0	22	22
2	2	22	22		GHS Rating	2	2	2	2	22	22
2.5	1.833333	22	22		2,3,5	1.0	1.0	2.5	2.2	22	22
2	4	22	22		GHS Rating	2	2	2	2	22	22

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZL	24	1	4	1	2	1	2	35	EPA	
			48	1	1	0	2	1	1	13	7	
			72	1	1	0	1	1	0	9	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZL	35	1	2	0.333333	1.666666667	1	1	7	7	
Redness	Chemosis	DtC EPA	DtC GHS		Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
2.5	1.333333	22	22	Combinatio n block #3	1,4,6	1.0	1.0	2.5	1.7	22	22	
2	4	22	22		GHS Rating	2	2	2	4	22	22	
2.666667	1.5	22	22		1,5,6	1.0	1.0	2.7	1.8	22	22	
2	4	22	22		GHS Rating	2	2	2	4	22	22	
2.333333	1.333333	22	22		2,3,4	1.0	0.5	2.3	1.5	7	7	
2	4	22	22		GHS Rating	2	4	2	4	7	7	
2.833333	1.833333	22	22		2,3,5	1.0	0.7	2.5	1.7	22	22	
2	4	22	22		GHS Rating	2	4	2	4	22	22	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZK	24	1	4	1	2	2	1	35	EPA	
			48	1	4	1	2	2	1	35	22	
			72	1	4	1	2	1	1	33	GHS	
			7 days	1	2	1	2	1	0	21	22	
			14 days	1	2	0	1	1	0	14		
			21 days	1	1	0	1	0	0	7		
	4	HZK	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZK	35	1	4	1	2	1.666666667	1	22	22	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	1.0	2.7	2.2	22	22	Combinatio block #5	3,4,5	1.0	1.0	
	GHS Rating	2	2	2	22	22	22		GHS Rating	2	2	
	2,4,5	1.0	1.0	2.5	1.8	22	22		3,4,6	1.0	1.0	
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2	
	2,4,6	1.0	1.0	2.7	1.8	22	22		3,5,6	1.0	1.0	
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2	
	2,5,6	1.0	1.0	2.7	2.0	22	22		4,5,6	1.0	1.0	
GHS Rating	2	2	2	2	22	22	GHS Rating	2	2			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZL	24	1	4	1	3	2	3	41	EPA	
			48	1	3	1	3	2	0	30	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	4	HZL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZL	41	1	2.666667	0.666667	2.66666667	1.666666667	1	7	7	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	0.7	2.2	1.5	7	22	Combinatio block #5	3,4,5	1.0	0.8	
	GHS Rating	2	4	2	4	7	22		GHS Rating	2	4	
	2,4,5	1.0	0.8	2.8	1.8	22	22		3,4,6	1.0	0.8	
	GHS Rating	2	4	2	4	22	22		GHS Rating	2	4	
	2,4,6	1.0	0.8	2.5	1.7	7	22		3,5,6	1.0	1.0	
	GHS Rating	2	4	2	4	7	22		GHS Rating	2	4	
	2,5,6	1.0	1.0	2.7	1.8	22	22		4,5,6	1.0	1.0	
GHS Rating	2	4	2	4	22	22	GHS Rating	2	2			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	5	HZK	24	1	4	1	3	2	3	41	EPA
			48	1	4	1	2	2	2	37	22
			72	1	4	1	2	2	2	37	GHS
			7 days	1	2	1	2	2	2	27	22
			14 days	2	1	1	2	2	2	27	
			21 days	3	1	0	2	2	1	25	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	5	HZK	41	1	4	1	2.33333333	2	2.33333333	22	22
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	2	22	
2.3	2.2	22	22				HZK	1,2,4	2	22	
2	2	22	22					1,2,5	2	22	
2.5	2.2	22	22					1,2,6	2	22	
2	2	22	22					1,3,4	2	22	
2.5	2.2	22	22					1,3,5	2	22	
2	2	22	22					1,3,6	2	22	
2.5	2.0	22	22					1,4,5	2	22	
2	2	22	22					1,4,6	2	22	
								1,5,6	2	22	
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	5	HZL	24	1	4	1	3	2	3	41	EPA
			48	1	1	1	3	2	2	24	22
			72	1	1	1	3	2	2	24	GHS
			7 days	1	1	0	2	1	1	13	22
			14 days	2	1	0	2	1	1	18	
			21 days	2	1	0	1	1	0	14	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	5	HZL	41	1	2	1	3	2	2.33333333	22	22
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	2	22	
2.8	1.8	22	22				HZL	1,2,4	2	22	
2	4	22	22					1,2,5	2	22	
2.5	1.7	7	22					1,2,6	2	22	
2	4	7	22					1,3,4	2	22	
2.7	1.8	22	22					1,3,5	2	22	
2	4	22	22					1,3,6	2	22	
2.8	1.8	22	22					1,4,5	2	22	
2	4	22	22					1,4,6	2	22	
								1,5,6	2	22	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZK	24	1	4	1	3	2	3	41	EPA
			48	1	3	1	3	2	3	36	22
			72	1	2	1	2	2	1	25	GHS
			7 days	1	2	1	2	2	2	27	22
			14 days	1	1	0	1	1	0	9	
			21 days	1	1	0	1	1	0	9	
						MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS
	6	HZK	41	1	3	1	2.66666667	2	2.333333333	22	22
22		2,3,4		2	22						
22		2,3,5		2	22						
22		2,3,6		2	22						
22		2,4,5		2	22						
22		2,4,6		2	22						
22		2,5,6		2	22						
22		3,4,5		2	22						
22		3,4,6		2	22						
22		3,5,6		2	22						
22		4,5,6		2	22						
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZL	24	1	4	1	2	2	2	37	22
			48	1	3	1	3	2	2	34	
			72	1	2	1	2	1	1	23	GHS
			7 days	1	1	0	2	1	0	11	22
			14 days	1	1	0	0	0	0	5	
			21 days	1	1	0	0	0	0	5	
						MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS
	6	HZL	37	1	3	1	2.33333333	1.666666667	1.666666667	0	22
22		2,3,4		2	7						
22		2,3,5		2	22						
22		2,3,6		2	22						
22		2,4,5		2	22						
22		2,4,6		2	22						
22		2,5,6		2	22						
22		3,4,5		2	22						
22		3,4,6		2	22						
22		3,5,6		2	22						
22		4,5,6		2	22						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZM*	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
GHS Tissue		1 HZM*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZM*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	2	HZM*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	3	HZM*	11	0.3	0.3	0.0	1.7	0.7	0.0	3	7	
	4	HZM*	7	0.3	0.3	0.0	0.7	0.0	0.0	0	3	
	5	HZM*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	6	HZM*	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZN*	24	1	1	0	2	1	0	11	EPA	
			48	0	0	0	1	1	0	4	3	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
GHS Tissue		1 HZN*	11	0.3	0.3	0.0	1.0	0.7	0.0	3	3	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZN*	11	0.3	0.3	0.0	1.0	0.7	0.0	3	3	
	2	HZN*	7	0.3	0.3	0.0	0.7	0.0	0.0	2	3	
	3	HZN*	20	0.7	1.0	0.0	1.3	1.0	0.3	3	3	
	4	HZN*	25	0.7	1.0	0.3	1.0	0.3	0.7	3	3	
	5	HZN*	20	0.7	0.7	0.3	1.3	0.7	0.7	3	3	
	6	HZN*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZM*	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	2	HZM*	2	0	0	0	0.5	0	0	0	2	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0.166667	0	1.083333	0.333333	3	7	Combina- tion block #2	1,3,4	0.333333	0	
	GHS Rating	4	4	4	4	3	7		GHS Rating	4	4	
	1,2,4	0.166667	0	0.583333	0	0	3		1,3,5	0.166667	0	
	GHS Rating	4	4	4	4	0	3		GHS Rating	4	4	
	1,2,5	0	0	0.5	0	0	2		1,3,6	0.166667	0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	1,2,6	0	0	0.5	0	0	2		1,4,5	0.166667	0	
GHS Rating	4	4	4	4	0	2	GHS Rating	4	4			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZN*	24	1	1	0	1	0	0	7	EPA	
			48	0	0	0	1	0	0	2	2	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
	2	HZN*	7	0.333333	0.333333	0	0.666666667	0	0	2	3	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0.5	0	1.166667	0.833333	3	3	Combina- tion block #2	1,3,4	0.666667	0.166667	
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4	
	1,2,4	0.5	0.166667	1	0.5	3	3		1,3,5	0.666667	0.166667	
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4	
	1,2,5	0.5	0.166667	1.166667	0.666667	3	3		1,3,6	0.5	0	
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4	
	1,2,6	0.333333	0	0.833333	0.333333	3	3		1,4,5	0.666667	0.333333	
GHS Rating	4	4	4	4	3	3	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZM*	24	1	1	0	2	1	0	11	EPA	
			48	0	0	0	2	1	0	6	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZM*	11	0.333333	0.333333	0	1.666666667	0.66666667	0	3	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.166667	0.333333	3	7	Combina- tion block #3	1,4,6 GHS Rating	0.2	0.0	0.6	0.0	0	3	
4	4	3	7		1,5,6 GHS Rating	4	4	4	4	0	3	
1.083333	0.333333	3	7		2,3,4 GHS Rating	0.0	0.0	0.5	0.0	0	2	
4	4	3	7		2,3,5 GHS Rating	4	4	4	4	0	2	
1.083333	0.333333	3	7		2,3,4 GHS Rating	0.3	0.0	1.2	0.3	3	7	
4	4	3	7		2,3,5 GHS Rating	4	4	4	4	3	7	
0.583333	0	0	3		2,3,5 GHS Rating	0.2	0.0	1.1	0.3	3	7	
4	4	0	3			4	4	4	4	3	7	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZN*	24	1	2	0	2	2	1	20	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	3
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZN*	20	0.666667	1	0	1.333333333	1	0.333333333	3	3	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.166667	0.833333	3	3	Combina- tion block #3	1,4,6 GHS Rating	0.5	0.2	1.0	0.5	3	3	
4	4	3	3		1,5,6 GHS Rating	4	4	4	4	3	3	
1.333333	0.833333	3	3		2,3,4 GHS Rating	0.5	0.2	1.2	0.7	3	3	
4	4	3	3		2,3,5 GHS Rating	4	4	4	4	3	3	
1.166667	0.833333	3	3		2,3,4 GHS Rating	0.7	0.2	1.2	0.7	3	3	
4	4	3	3		2,3,5 GHS Rating	4	4	4	4	3	3	
1.166667	0.666667	3	3		2,3,5 GHS Rating	0.7	0.2	1.3	0.8	3	3	
4	4	3	3			4	4	4	4	3	3	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZM*	24	1	1	0	1	0	0	7	EPA	
			48	0	0	0	1	0	0	2	0	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	3
			14 days								0	
			21 days								0	
	4	HZM*	MAS	0.333333	0.333333	0	0.66666667	0	0	0	3	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	0.2	0.0	1.1	0.3	3	7	Combina- tion block #5	3,4,5	0.3	0.0	
	GHS Rating	4	4	4	4	3	7		GHS Rating	4	4	
	2,4,5	0.2	0.0	0.6	0.0	0	3		3,4,6	0.3	0.0	
	GHS Rating	4	4	4	4	0	3		GHS Rating	4	4	
	2,4,6	0.2	0.0	0.6	0.0	0	3		3,5,6	0.2	0.0	
	GHS Rating	4	4	4	4	0	3		GHS Rating	4	4	
	2,5,6	0.0	0.0	0.5	0.0	0	2		4,5,6	0.2	0.0	
GHS Rating	4	4	4	4	0	2	GHS Rating	4	4			
	4	HZN*	MAS	0.666667	1	0.333333	1	0.333333333	0.666666667	3	3	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	0.5	0.0	1.0	0.5	3	3	Combina- tion block #5	3,4,5	0.7	0.3	
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4	
	2,4,5	0.7	0.3	1.2	0.5	3	3		3,4,6	0.7	0.2	
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4	
	2,4,6	0.5	0.2	0.8	0.2	3	3		3,5,6	0.7	0.2	
	GHS Rating	4	4	4	4	3	3		GHS Rating	4	4	
	2,5,6	0.5	0.2	1.0	0.3	3	3		4,5,6	0.7	0.3	
GHS Rating	4	4	4	4	3	3	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZM*	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZM*	2	0	0	0	0.5	0	0	0	2	
Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	4	7	
1.2	0.3	3	7					HZM*	1,2,4	4	3	
4	4	3	7						1,2,5	4	2	
1.2	0.3	3	7						1,2,6	4	2	
4	4	3	7						1,3,4	4	7	
1.1	0.3	3	7						1,3,5	4	7	
4	4	3	7						1,3,6	4	7	
0.6	0.0	0	3						1,4,5	4	3	
4	4	0	3						1,4,6	4	3	
									1,5,6	4	2	
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZN*	24	1	1	1	2	1	2	20	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZN*	20	0.666667	0.666667	0.333333	1.33333333	0.666666667	0.666666667	3	3	
Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	4	3	
1.3	0.8	3	3					HZN*	1,2,4	4	3	
4	4	3	3						1,2,5	4	3	
1.2	0.7	3	3						1,2,6	4	3	
4	4	3	3						1,3,4	4	3	
1.3	0.8	3	3						1,3,5	4	3	
4	4	3	3						1,3,6	4	3	
1.2	0.5	3	3						1,4,5	4	3	
4	4	3	3						1,4,6	4	3	
									1,5,6	4	3	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZM*	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days									0
			14 days									0
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZM*	0	0	0	0	0	0	0	0	0	
3		2,3,4		4	7							
0		2,3,5		4	7							
0		2,3,6		4	7							
0		2,4,5		4	3							
3		2,4,6		4	3							
3		2,5,6		4	2							
3		3,4,5		4	7							
0		3,4,6		4	7							
0		3,5,6		4	7							
0		4,5,6		4	3							
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZN*	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days									2
			14 days									0
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZN*	2	0	0	0	0.5	0	0	0	2	
3		2,3,4		4	3							
3		2,3,5		4	3							
3		2,3,6		4	3							
3		2,4,5		4	3							
3		2,4,6		4	3							
3		2,5,6		4	3							
3		3,4,5		4	3							
3		3,4,6		4	3							
3		3,5,6		4	3							
3		4,5,6		4	3							

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZP	24	0	0	0	2	0	0	0	4	EPA
			48	0	0	0	1	0	0	0	2	2
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
GHS Tissue		ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
		1	HZP	4	0.0	0.0	0.0	1.0	0.0	0.0	2	3
Summary block used analysis of the twenty combinations	ANIMAL ID											
	1	HZP	4	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2	3
	2	HZP	4	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2	2
	3	HZP	2	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0	3
	4	HZP	2	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0	3
	5	HZP	6	0.0	0.0	0.0	1.0	0.3	0.0	0.0	2	3
6	HZP	2	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0	2	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZQ	24	0	0	0	0	0	0	0	0	EPA
			48	0	0	0	0	0	0	0	0	0
			72								0	GHS
			7 days								0	0
			14 days								0	
			21 days								0	
GHS Tissue		ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
		1	HZQ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Summary block used analysis of the twenty combinations	ANIMAL ID											
	1	HZQ	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
	2	HZQ	34	1.0	1.7	0.7	2.0	1.3	1.0	1.0	7	7
	3	HZQ	8	0.0	0.0	0.0	1.0	0.3	0.3	0.3	2	3
	4	HZQ	6	0.0	0.0	0.0	1.3	0.0	0.3	0.3	3	3
	5	HZQ	6	0.0	0.0	0.0	1.0	0.3	0.0	0.0	2	3
6	HZQ	11	0.3	0.3	0.0	1.7	0.7	0.0	0.0	3	7	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZP	24	0	0	0	2	0	0	4	EPA	
			48	0	0	0	0	0	0	0	2	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	2	HZP	4	0	0	0	1	0	0	2	2	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0	0	1	0	2	3	Combina- tion block #2	1,3,4	0	0	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	1,2,4	0	0	1	0	2	3		1,3,5	0	0	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	1,2,5	0	0	1	0.166667	2	3		1,3,6	0	0	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	1,2,6	0	0	1	0	2	3		1,4,5	0	0	
GHS Rating	4	4	4	4	2	3	GHS Rating	4	4			
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZQ	24	1	3	1	3	2	2	34	EPA	
			48	1	1	1	2	1	1	18	7	
			72	1	1	0	1	1	0	9	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	2	HZQ	34	1	1.666667	0.666667	2	1.333333333	1	7	7	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0.5	0.333333	1.5	0.833333	7	7	Combina- tion block #2	1,3,4	0	0	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	1,2,4	0.5	0.333333	1.666667	0.666667	7	7		1,3,5	0	0	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	1,2,5	0.5	0.333333	1.5	0.833333	7	7		1,3,6	0.166667	0	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	1,2,6	0.666667	0.333333	1.833333	1	7	7		1,4,5	0	0	
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA		REDNESS	CHEMOSIS	DISCHARGE		
0.1	3	HZP	24	0	0	0	1	0	0	2	EPA
			48	0	0	0	1	0	0	2	0
			72	0	0	0	0	0	0	0	GHS
			7 days							0	3
			14 days							0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZP	2	0	0	0	0.666666667	0	0	0	3
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
0.833333	0	2	3	Combina- tion block #3	1,4,6	0.0	0.0	0.8	0.0	2	3
4	4	2	3		GHS Rating	4	4	4	4	2	3
1	0.166667	2	3		1,5,6	0.0	0.0	1.0	0.2	2	3
4	4	2	3		GHS Rating	4	4	4	4	2	3
0.833333	0	2	3		2,3,4	0.0	0.0	0.8	0.0	2	3
4	4	2	3		GHS Rating	4	4	4	4	2	3
1	0.166667	2	3		2,3,5	0.0	0.0	1.0	0.2	2	3
4	4	2	3		GHS Rating	4	4	4	4	2	3

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA		REDNESS	CHEMOSIS	DISCHARGE		
0.1	3	HZQ	24	0	0	0	2	1	1	8	EPA
			48	0	0	0	1	0	0	2	2
			72	0	0	0	0	0	0	0	GHS
			7 days							0	3
			14 days							0	
			21 days							0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	3	HZQ	8	0	0	0	1	0.33333333	0.33333333	2	3
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	
1.166667	0.166667	3	3	Combina- tion block #3	1,4,6	0.2	0.0	1.5	0.3	3	7
4	4	3	3		GHS Rating	4	4	4	4	3	7
1	0.333333	2	3		1,5,6	0.2	0.0	1.3	0.5	3	7
4	4	2	3		GHS Rating	4	4	4	4	3	7
1.333333	0.5	3	7		2,3,4	0.5	0.3	1.7	0.8	7	7
4	4	3	7		GHS Rating	4	4	4	4	7	7
1.166667	0.166667	3	3		2,3,5	0.5	0.3	1.5	0.8	7	7
4	4	3	3		GHS Rating	4	4	4	4	7	7

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZP	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	1	0	0	2	0	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
	4	HZP	MAS	0	0	0	0.66666667	0	0	0	3	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	0.0	0.0	0.8	0.0	2	3	Combina- tion block #5	3,4,5	0.0	0.0	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	2,4,5	0.0	0.0	1.0	0.2	2	3		3,4,6	0.0	0.0	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	2,4,6	0.0	0.0	0.8	0.0	2	3		3,5,6	0.0	0.0	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	2,5,6	0.0	0.0	1.0	0.2	2	3		4,5,6	0.0	0.0	
GHS Rating	4	4	4	4	2	3	GHS Rating	4	4			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZQ	24	0	0	0	2	0	0	4	EPA	
			48	0	0	0	2	0	1	6	3	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days								0	
	4	HZQ	MAS	0	0	0	1.33333333	0	0.33333333	3	3	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	0.7	0.3	1.8	1.0	7	7	Combina- tion block #5	3,4,5	0.0	0.0	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	2,4,5	0.5	0.3	1.7	0.8	7	7		3,4,6	0.2	0.0	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	2,4,6	0.7	0.3	1.8	1.0	7	7		3,5,6	0.2	0.0	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	2,5,6	0.7	0.3	1.8	1.0	7	7		4,5,6	0.2	0.0	
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE					
0.1	5	HZP	24	0	0	0	2	1	0	6	EPA			
			48	0	0	0	1	0	0	2	2			
			72	0	0	0	0	0	0	0	GHS			
			7 days							0	3			
			14 days							0				
			21 days							0				
			ANIMAL ID		MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
			5		HZP	6	0	0	0	1	0.33333333	0	2	3
			Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	4	3
			0.8	0.2	2	3					HZP	1,2,4	4	3
4	4	2	3						1,2,5	4	3			
0.7	0.0	0	3						1,2,6	4	3			
4	4	0	3						1,3,4	4	3			
0.8	0.2	2	3						1,3,5	4	3			
4	4	2	3						1,3,6	4	3			
0.8	0.2	2	3						1,4,5	4	3			
4	4	2	3						1,4,6	4	3			
									1,5,6	4	3			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO-CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE					
0.1	5	HZQ	24	0	0	0	2	1	0	6	EPA			
			48	0	0	0	1	0	0	2	2			
			72	0	0	0	0	0	0	0	GHS			
			7 days							0	3			
			14 days							0				
			21 days							0				
			ANIMAL ID		MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
			5		HZQ	6	0	0	0	1	0.33333333	0	2	3
			Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	4	7
			1.2	0.3	3	3					HZQ	1,2,4	4	7
4	4	3	3						1,2,5	4	7			
1.5	0.5	3	7						1,2,6	4	7			
4	4	3	7						1,3,4	4	3			
1.3	0.5	3	7						1,3,5	4	3			
4	4	3	7						1,3,6	4	7			
1.5	0.5	3	7						1,4,5	4	3			
4	4	3	7						1,4,6	4	7			
									1,5,6	4	7			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZP	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZP	2	0	0	0	0.5	0	0	0	2	
2		2,3,4	4	3		2						
2		2,3,5	4	3		2						
2		2,3,6	4	3		2						
2		2,4,5	4	3		2						
2		2,4,6	4	3		2						
2		2,5,6	4	3		2						
2		3,4,5	4	3		2						
2		3,4,6	4	3		0						
2		3,5,6	4	3		2						
2		4,5,6	4	3		2						
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZQ	24	1	1	0	2	1	0	11	EPA	
			48	0	0	0	2	1	0	6	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	0	7
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZQ	11	0.333333	0.333333	0	1.6666667	0.66666667	0	3	7	
7		2,3,4	4	7		7						
7		2,3,5	4	7		7						
7		2,3,6	4	7		7						
7		2,4,5	4	7		7						
3		2,4,6	4	7		7						
2		2,5,6	4	7		7						
3		3,4,5	4	3		3						
3		3,4,6	4	7		3						
3		3,5,6	4	7		3						
3		4,5,6	4	7		3						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	1	HZR*	24	1	3	1	3	3	1	34	EPA		
			48	1	1	1	3	2	1	22	7		
			72	0	0	0	2	1	0	6	GHS		
			7 days	0	0	0	0	0	0	0	7		
			14 days							0			
			21 days							0			
GHS Tissue			1	HZR*	34	0.7	1.3	0.7	2.7	2.0	0.7	7	7
Summary block used analysis of the twenty combinations			ANIMAL ID										
	1	HZR*	34	0.7	1.3	0.7	2.7	2.0	0.7	7	7		
	2	HZR*	23	0.7	1.0	0.3	1.7	1.0	0.3	3	7		
	3	HZR*	13	0.3	0.3	0.0	1.7	0.7	1.0	3	7		
	4	HZR*	31	1.0	1.7	1.0	2.0	2.3	2.0	22	22		
	5	HZR*	29	0.7	1.0	0.3	1.7	1.0	1.0	3	7		
	6	HZR*	34	1.0	1.7	0.7	2.0	1.3	1.0	7	7		
Dose Vol			0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	F40824	HZS	24	1	4	1	3	2	2	39	EPA		
			48	1	4	1	2	1	1	33	14		
			72	1	2	1	2	1	1	23	GHS		
			7 days	1	1	0	1	1	0	9	14		
			14 days	0	0	0	0	0	0	0			
			21 days							0			
GHS Tissue			F40824	HZS	39	1.0	3.3	1.0	2.3	1.3	1.3	14	14
Summary block used analysis of the twenty combinations			ANIMAL ID										
	F40824	HZS	39	1.0	3.3	1.0	2.3	1.3	1.3	14	14		
	F40863	HZS	39	1.0	3.3	1.0	2.3	1.7	1.3	22	22		
	F40885	HZS	37	1.0	3.3	1.0	2.0	2.0	2.0	7	7		
	F41368	HZS	41	1.0	4.0	1.0	2.0	2.0	2.3	22	22		
	5	HZS	39	1.0	2.7	1.0	2.0	1.7	2.0	7	7		
	6	HZS	39	1.0	3.0	1.0	2.0	2.0	2.3	22	22		
Dose Vol			0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	2	HZR*	24	1	2	1	2	1	1	23	EPA
			48	1	1	0	2	1	0	11	3
			72	0	0	0	1	1	0	4	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	2	HZR*	23	0.666667	1	0.333333	1.666666667	1	0.333333333	3	7
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	0.666667	0.5	2.166667	1.5	7	7	Combina- tion block #2	1,3,4	0.833333	0.833333
	GHS Rating	4	4	2	4	7	7		GHS Rating	4	4
	1,2,4	0.833333	0.833333	2.333333	2.166667	22	22		1,3,5	0.666667	0.5
	GHS Rating	4	4	2	2	22	22		GHS Rating	4	4
	1,2,5	0.666667	0.5	2.166667	1.5	7	7		1,3,6	0.833333	0.666667
	GHS Rating	4	4	2	4	7	7		GHS Rating	4	4
	1,2,6	0.833333	0.666667	2.333333	1.666667	7	7		1,4,5	0.833333	0.833333
GHS Rating	4	4	2	4	7	7	GHS Rating	4	4		

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	F40863	HZS	24	1	4	1	2	2	3	39	EPA
			48	1	4	1	3	1	1	35	22
			72	1	2	1	2	2	0	23	GHS
			7 days	1	1	0	2	1	0	11	22
			14 days	1	1	0	2	1	1	13	
			21 days	0	0	0	1	1	1	6	
	F40863	HZS	39	1	3.333333	1	2.333333333	1.666666667	1.333333333	22	22
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	1	1	2.333333	1.833333	22	22	Combina- tion block #2	1,3,4	1	1
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2
	1,2,4	1	1	2.333333	1.833333	22	22		1,3,5	1	1
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2
	1,2,5	1	1	2.333333	1.666667	22	22		1,3,6	1	1
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2
	1,2,6	1	1	2.333333	1.833333	22	22		1,4,5	1	1
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZR*	24	1	1	0	2	1	1	13	EPA	
			48	0	0	0	2	1	2	10	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZR*	13	0.333333	0.333333	0	1.666666667	0.666666667	1	3	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
2.333333	2.166667	22	22	Combina- tion block #3	1,4,6 GHS Rating	1.0	0.8	2.3	2.2	22	22	
2	2	22	22		1,5,6 GHS Rating	2	4	2	2	22	22	
2.166667	1.5	7	7		1,5,6 GHS Rating	0.8	0.7	2.3	1.7	7	7	
2	4	7	7		2,3,4 GHS Rating	4	4	2	4	7	7	
2.333333	1.666667	7	7		2,3,4 GHS Rating	0.8	0.7	1.8	1.7	22	22	
2	4	7	7		2,3,5 GHS Rating	4	4	4	4	22	22	
2.333333	2.166667	22	22		2,3,5 GHS Rating	0.7	0.3	1.7	1.0	3	7	
2	2	22	22			4	4	4	4	3	7	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F40885	HZS	24	1	4	1	2	2	2	37	EPA	
			48	1	3	1	2	2	2	32	7	
			72	1	3	1	2	2	2	32	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	F40885	HZS	37	1	3.333333	1	2	2	2	7	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
2.166667	2	22	22	Combina- tion block #3	1,4,6 GHS Rating	1.0	1.0	2.2	2.0	22	22	
2	2	22	22		1,5,6 GHS Rating	2	2	2	2	22	22	
2.166667	1.833333	14	14		1,5,6 GHS Rating	1.0	1.0	2.2	1.8	22	22	
2	4	14	14		2,3,4 GHS Rating	2	2	2	4	22	22	
2.166667	2	22	22		2,3,4 GHS Rating	1.0	1.0	2.2	2.0	22	22	
2	2	22	22		2,3,5 GHS Rating	2	2	2	2	22	22	
2.166667	1.833333	22	22		2,3,5 GHS Rating	1.0	1.0	2.2	1.8	22	22	
2	4	22	22			2	2	2	4	22	22	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZR*	24	1	2	1	2	3	3	31	EPA	
			48	1	2	1	2	2	2	27	22	
			72	1	1	1	2	2	1	20	GHS	
			7 days	1	1	0	2	1	1	13	22	
			14 days	2	1	0	1	1	0	14		
			21 days	1	1	0	0	0	0	5		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZR*	31	1	1.666667	1	2	2.333333333	2	22	22	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	0.8	0.5	1.8	1.2	7	7	Combinatio block #5	3,4,5	0.8	0.7	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	2,4,5	0.8	0.7	1.8	1.7	22	22		3,4,6	1.0	0.8	
	GHS Rating	4	4	4	4	22	22		GHS Rating	4	4	
	2,4,6	1.0	0.8	2.0	1.8	22	22		3,5,6	0.8	0.5	
	GHS Rating	2	4	2	4	22	22		GHS Rating	4	4	
	2,5,6	0.8	0.5	1.8	1.2	7	7		4,5,6	1.0	0.8	
GHS Rating	4	4	4	4	7	7	GHS Rating	2	4			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	F41368	HZS	24	1	4	1	2	3	3	41	EPA	
			48	1	4	1	2	2	2	37	22	
			72	1	4	1	2	1	2	35	GHS	
			7 days	1	2	1	2	2	2	27	22	
			14 days	3	1	0	3	2	3	31		
			21 days	2	1	0	2	2	1	20		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	F41368	HZS	41	1	4	1	2	2.333333333	2	22	22	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	1.0	2.2	2.0	22	22	Combinatio block #5	3,4,5	1.0	1.0	
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	2	
	2,4,5	1.0	1.0	2.2	1.8	22	22		3,4,6	1.0	1.0	
	GHS Rating	2	2	2	4	22	22		GHS Rating	2	2	
	2,4,6	1.0	1.0	2.2	2.0	22	22		3,5,6	1.0	1.0	
	GHS Rating	2	2	2	2	22	22		GHS Rating	2	2	
	2,5,6	1.0	1.0	2.2	1.8	22	22		4,5,6	1.0	1.0	
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZR*	24	1	2	1	2	2	3	29	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZR*	29	0.666667	1	0.333333	1.66666667	1	1	3	7	
Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	2	7	
1.8	1.7	22	22					HZR*	1,2,4	2	22	
4	4	22	22						1,2,5	2	7	
2.0	1.8	22	22						1,2,6	2	7	
2	4	22	22						1,3,4	2	22	
1.8	1.2	7	7						1,3,5	2	7	
4	4	7	7						1,3,6	2	7	
2.0	1.8	22	22						1,4,5	2	22	
2	4	22	22						1,4,6	2	22	
									1,5,6	2	7	
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZS	24	1	4	1	2	2	3	39	EPA	
			48	1	2	1	2	2	2	27	7	
			72	1	2	1	2	1	1	23	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZS	39	1	2.666667	1	2	1.666666667	2	7	7	
Redness	Chemosis	DtC EPA	DtC GHS					Summary	1,2,3	2	22	
2.0	2.0	22	22					HZS	1,2,4	2	22	
2	2	22	22						1,2,5	2	22	
2.0	2.0	22	22						1,2,6	2	22	
2	2	22	22						1,3,4	2	22	
2.0	2.0	22	22						1,3,5	2	14	
2	2	22	22						1,3,6	2	22	
2.0	2.0	22	22						1,4,5	2	22	
2	2	22	22						1,4,6	2	22	
									1,5,6	2	22	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZR*	24	1	3	1	2	2	3	34	EPA
			48	1	1	1	2	1	0	16	7
			72	1	1	0	2	1	0	11	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days						0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	6	HZR*	34	1	1.666667	0.666667	2	1.333333333	1	7	7
7		2,3,4	4	22		22					
22		2,3,5	4	7		3					
7		2,3,6	4	7		7					
7		2,4,5	4	22		22					
22		2,4,6	2	22		22					
7		2,5,6	4	7		7					
7		3,4,5	4	22		22					
22		3,4,6	2	22		22					
22		3,5,6	4	7		7					
7		4,5,6	2	22		22					
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZS	24	1	4	1	2	2	3	39	EPA
			48	1	2	1	2	2	2	27	22
			72	1	3	1	2	2	2	32	GHS
			7 days	1	2	1	2	2	2	27	22
			14 days	3	1	1	2	2	3	34	
			21 days	4	1	0	2	2	3	34	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	6	HZS	39	1	3	1	2	2	2.333333333	22	22
22		2,3,4	2	22		22					
22		2,3,5	2	22		22					
22		2,3,6	2	22		22					
22		2,4,5	2	22		22					
22		2,4,6	2	22		22					
14		2,5,6	2	22		22					
22		3,4,5	2	22		22					
22		3,4,6	2	22		22					
22		3,5,6	2	22		22					
22		4,5,6	2	22		22					

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZT	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days									0
			14 days									0
			21 days									0
GHS Tissue		1 HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	2	HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	3	HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	4	HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	5	HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	6	HZT	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZU*	24	1	2	1	3	2	2	29	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	3
			14 days								0	
			21 days								0	
GHS Tissue		1 HZU*	29	0.7	1.0	0.3	1.7	1.0	0.7	3	3	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZU*	29	0.7	1.0	0.3	1.7	1.0	0.7	3	3	
	2	HZU*	31	1.0	2.0	0.3	1.7	1.0	0.0	7	7	
	3	HZU*	22	1.0	1.3	0.0	2.0	1.3	0.7	7	7	
	4	HZU*	25	0.7	1.0	0.3	1.3	0.7	0.7	3	3	
	5	HZU*	24	0.7	0.7	0.3	1.7	1.0	1.0	3	7	
	6	HZU*	13	0.3	0.3	0.0	1.3	0.3	0.3	3	3	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZT	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days									0
			14 days									0
			21 days									0
	2	HZT	0	0	0	0	0	0	0	0	0	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0	0	0	0	0	0	Combina- tion block #2	1,3,4	0	0	
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4	
	1,2,4	0	0	0	0	0	0		1,3,5	0	0	
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4	
	1,2,5	0	0	0	0	0	0		1,3,6	0	0	
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4	
	1,2,6	0	0	0	0	0	0		1,4,5	0	0	
GHS Rating	4	4	4	4	0	0	GHS Rating	4	4			
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
0.1	2	HZU*	24	1	4			1	2			1
			48	1	1	0	2	1	0	11	7	
			72	1	1	0	1	1	0	9	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	2	HZU*	31	1	2	0.333333	1.666666667	1	0	7	7	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	1	0.333333	1.833333	1.166667	7	7	Combina- tion block #2	1,3,4	0.833333	0.333333	
	GHS Rating	2	4	4	4	7	7		GHS Rating	4	4	
	1,2,4	0.833333	0.333333	1.666667	1	7	7		1,3,5	0.833333	0.333333	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	1,2,5	0.833333	0.333333	1.666667	1	7	7		1,3,6	0.833333	0.166667	
	GHS Rating	4	4	4	4	7	7		GHS Rating	4	4	
	1,2,6	0.833333	0.333333	1.666667	1	7	7		1,4,5	0.666667	0.333333	
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	3	HZT	24	0	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	0	GHS
			72										0
			7 days										0
			14 days										0
			21 days										0
	3	HZT	0	0	0	0	0	0	0	0	0	0	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS			
0	0	0	0	Combinatio	1,4,6	0.0	0.0	0.0	0.0	0	0	0	
4	4	0	0	tion block	GHS Rating	4	4	4	4	0	0	0	
0	0	0	0	#3	1,5,6	0.0	0.0	0.0	0.0	0	0	0	
4	4	0	0		GHS Rating	4	4	4	4	0	0	0	
0	0	0	0		2,3,4	0.0	0.0	0.0	0.0	0	0	0	
4	4	0	0		GHS Rating	4	4	4	4	0	0	0	
0	0	0	0		2,3,5	0.0	0.0	0.0	0.0	0	0	0	
4	4	0	0		GHS Rating	4	4	4	4	0	0	0	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZU*	24	1	2	0	2	2	2	2	22	EPA
			48	1	1	0	2	1	0	11	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	3	HZU*	22	1	1.333333	0	2	1.33333333	0.66666667	7	7	7
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.833333	1.166667	7	7	Combinatio	1,4,6	0.7	0.3	1.5	0.8	3	3	3
4	4	7	7	tion block	GHS Rating	4	4	4	4	3	3	3
1.833333	1.166667	7	7	#3	1,5,6	0.7	0.3	1.7	1.0	3	7	7
4	4	7	7		GHS Rating	4	4	4	4	3	7	7
1.833333	1.166667	7	7		2,3,4	1.0	0.3	1.8	1.2	7	7	7
4	4	7	7		GHS Rating	2	4	4	4	7	7	7
1.666667	1	3	7		2,3,5	1.0	0.3	1.8	1.2	7	7	7
4	4	3	7		GHS Rating	2	4	4	4	7	7	7

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	4	HZT	24	0	0	0	0	0	0	0	EPA		
			48	0	0	0	0	0	0	0	0	GHS	
			72										0
			7 days										0
			14 days										0
			21 days										0
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	4	HZT	0	0	0	0	0	0	0	0	0		
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris		
Combina- tion block #4	2,3,6	0.0	0.0	0.0	0.0	0	0	0	3,4,5	0.0	0.0		
	GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4		
	2,4,5	0.0	0.0	0.0	0.0	0	0	0	3,4,6	0.0	0.0		
	GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4		
	2,4,6	0.0	0.0	0.0	0.0	0	0	0	3,5,6	0.0	0.0		
	GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4		
	2,5,6	0.0	0.0	0.0	0.0	0	0	0	4,5,6	0.0	0.0		
GHS Rating	4	4	4	4	0	0	0	GHS Rating	4	4			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	4	HZU*	25	0.666667	1	0.333333	1.333333	0.666666667	0.666666667	3	3		
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris		
Combina- tion block #4	2,3,6	1.0	0.2	1.8	1.2	7	7	7	3,4,5	0.8	0.3		
	GHS Rating	2	4	4	4	7	7	7	GHS Rating	4	4		
	2,4,5	0.8	0.3	1.7	1.0	7	7	7	3,4,6	0.8	0.2		
	GHS Rating	4	4	4	4	7	7	7	GHS Rating	4	4		
	2,4,6	0.8	0.3	1.5	0.8	7	7	7	3,5,6	0.8	0.2		
	GHS Rating	4	4	4	4	7	7	7	GHS Rating	4	4		
	2,5,6	0.8	0.3	1.7	1.0	7	7	7	4,5,6	0.7	0.3		
GHS Rating	4	4	4	4	7	7	7	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE					
0.1	5	HZT	24	0	0	0	0	0	0	0	0	EPA		
			48	0	0	0	0	0	0	0	0	0	GHS	
			72											
			7 days											0
			14 days											0
			21 days											0
	5	HZT	0	0	0	0	0	0	0	0	0	0		
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3		4	0			
0.0	0.0	0	0				HZT	1,2,4		4	0			
4	4	0	0					1,2,5		4	0			
0.0	0.0	0	0					1,2,6		4	0			
4	4	0	0					1,3,4		4	0			
0.0	0.0	0	0					1,3,5		4	0			
4	4	0	0					1,3,6		4	0			
0.0	0.0	0	0					1,4,5		4	0			
4	4	0	0					1,4,6		4	0			
								1,5,6		4	0			
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE					
0.1	5	HZU*	24	1	1	1	2	2	3	24	EPA			
			48	1	1	0	2	1	0	11	3			
			72	0	0	0	1	0	0	2	GHS			
			7 days	0	0	0	0	0	0	0	7			
			14 days											
			21 days											
	5	HZU*	24	0.666667	0.666667	0.333333	1.66666667	1	1	3	7			
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3		2	7			
1.8	1.2	7	7				HZU*	1,2,4		4	7			
4	4	7	7					1,2,5		4	7			
1.7	1.0	7	7					1,2,6		4	7			
4	4	7	7					1,3,4		4	7			
1.8	1.2	7	7					1,3,5		4	7			
4	4	7	7					1,3,6		4	7			
1.5	0.8	3	7					1,4,5		4	7			
4	4	3	7					1,4,6		4	3			
								1,5,6		4	7			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZT	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days									0
			14 days									0
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZT	0	0	0	0	0	0	0	0	0	
0		2,3,4	4	0		0						
0		2,3,5	4	0		0						
0		2,3,6	4	0		0						
0		2,4,5	4	0		0						
0		2,4,6	4	0		0						
0		2,5,6	4	0		0						
0		3,4,5	4	0		0						
0		3,4,6	4	0		0						
0		3,5,6	4	0		0						
0		4,5,6	4	0		0						
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZU*	24	1	1	0	2	1	1	13	EPA	
			48	0	0	0	2	0	0	4	3	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	3
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZU*	13	0.333333	0.333333	0	1.33333333	0.333333333	0.333333333	3	3	
7		2,3,4	2	7		7						
7		2,3,5	2	7		7						
7		2,3,6	2	7		7						
7		2,4,5	4	7		7						
7		2,4,6	4	7		7						
7		2,5,6	4	7		7						
7		3,4,5	4	7		7						
3		3,4,6	4	7		7						
3		3,5,6	4	7		7						
3		4,5,6	4	7		3						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZV*	24	1	3	1	3	2	3	36	EPA	
			48	1	1	0	2	1	0	11	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
GHS Tissue		1 HZV*	36	1.0	1.7	0.3	2.3	1.3	1.0	7	7	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZV*	36	1.0	1.7	0.3	2.3	1.3	1.0	7	7	
	2	HZV*	11	0.3	0.3	0.0	0.7	0.3	0.0	2	2	
	3	HZV*	16	0.7	1.0	0.0	1.3	0.7	0.0	3	7	
	4	HZV*	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	5	HZV*	20	0.7	0.7	0.3	1.7	1.0	0.3	3	7	
	6	HZV*	7	0.3	0.3	0.0	0.7	0.0	0.0	2	3	
Dose Vol		0.1										

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZW*	24	1	4	1	2	1	1	33	EPA	
			48	1	2	1	2	1	0	21	7	
			72	1	2	1	2	1	1	23	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
GHS Tissue		1 HZW*	33	1.0	2.7	1.0	2.0	1.0	0.7	7	7	
Summary block used analysis of the twenty combinations		ANIMAL ID										
	1	HZW*	33	1.0	2.7	1.0	2.0	1.0	0.7	7	7	
	2	HZW*	32	1.0	1.7	0.7	2.0	1.3	0.7	7	7	
	3	HZW*	28	1.0	2.0	0.3	2.0	1.0	0.7	7	7	
	4	HZW*	11	0.7	0.7	0.0	1.7	0.3	0.0	3	7	
	5	HZW*	29	1.0	1.3	0.3	1.7	1.0	1.0	7	7	
	6	HZW*	25	0.7	1.0	0.3	1.7	1.3	0.3	3	7	
Dose Vol		0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZV*	24	1	1	0	2	1	0	11	EPA	
			48	0	0	0	0	0	0	0	2	
			72	0	0	0	0	0	0	0	GHS	
			7 days								0	2
			14 days								0	
			21 days								0	
	2	HZV*	11	0.333333	0.333333	0	0.666666667	0.333333333	0	2	2	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	0.833333	0.166667	1.833333	1	7	7	Combina- tion block #2	1,3,4	0.833333	0.166667	
	GHS Rating	4	4	4	4	7	7	GHS Rating	4	4	4	
	1,2,4	0.666667	0.166667	1.5	0.833333	7	7	1,3,5	0.833333	0.333333	0.333333	
	GHS Rating	4	4	4	4	7	7	GHS Rating	4	4	4	
	1,2,5	0.833333	0.333333	2	1.166667	7	7	1,3,6	0.833333	0.166667	0.166667	
	GHS Rating	4	4	2	4	7	7	GHS Rating	4	4	4	
	1,2,6	0.666667	0.166667	1.5	0.833333	7	7	1,4,5	0.833333	0.333333	0.333333	
GHS Rating	4	4	4	4	7	7	GHS Rating	4	4	4		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	2	HZW*	24	1	3	1	2	2	2	32	EPA	
			48	1	1	1	2	1	0	16	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	2	HZW*	32	1	1.666667	0.666667	2	1.333333333	0.666666667	7	7	
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris	
Combina- tion block #1	1,2,3	1	0.833333	2	1.166667	7	7	Combina- tion block #2	1,3,4	1	0.666667	
	GHS Rating	2	4	2	4	7	7	GHS Rating	2	4	4	
	1,2,4	1	0.833333	2	1.166667	7	7	1,3,5	1	0.666667	0.666667	
	GHS Rating	2	4	2	4	7	7	GHS Rating	2	4	4	
	1,2,5	1	0.833333	2	1.166667	7	7	1,3,6	1	0.666667	0.666667	
	GHS Rating	2	4	2	4	7	7	GHS Rating	2	4	4	
	1,2,6	1	0.833333	2	1.333333	7	7	1,4,5	1	0.666667	0.666667	
GHS Rating	2	4	2	4	7	7	GHS Rating	2	4	4		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZV*	24	1	2	0	2	1	0	16	EPA	
			48	1	1	0	1	1	0	9	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZV*	16	0.666667	1	0	1.333333333	0.66666667	0	3	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
1.833333	1	7	7	Combinatio n block #3	1,4,6	0.7	0.2	1.5	0.7	7	7	
4	4	7	7		GHS Rating	4	4	4	4	7	7	
2	1.166667	7	7		1,5,6	0.8	0.3	2.0	1.2	7	7	
2	4	7	7		GHS Rating	4	4	2	4	7	7	
1.833333	1	7	7		2,3,4	0.5	0.0	1.0	0.5	3	7	
4	4	7	7		GHS Rating	4	4	4	4	3	7	
2	1.166667	7	7		2,3,5	0.7	0.2	1.5	0.8	3	7	
2	4	7	7		GHS Rating	4	4	4	4	3	7	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZW*	24	1	3	1	2	1	1	28	EPA	
			48	1	2	0	2	1	1	18	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZW*	28	1	2	0.333333	2	1	0.666666667	7	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
2	1	7	7	Combinatio n block #3	1,4,6	0.8	0.7	1.8	1.2	7	7	
2	4	7	7		GHS Rating	4	4	4	4	7	7	
2	1	7	7		1,5,6	1.0	0.7	1.8	1.2	7	7	
2	4	7	7		GHS Rating	2	4	4	4	7	7	
2	1.166667	7	7		2,3,4	1.0	0.5	2.0	1.2	7	7	
2	4	7	7		GHS Rating	2	4	2	4	7	7	
1.833333	1	7	7		2,3,5	1.0	0.5	2.0	1.2	7	7	
4	4	7	7		GHS Rating	2	4	2	4	7	7	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZV*	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days								0	
	4	HZV*	2	0	0	0	0.5	0	0	0	2	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	0.5	0.0	1.0	0.5	3	7	Combina- tion block #5	3,4,5	0.7	0.2	
	GHS Rating	4	4	4	4	3	7		GHS Rating	4	4	
	2,4,5	0.5	0.2	1.2	0.7	3	7		3,4,6	0.5	0.0	
	GHS Rating	4	4	4	4	3	7		GHS Rating	4	4	
	2,4,6	0.3	0.0	0.7	0.2	2	3		3,5,6	0.7	0.2	
	GHS Rating	4	4	4	4	2	3		GHS Rating	4	4	
	2,5,6	0.5	0.2	1.2	0.7	3	7		4,5,6	0.5	0.2	
GHS Rating	4	4	4	4	3	7	GHS Rating	4	4			
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZW*	24	1	1	0	2	1	0	11	EPA	
			48	1	1	0	2	0	0	9	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	4	HZW*	11	0.666667	0.666667	0	1.66666667	0.333333333	0	3	7	
	Combinatio		Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris	
Combina- tion block #4	2,3,6	1.0	0.5	2.0	1.3	7	7	Combina- tion block #5	3,4,5	1.0	0.3	
	GHS Rating	2	4	2	4	7	7		GHS Rating	2	4	
	2,4,5	1.0	0.5	1.8	1.2	7	7		3,4,6	0.8	0.3	
	GHS Rating	2	4	4	4	7	7		GHS Rating	4	4	
	2,4,6	0.8	0.5	1.8	1.3	7	7		3,5,6	1.0	0.3	
	GHS Rating	4	4	4	4	7	7		GHS Rating	2	4	
	2,5,6	1.0	0.5	1.8	1.3	7	7		4,5,6	0.8	0.3	
GHS Rating	2	4	4	4	7	7	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZV*	24	1	1	1	2	2	1	20	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	1	0	0	2	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	5	HZV*	20	0.666667	0.666667	0.333333	1.66666667	1	0.333333333	3	7	
Redness	Chemosis	DtC EPA	DtC GHS				Summary					
1.5	0.8	3	7				HZV*	1,2,3	4	7		
4	4	3	7					1,2,4	4	7		
1.0	0.3	3	7					1,2,5	2	7		
4	4	3	7					1,2,6	4	7		
1.5	0.8	3	7					1,3,4	4	7		
4	4	3	7					1,3,5	2	7		
1.2	0.5	3	7					1,3,6	4	7		
4	4	3	7					1,4,5	2	7		
								1,4,6	4	7		
								1,5,6	2	7		

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZW*	24	1	2	1	2	2	3	29	EPA	
			48	1	1	0	2	1	0	11	7	
			72	1	1	0	1	0	0	7	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
	5	HZW*	29	1	1.333333	0.333333	1.66666667	1	1	7	7	
Redness	Chemosis	DtC EPA	DtC GHS				Summary					
1.8	1.0	7	7				HZW*	1,2,3	2	7		
4	4	7	7					1,2,4	2	7		
1.8	1.2	7	7					1,2,5	2	7		
4	4	7	7					1,2,6	2	7		
1.8	1.2	7	7					1,3,4	2	7		
4	4	7	7					1,3,5	2	7		
1.7	1.2	7	7					1,3,6	2	7		
4	4	7	7					1,4,5	2	7		
								1,4,6	4	7		
								1,5,6	2	7		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZV*	24	1	1	0	1	0	0	7	EPA	
			48	0	0	0	1	0	0	2	2	
			72	0	0	0	0	0	0	0	0	GHS
			7 days								0	3
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZV*	7	0.333333	0.333333	0	0.66666667	0	0	2	3	
7		2,3,4	4	7		3						
7		2,3,5	4	7		3						
7		2,3,6	4	7		3						
7		2,4,5	4	7		3						
7		2,4,6	4	3		2						
7		2,5,6	4	7		3						
7		3,4,5	4	7		3						
7		3,4,6	4	7		3						
7		3,5,6	4	7		3						
7		4,5,6	4	7		3						
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO-CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZW*	24	1	2	1	2	2	1	25	EPA	
			48	1	1	0	2	1	0	11	3	
			72	0	0	0	1	1	0	4	GHS	
			7 days	0	0	0	0	0	0	0	0	7
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZW*	25	0.666667	1	0.333333	1.66666667	1.333333333	0.333333333	3	7	
7		2,3,4	2	7		7						
7		2,3,5	2	7		7						
7		2,3,6	2	7		7						
7		2,4,5	2	7		7						
7		2,4,6	4	7		7						
7		2,5,6	2	7		7						
7		3,4,5	2	7		7						
7		3,4,6	4	7		7						
7		3,5,6	2	7		7						
7		4,5,6	4	7		7						

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZX	24	1	4	1	2	2	2	2	37	EPA
			48	1	4	1	2	2	2	2	37	22
			72	1	4	1	2	2	2	2	37	GHS
			7 days	1	2	0	2	2	2	2	22	22
			14 days	1	1	0	2	2	2	2	17	
			21 days	1	1	0	2	1	0	0	11	
GHS Tissue		1 HZX	37	1.0	4.0	1.0	2.0	2.0	2.0	22	22	
		ANIMAL ID										
Summary block used analysis of the twenty combinations		1	37	1.0	4.0	1.0	2.0	2.0	2.0	22	22	
		2	41	1.0	2.3	0.7	2.3	1.3	1.3	7	7	
		3	39	1.0	2.7	0.7	2.7	1.3	1.3	7	7	
		4	41	1.0	3.3	1.0	2.3	2.0	2.0	21	22	
		5	39	1.0	4.0	1.0	2.3	2.0	2.0	22	22	
		6	41	1.0	2.7	1.0	2.3	1.3	1.7	14	14	
		Dose Vol	0.1									

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZY	24	1	4	1	2	3	3	41	EPA	
			48	1	4	1	3	1	1	35	7	
			72	1	3	1	2	1	1	28	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days								0	
			21 days								0	
GHS Tissue		1 HZY	41	1.0	3.7	1.0	2.3	1.7	1.7	7	7	
		ANIMAL ID										
Summary block used analysis of the twenty combinations		1	41	1.0	3.7	1.0	2.3	1.7	1.7	7	7	
		2	37	1.0	4.0	1.0	2.7	1.7	1.7	14	14	
		3	41	1.0	3.3	1.0	2.7	2.0	1.7	7	7	
		4	37	1.0	3.7	1.0	2.3	2.0	1.7	21	21	
		5	39	1.0	3.7	1.0	2.7	2.0	2.0	22	22	
		6	31	1.0	4.0	0.3	2.0	1.0	1.0	22	22	
		Dose Vol	0.1									

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	2	HZX	24	1	4	1	3	2	3	41	EPA
			48	1	2	1	2	1	1	23	7
			72	1	1	0	2	1	0	11	GHS
			7 days	0	0	0	0	0	0	0	7
			14 days							0	
			21 days							0	
	2	HZX	41	1	2.333333	0.666667	2.333333333	1.333333333	1.333333333	7	7
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	1	0.833333	2.5	1.666667	22	22	Combina- tion block #2	1,3,4	1	1
	GHS Rating	2	4	2	4	22	22	GHS Rating	2	2	
	1,2,4	1	1	2.333333	2	22	22	1,3,5	1	1	
	GHS Rating	2	2	2	2	22	22	GHS Rating	2	2	
	1,2,5	1	1	2.333333	2	22	22	1,3,6	1	1	
	GHS Rating	2	2	2	2	22	22	GHS Rating	2	2	
	1,2,6	1	1	2.333333	1.666667	22	22	1,4,5	1	1	
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2		

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	2	HZY	24	1	4	1	2	2	2	37	EPA
			48	1	4	1	3	1	2	37	14
			72	1	4	1	3	2	1	37	GHS
			7 days	1	1	0	2	1	0	11	14
			14 days	0	0	0	0	0	0	0	
			21 days							0	
	2	HZY	37	1	4	1	2.666666667	1.666666667	1.666666667	14	14
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris
Combina- tion block #1	1,2,3	1	1	2.666667	1.833333	14	14	Combina- tion block #2	1,3,4	1	1
	GHS Rating	2	2	2	4	14	14	GHS Rating	2	2	
	1,2,4	1	1	2.5	1.833333	21	21	1,3,5	1	1	
	GHS Rating	2	2	2	4	21	21	GHS Rating	2	2	
	1,2,5	1	1	2.666667	1.833333	22	22	1,3,6	1	1	
	GHS Rating	2	2	2	4	22	22	GHS Rating	2	2	
	1,2,6	1	1	2.5	1.666667	22	22	1,4,5	1	1	
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZX	24	1	4	1	3	2	2	39	EPA	
			48	1	3	1	3	1	2	32	7	
			72	1	1	0	2	1	0	11	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZX	39	1	2.666667	0.666667	2.666666667	1.33333333	1.333333333	7	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
2.5	2	22	22	Combina- tion block #3	1,4,6 GHS Rating	1.0	1.0	2.3	2.0	22	22	
2	2	22	22		1,5,6 GHS Rating	2	2	2	2	22	22	
2.5	2	22	22		1,5,6 GHS Rating	1.0	1.0	2.3	2.0	22	22	
2	2	22	22		2,3,4 GHS Rating	2	2	2	2	22	22	
2.5	1.666667	22	22		2,3,4 GHS Rating	1.0	0.8	2.5	1.7	21	22	
2	4	22	22		2,3,5 GHS Rating	2	4	2	4	21	22	
2.333333	2	22	22		2,3,5 GHS Rating	1.0	0.8	2.5	1.7	22	22	
2	2	22	22		2,3,5 GHS Rating	2	4	2	4	22	22	

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	3	HZY	24	1	4	1	3	2	3	41	EPA	
			48	1	4	1	3	2	2	39	7	
			72	1	2	1	2	2	0	23	GHS	
			7 days	0	0	0	0	0	0	0	7	
			14 days							0		
			21 days							0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	3	HZY	41	1	3.333333	1	2.666666667	2	1.666666667	7	7	
Redness	Chemosis	DtC EPA	DtC GHS	Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
2.5	2	21	21	Combina- tion block #3	1,4,6 GHS Rating	1.0	1.0	2.3	1.8	22	22	
2	2	21	21		1,5,6 GHS Rating	2	2	2	4	22	22	
2.666667	2	22	22		1,5,6 GHS Rating	1.0	1.0	2.5	1.8	22	22	
2	2	22	22		2,3,4 GHS Rating	2	2	2	4	22	22	
2.5	1.833333	22	22		2,3,4 GHS Rating	1.0	1.0	2.7	2.0	21	21	
2	4	22	22		2,3,5 GHS Rating	2	2	2	2	21	21	
2.5	2	22	22		2,3,5 GHS Rating	1.0	1.0	2.7	2.0	22	22	
2	2	22	22		2,3,5 GHS Rating	2	2	2	2	22	22	

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZX	24	1	4	1	3	2	3	41	EPA	
			48	1	3	1	2	2	1	30	21	
			72	1	3	1	2	2	2	32	GHS	
			7 days	1	2	1	2	2	2	27	22	
			14 days	1	1	0	2	2	2	17		
			21 days	0	0	0	1	1	0	4		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZX	41	1	3.333333	1	2.33333333	2	2	21	22	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	0.8	2.5	1.3	14	14	Combinatio block #5	3,4,5	1.0	1.0	
	GHS Rating	2	4	2	4	14	14	GHS Rating	2	2		
	2,4,5	1.0	1.0	2.3	2.0	22	22	3,4,6	1.0	1.0		
	GHS Rating	2	2	2	2	22	22	GHS Rating	2	2		
	2,4,6	1.0	1.0	2.3	1.7	21	22	3,5,6	1.0	1.0		
	GHS Rating	2	2	2	4	21	22	GHS Rating	2	2		
	2,5,6	1.0	1.0	2.3	1.7	22	22	4,5,6	1.0	1.0		
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2			

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZY	24	1	4	1	2	2	2	37	EPA	
			48	1	4	1	2	2	2	37	21	
			72	1	3	1	3	2	1	32	GHS	
			7 days	1	1	1	2	1	0	16	21	
			14 days	1	1	0	1	1	1	11		
			21 days	0	0	0	0	0	0	0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZY	37	1	3.666667	1	2.33333333	2	1.66666667	21	21	
	Combinatio			Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations	Opacity	Iris
Combinatio block #4	2,3,6	1.0	1.0	2.7	1.8	22	22	Combinatio block #5	3,4,5	1.0	1.0	
	GHS Rating	2	2	2	4	22	22	GHS Rating	2	2		
	2,4,5	1.0	1.0	2.7	2.0	22	22	3,4,6	1.0	1.0		
	GHS Rating	2	2	2	2	22	22	GHS Rating	2	2		
	2,4,6	1.0	1.0	2.5	1.8	22	22	3,5,6	1.0	1.0		
	GHS Rating	2	2	2	4	22	22	GHS Rating	2	2		
	2,5,6	1.0	1.0	2.7	1.8	22	22	4,5,6	1.0	1.0		
GHS Rating	2	2	2	4	22	22	GHS Rating	2	2			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZX	24	1	4	1	2	2	2	2	37	EPA
			48	1	4	1	3	2	2	2	39	22
			72	1	4	1	2	2	2	2	37	GHS
			7 days	1	1	0	2	1	1	1	13	22
			14 days	1	1	0	1	1	0	0	9	
			21 days	1	1	0	0	0	0	0	5	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZX	39	1	4	1	2.33333333	2	2	22	22	
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	2	22		
2.5	2.0	22	22				HZX	1,2,4	2	22		
2	2	22	22					1,2,5	2	22		
2.5	1.7	21	22					1,2,6	2	22		
2	4	21	22					1,3,4	2	22		
2.5	1.7	22	22					1,3,5	2	22		
2	4	22	22					1,3,6	2	22		
2.3	2.0	22	22					1,4,5	2	22		
2	2	22	22					1,4,6	2	22		
								1,5,6	2	22		
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	5	HZY	24	1	4	1	2	2	2	2	37	EPA
			48	1	4	1	3	2	2	2	39	22
			72	1	3	1	3	2	2	2	34	GHS
			7 days	1	2	0	2	2	1	1	20	22
			14 days	2	1	0	2	2	1	1	20	
			21 days	2	1	0	2	2	1	1	20	
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	5	HZY	39	1	3.666667	1	2.66666667	2	2	22	22	
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3	2	14		
2.7	2.0	22	22				HZY	1,2,4	2	21		
2	2	22	22					1,2,5	2	22		
2.5	2.0	22	22					1,2,6	2	22		
2	2	22	22					1,3,4	2	21		
2.7	2.0	22	22					1,3,5	2	22		
2	2	22	22					1,3,6	2	22		
2.5	2.0	22	22					1,4,5	2	22		
2	2	22	22					1,4,6	2	22		
								1,5,6	2	22		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZX	24	1	4	1	3	2	3	41	EPA
			48	1	2	1	2	1	2	25	14
			72	1	2	1	2	1	0	21	GHS
			7 days	1	1	0	0	0	0	5	14
			14 days	0	0	0	0	0	0	0	
			21 days						0		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	6	HZX	41	1	2.666667	1	2.33333333	1.333333333	1.666666667	14	14
22		2,3,4	2	22		21					
22		2,3,5	2	22		22					
22		2,3,6	2	14		14					
22		2,4,5	2	22		22					
22		2,4,6	2	22		21					
22		2,5,6	2	22		22					
22		3,4,5	2	22		22					
22		3,4,6	2	22		21					
22		3,5,6	2	22		22					
22		4,5,6	2	22		22					
Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR
				OPACITY	AREA			CHEMOSIS	DISCHARGE		
0.1	6	HZY	24	1	4	0	2	1	2	30	EPA
			48	1	4	0	2	1	1	28	22
			72	1	4	1	2	1	0	31	GHS
			7 days	1	4	1	2	1	0	31	22
			14 days	1	4	0	1	1	0	24	
			21 days	1	1	0	1	0	7		
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS
	6	HZY	31	1	4	0.333333	2	1	1	22	22
14		2,3,4	2	21		21					
21		2,3,5	2	22		22					
22		2,3,6	2	22		22					
22		2,4,5	2	22		22					
21		2,4,6	2	22		22					
22		2,5,6	2	22		22					
22		3,4,5	2	22		22					
22		3,4,6	2	22		22					
22		3,5,6	2	22		22					
22		4,5,6	2	22		22					

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	1	HZZ	24	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	
			72									GHS
			7 days									0
			14 days									0
			21 days									0
GHS Tissue	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	1	HZZ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
Summary block used analysis of the twenty combinations	ANIMAL ID											
	1	HZZ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	2	HZZ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	3	HZZ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
	4	HZZ	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2	
	5	HZZ	0	0.0	0.0	0.0	0.0	0.0	0.0	0	0	
6	HZZ	2	0.0	0.0	0.0	0.5	0.0	0.0	0	2		
	Dose Vol	0.1										

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR		
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	2	HZZ	24	0	0	0	0	0	0	0	EPA		
			48	0	0	0	0	0	0	0	0	GHS	
			72										
			7 days										
			14 days										
			21 days										
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	2	HZZ	0	0	0	0	0	0	0	0	0		
	Combinations	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		Combinations	Opacity	Iris		
Combina- tion block #1	1,2,3	0	0	0	0	0	0	Combina- tion block #2	1,3,4	0	0		
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4		
	1,2,4	0	0	0.25	0	0	2		1,3,5	0	0		
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4		
	1,2,5	0	0	0	0	0	0		1,3,6	0	0		
	GHS Rating	4	4	4	4	0	0		GHS Rating	4	4		
	1,2,6	0	0	0.25	0	0	2		1,4,5	0	0		
GHS Rating	4	4	4	4	0	2	GHS Rating	4	4				

IIVS Submission - In Vivo Data and Analysis for the Gettings et al. (1996) Study

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	3	HZZ	24	0	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	0	GHS
			72										0
			7 days										0
			14 days										0
			21 days										0
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	3	HZZ	0	0	0	0	0	0	0	0	0		
Redness	Chemosis	DtC EPA	DtC GHS		Combinatio	Opacity	Iris	Redness	Chemosis	DtC EPA	DtC GHS		
0.25	0	0	2	Combina- tion block #3	1,4,6	0.0	0.0	0.5	0.0	0	2		
4	4	0	2		GHS Rating	4	4	4	4	0	2		
0	0	0	0		1,5,6	0.0	0.0	0.3	0.0	0	2		
4	4	0	0		GHS Rating	4	4	4	4	0	2		
0.25	0	0	2		2,3,4	0.0	0.0	0.3	0.0	0	2		
4	4	0	2		GHS Rating	4	4	4	4	0	2		
0.25	0	0	2		2,3,5	0.0	0.0	0.0	0.0	0	0		
4	4	0	2		GHS Rating	4	4	4	4	0	0		

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	4	HZZ	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	GHS
			72								0	2
			7 days								0	
			14 days								0	
			21 days						0			
	4	HZZ	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	4	HZZ	2	0	0	0	0.5	0	0	0	2	
	Combinatio Opacity		Iris	Redness	Chemosis	DtC EPA	DtC GHS	Combinations		Opacity	Iris	
Combina- tion block #4	2,3,6	0.0	0.0	0.3	0.0	0	2	Combina- tion block #5	3,4,5	0.0	0.0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	2,4,5	0.0	0.0	0.3	0.0	0	2		3,4,6	0.0	0.0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	2,4,6	0.0	0.0	0.5	0.0	0	2		3,5,6	0.0	0.0	
	GHS Rating	4	4	4	4	0	2		GHS Rating	4	4	
	2,5,6	0.0	0.0	0.3	0.0	0	2		4,5,6	0.0	0.0	
GHS Rating	4	4	4	4	0	2	GHS Rating	4	4			

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Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL			DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE				
0.1	5	HZZ	24	0	0	0	0	0	0	0	0	EPA	
			48	0	0	0	0	0	0	0	0	0	
			72										GHS
			7 days										0
			14 days										
			21 days										
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS		
	5	HZZ	0	0	0	0	0	0	0	0	0		
Redness	Chemosis	DtC EPA	DtC GHS				Summary	1,2,3		4	0		
0.3	0.0	0	2				HZZ	1,2,4		4	2		
4	4	0	2					1,2,5		4	0		
0.5	0.0	0	2					1,2,6		4	2		
4	4	0	2					1,3,4		4	2		
0.3	0.0	0	2					1,3,5		4	0		
4	4	0	2					1,3,6		4	2		
0.5	0.0	0	2					1,4,5		4	2		
4	4	0	2					1,4,6		4	2		
								1,5,6		4	2		

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Gettings et al. (1996) Study**

Volume	ANIMAL ID	TEST MATL	TIME	CORNEAL		IRIS	REDNESS	CONJUNCTIVAL		DRAIZE	DAYS-TO- CLEAR	
				OPACITY	AREA			CHEMOSIS	DISCHARGE			
0.1	6	HZZ	24	0	0	0	1	0	0	2	EPA	
			48	0	0	0	0	0	0	0	0	
			72								0	GHS
			7 days								0	2
			14 days								0	
			21 days						0			
	ANIMAL ID	MATL	MAS	OPACITY	AREA	IRIS	REDNESS	CHEMOSIS	DISCHARGE	DtC EPA	DtC GHS	
	6	HZZ	2	0	0	0	0.5	0	0	0	2	
0		2,3,4		4	2	0						
0		2,3,5		4	0	0						
0		2,3,6		4	2	0						
0		2,4,5		4	2	0						
0		2,4,6		4	2	0						
0		2,5,6		4	2	0						
0		3,4,5		4	2	0						
0		3,4,6		4	2	0						
0		3,5,6		4	2	0						
0		4,5,6		4	2	0						

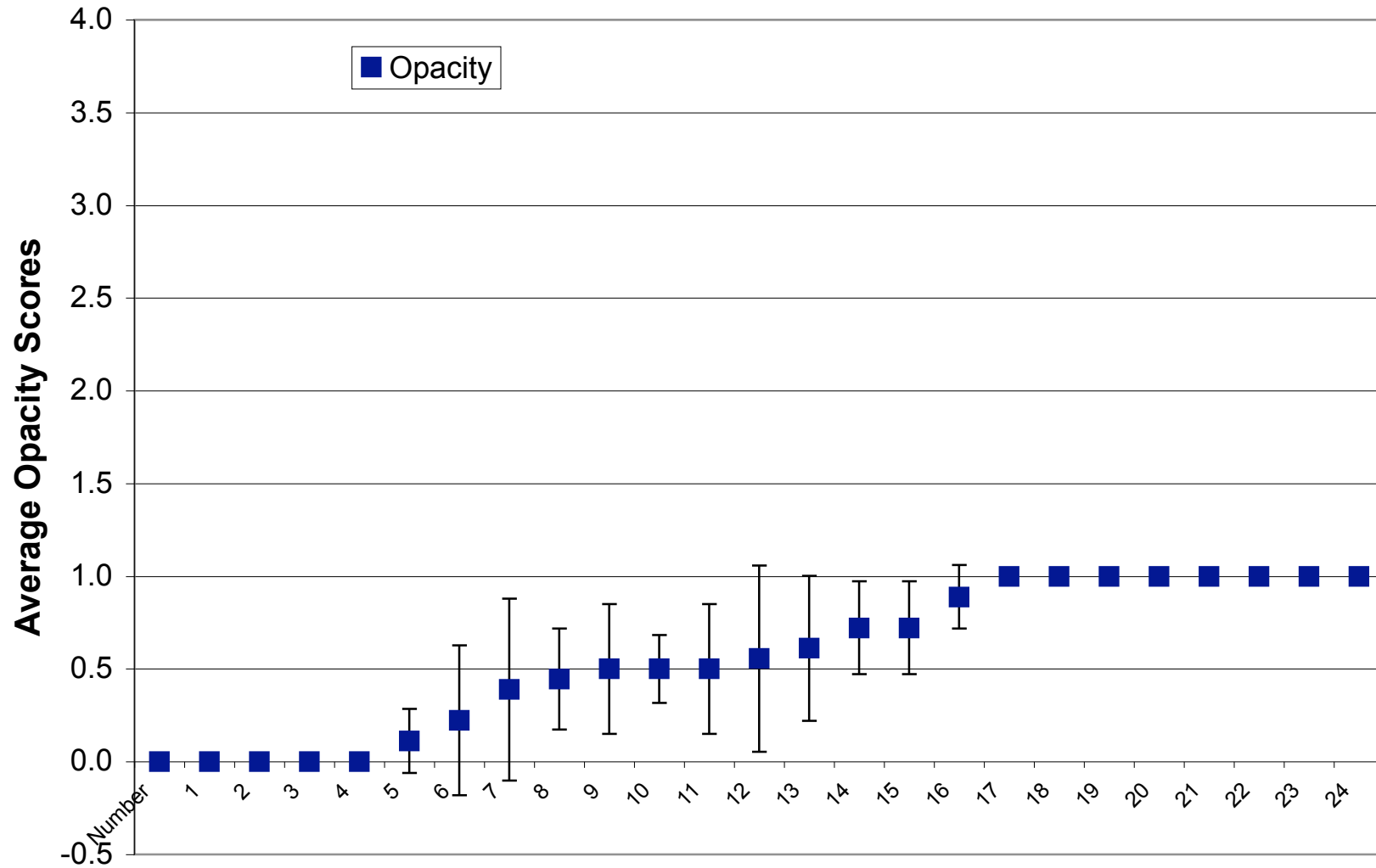
**Summary of Boot Strap Analysis for the
Gettings et al. (1996) Study**

Summary of the Animal Data

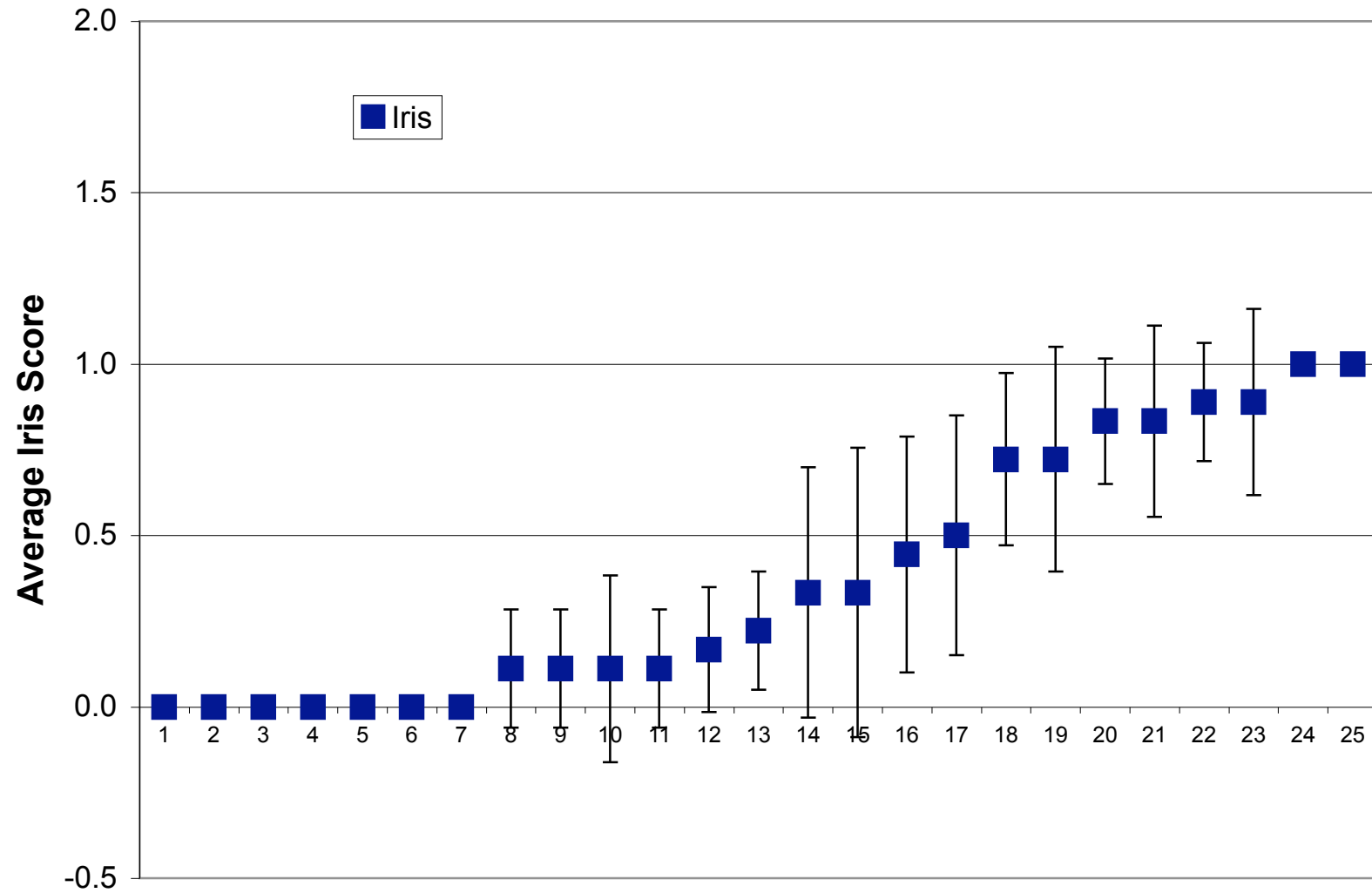
Name	Material	GHS 1	GHS 2a	GHS 2b	GHS NI	EPA 1	EPA 2	EPA 3	EPA 4	Mean OD490	SD OD490
Shampoo 7	HZA	16	4	0	0	16	4	0	0	0.41	0.16
Liquid Soap 1	HZB*	0	0	4	16	0	0	20	0	0.20	0.02
Shampoo 1	HZC*	0	0	10	10	0	0	20	0	0.96	0.31
Shampoo 5	HZD*	0	0	0	20	0	0	20	0	0.23	0.08
Gel Cleaner	HZE	10	0	0	10	10	0	10	0	0.19	0.05
Baby Shampoo 2	HZF	16	4	0	0	16	4	0	0	0.42	0.08
Shampoo 8	HZG*	0	0	0	20	0	0	20	0	0.20	0.06
Eye Makeup re.	HZH	0	0	0	20	0	0	0	20	0.02	0.02
Skin Cleaner	HZI	16	3	1	0	16	3	1	0	0.77	0.04
Mild Shampoo	HZJ	0	0	0	20	0	0	0	20	0.05	0.03
Bubble bath	HZK	20	0	0	0	20	0	0	0	0.96	0.32
Foam Bath	HZL	19	0	1	0	16	0	4	0	0.91	0.26
Shampoo 3	HZM*	0	0	10	10	0	0	10	10	0.21	0.05
Shampoo 6	HZN*	0	0	0	20	0	0	20	0	0.27	0.08
Baby Shampoo 1	HZP	0	0	0	20	0	0	19	1	0.26	0.05
Cleaning Gel	HZQ	0	0	0	20	0	0	20	0	0.16	0.05
Facial Ci Foam	HZR*	10	0	6	4	10	0	10	0	0.24	0.02
Shower Gel	HZS	19	1	0	0	19	1	0	0	1.55	0.09
Polishing Scrub	HZT	0	0	0	20	0	0	0	20	0.00	0.00
Hand Soap	HZU*	0	0	4	16	0	0	20	0	0.29	0.09
Shampoo 4	HZV*	0	0	4	16	0	0	20	0	0.27	0.04
Liquid Soap 2	HZW*	0	0	16	4	0	0	20	0	0.35	0.10
Shampoo 2	HZX	19	1	0	0	16	4	0	0	0.71	0.29
Shampoo AntiD	HZY	16	4	0	0	16	4	0	0	0.85	0.20
Facial Cleaner	HZZ	0	0	0	20	0	0	0	20	0.00	0.00

Name	Material	GHS 1	GHS 2a	GHS 2b	GHS NI	EPA 1	EPA 2	EPA 3	EPA 4	Mean OD490	SD OD490
Polishing Scrub	HZT	0	0	0	20	0	0	0	20	0.001	0.001
Facial Cleaner	HZZ	0	0	0	20	0	0	0	20	0.004	0.004
Eye Makeup re.	HZH	0	0	0	20	0	0	0	20	0.020	0.016
Mild Shampoo	HZJ	0	0	0	20	0	0	0	20	0.050	0.025
Cleaning Gel	HZQ	0	0	0	20	0	0	20	0	0.164	0.050
Gel Cleaner	HZE	10	0	0	10	10	0	10	0	0.194	0.048
Shampoo 8	HZG*	0	0	0	20	0	0	20	0	0.197	0.058
Liquid Soap 1	HZB*	0	0	4	16	0	0	0	0	0.199	0.024
Shampoo 3	HZM*	0	0	10	10	0	0	10	10	0.214	0.049
Shampoo 5	HZD*	0	0	0	20	0	0	20	0	0.231	0.084
Facial Ci Foam	HZR*	10	0	6	4	10	0	10	0	0.239	0.022
Baby Shampoo 1	HZP	0	0	0	20	0	0	19	1	0.261	0.051
Shampoo 6	HZN*	0	0	0	20	0	0	20	0	0.267	0.076
Shampoo 4	HZV*	0	0	4	16	0	0	20	0	0.268	0.045
Hand Soap	HZU*	0	0	4	16	0	0	20	0	0.293	0.092
Liquid Soap 2	HZW*	0	0	16	4	0	0	20	0	0.352	0.100
Shampoo 7	HZA	16	4	0	0	16	4	0	0	0.406	0.156
Baby Shampoo 2	HZF	16	4	0	0	16	4	0	0	0.425	0.082
Shampoo 2	HZX	19	1	0	0	16	4	0	0	0.705	0.289
Skin Cleaner	HZI	16	3	1	0	16	3	1	0	0.769	0.036
Shampoo AntiD	HZY	16	4	0	0	16	4	0	0	0.847	0.199
Foam Bath	HZL	19	0	1	0	16	0	4	0	0.912	0.261
Bubble bath	HZK	20	0	0	0	20	0	0	0	0.956	0.324
Shampoo 1	HZC*	0	0	10	10	0	0	20	0	0.957	0.306
Shower Gel	HZS	19	1	0	0	19	1	0	0	1.548	0.093

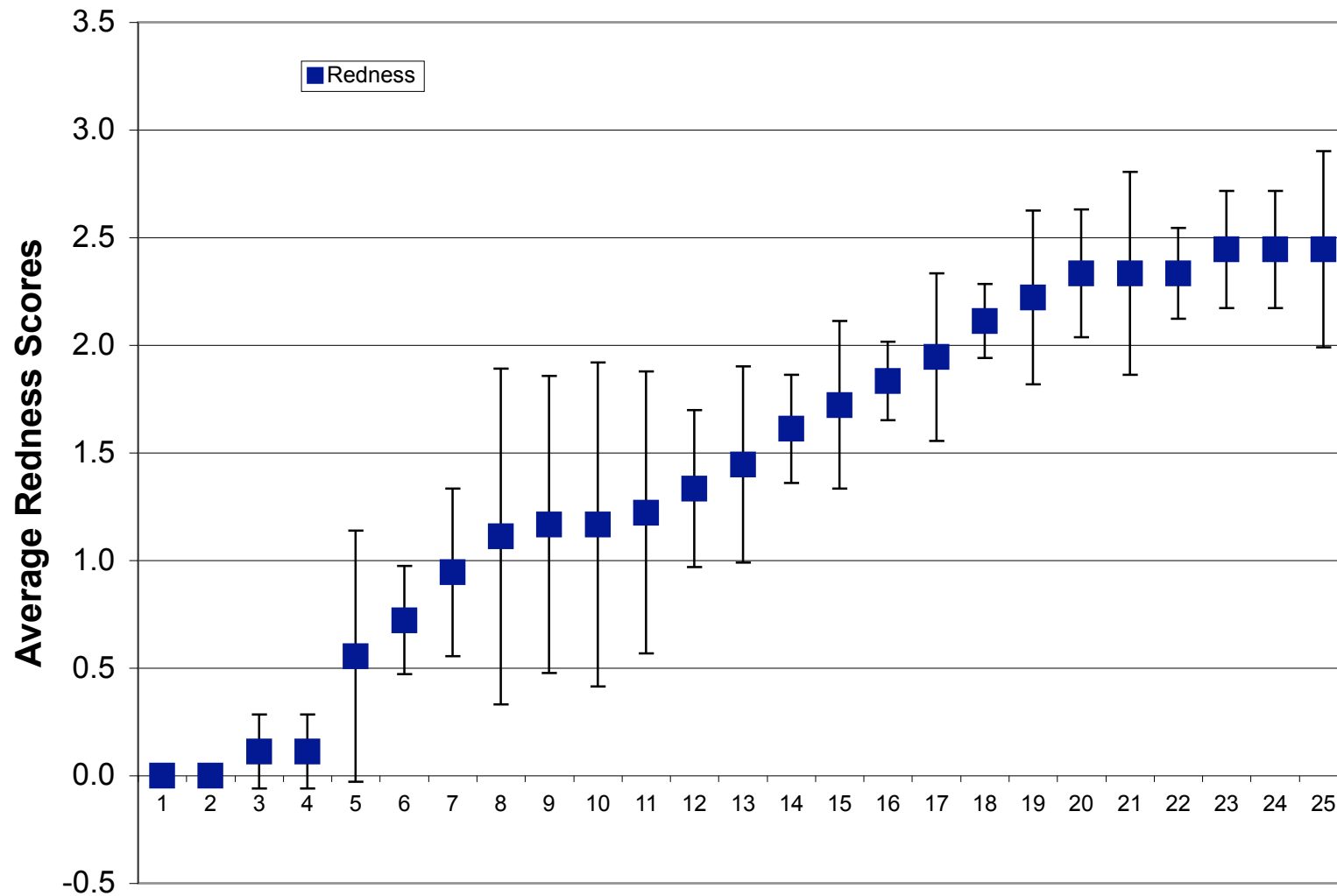
IIVS Submission - Analysis of In Vivo Data for Gettings et al. (1996)



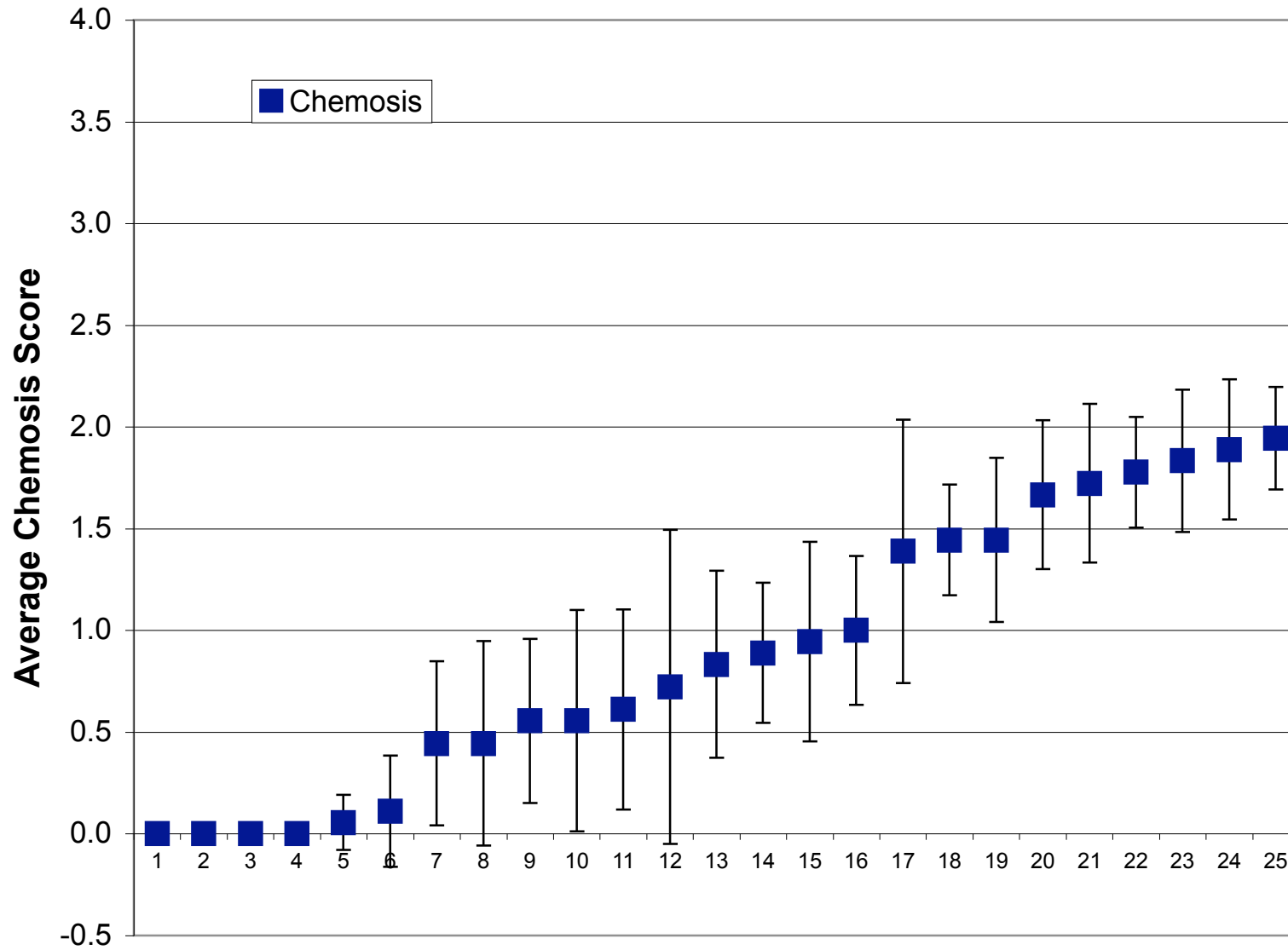
IIVS Submission - Analysis of In Vivo Data for Gettings et al. (1996)



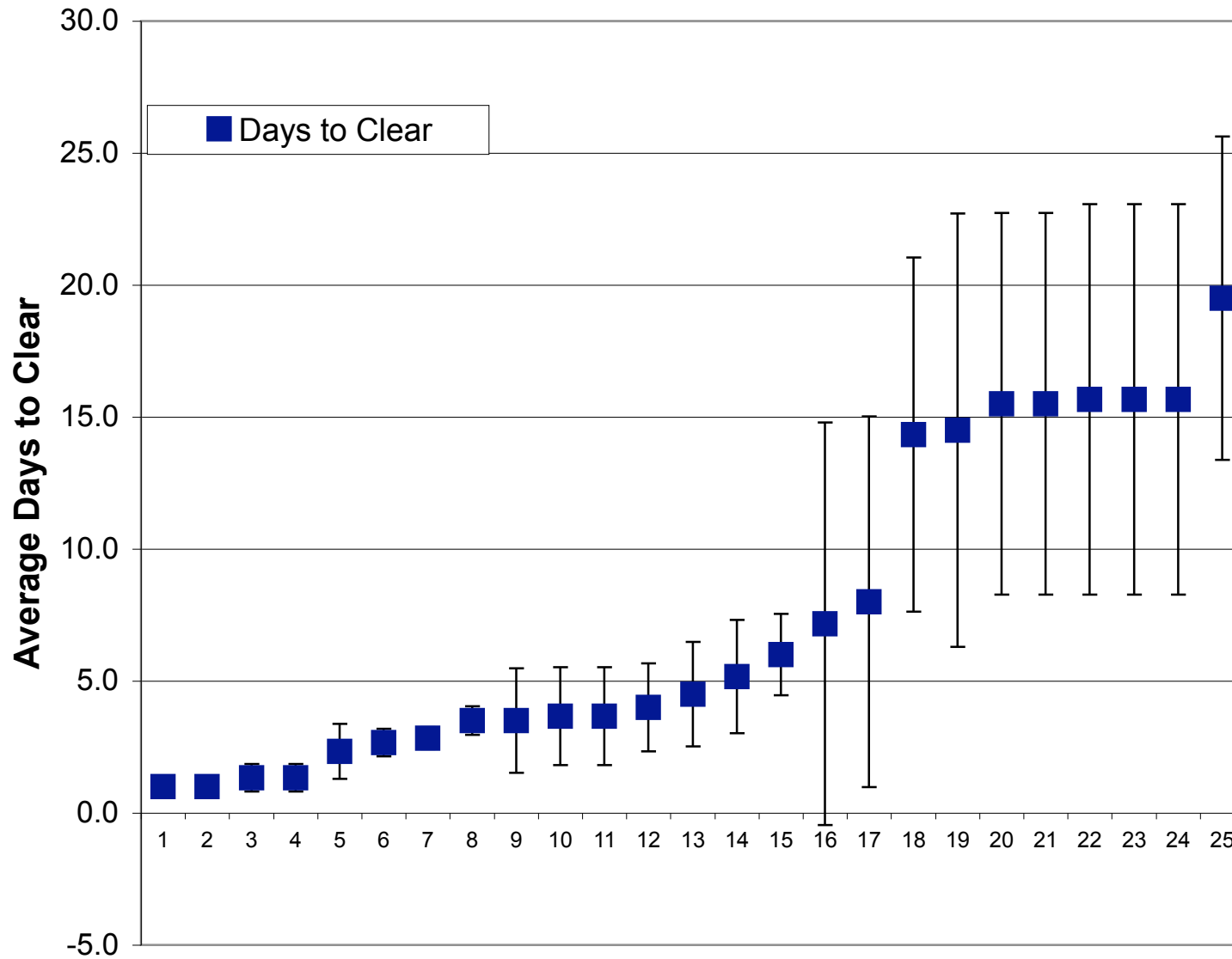
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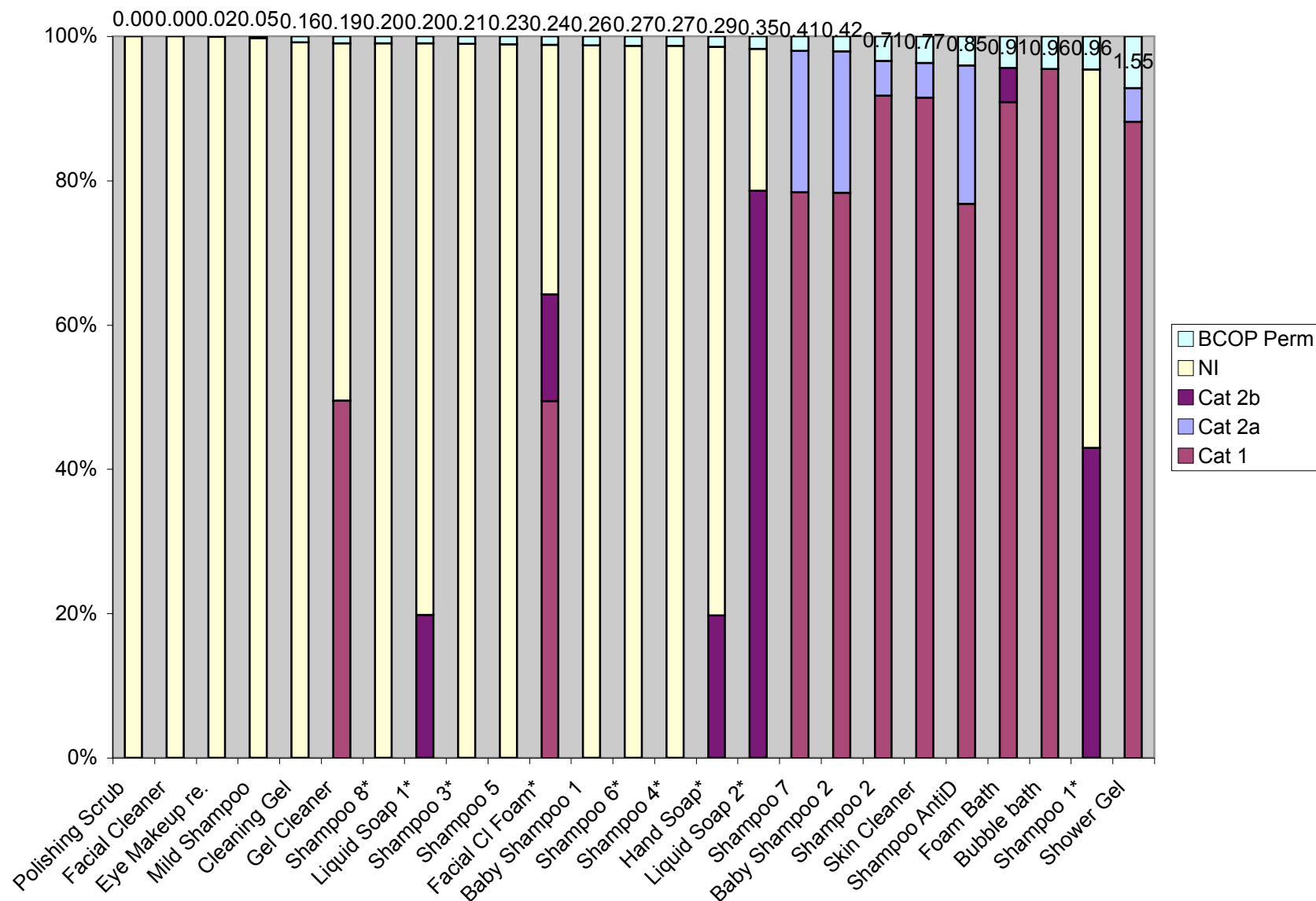
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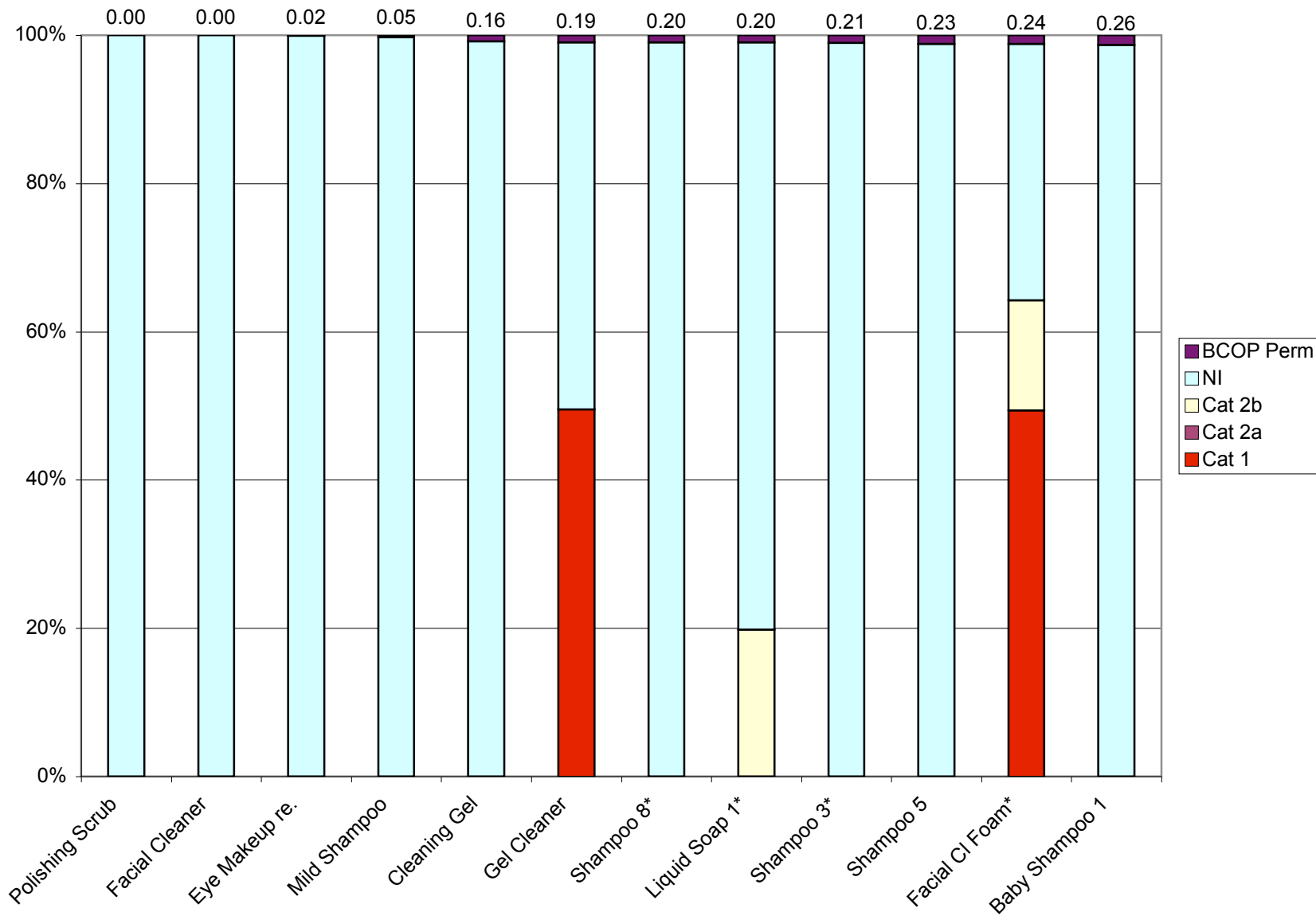
IIVS Submission - Analysis of In Vivo Data for Gettings et al. (1996)



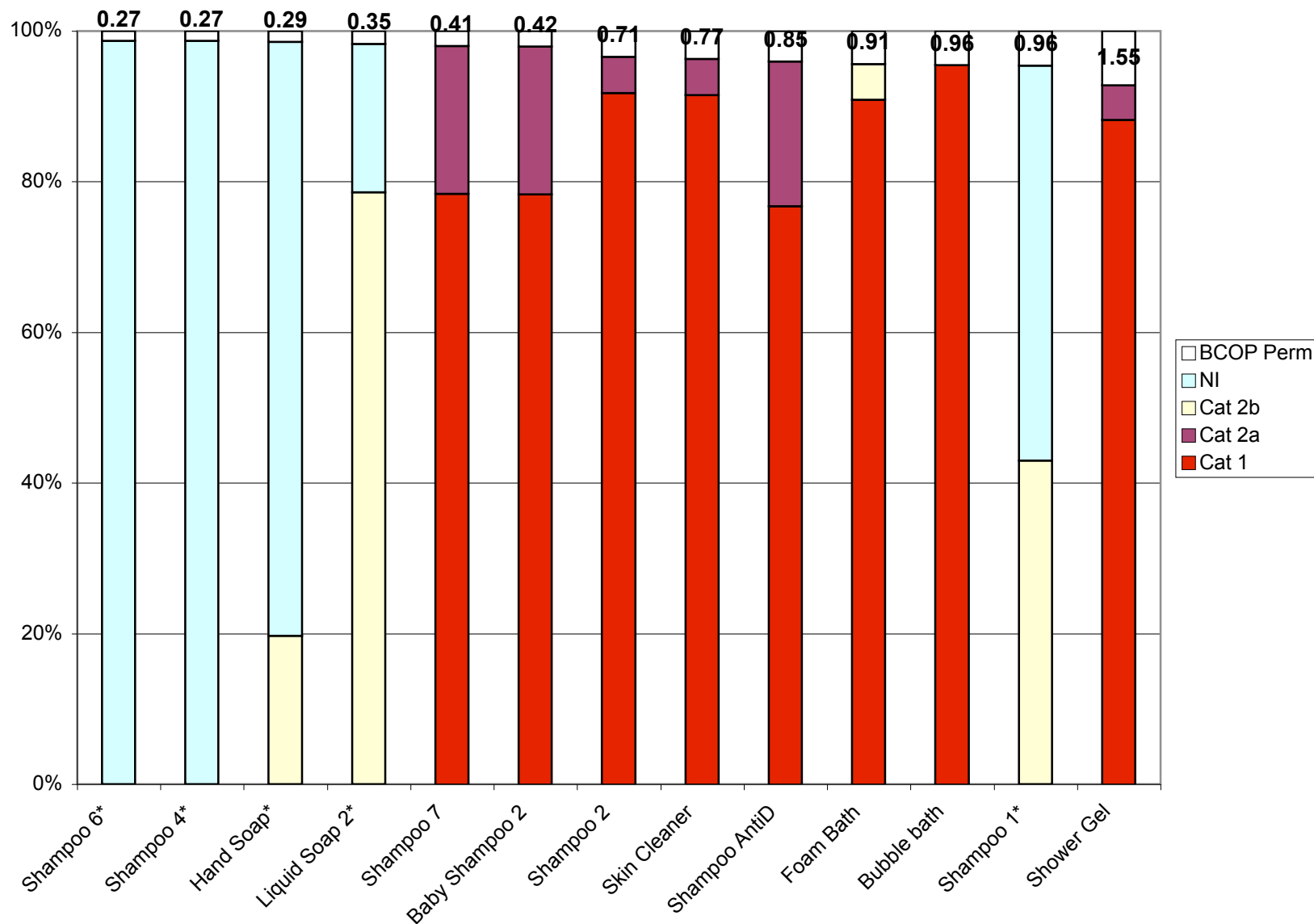
IIVS Submission - Comparison of BCOP Permeability Data with GHS Categories for In Vivo Data



IIVS Submission - Comparison of BCOP Permeability Data with GHS Categories for In Vivo Data



IIVS Submission - Comparison of BCOP Permeability Data with GHS Categories for In Vivo Data



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Appendix G6

Dataset Received from Johnson & Johnson Pharmaceutical Research and Development – A Division of Janssen Pharmaceutica N.V. (Laboratory No. 9 in Gautheron et al. 1994)

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Johnson & Johnson
PHARMACEUTICAL RESEARCH
& DEVELOPMENT

DIVISION OF JANSSEN PHARMACEUTICA N.V.



Pergamon

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INTERLABORATORY ASSESSMENT OF THE BOVINE CORNEAL OPACITY AND PERMEABILITY (BCOP) ASSAY*

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This document contains the individual cornea data collected in laboratory
no. 09 (Janssen Pharmaceutica) => 52 compounds were tested.

Compounds tested

Table 1. Test chemicals and suppliers

Chemical			Supplier:
Code no.	Name	CAS no.*	catalogue no.
1	2-Ethoxyethanol	110-80-5	Aldrich: 25,637-4
2	Anthracene	120-12-7	Aldrich: 14,106-2
3	Allyl alcohol	107-18-6	Aldrich: 24,053-2
4	EDTA, di-potassium salt	25102-12-9	Aldrich: 22,600-9
5	Hexane	110-54-3	Aldrich: 13,936-6
6	2,4-Pentanedione	123-54-6	Aldrich: P 775-4
7	Phenylbutazone	50-33-9	Aldrich: 21,186-9
8	1-Nitropropane	108-03-2	Aldrich: N2,285-1
9	3-Glycidoxypropyltrimethoxysilane	2530-83-8	Aldrich: 23,578-4
10	Aluminium hydroxide	21645-51-2	Aldrich: 23,918-6
11	1,2,4-Trimethylbenzene	95-63-6	Aldrich: 24,027-3
12	2-Mercaptopyrimidine	1450-85-7	Aldrich: 12,962-3
13	Betaine monohydrate	590-47-6	Aldrich: 21,913-4
14	Sodium oxalate	62-76-0	Aldrich: 22,343-3
15	D,L-Glutamic acid	19285-83-7	Aldrich: G 279-6
16	Petroleum ether	8032-32-4	Aldrich: 26,173-4
17	Butyrolactone	96-48-0	Aldrich: B10 360-84
18	2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	Aldrich: 14,739-7
19	Furan	110-00-9	Aldrich: 18,592-2
20	Imidazole	288-32-4	Aldrich: I 20-2
21	1-phenyl-3-pyrazolidone	92-43-3	Aldrich: 12,791-4
22	2-Aminophenol	95-55-6	Aldrich: A7 130-1
23	Gluconolactone	90-80-2	Aldrich: G200-1
24	2-Methoxyethanol	109-86-4	Aldrich: 27,048-2
25	Dimethyl sulfoxide	67-68-5	Aldrich: 27,043-1
26	Magnesium carbonate	56378-72-4	Aldrich: 22,766-8
27	Propyl-4-Hydroxybenzoate	94-13-3	Aldrich: P5 335-7
28	Iminodibenzyl	494-19-9	Aldrich: I 130-8
29	Octanol	111-87-5	Aldrich: 29,324-5
30	Methylisobutyl ketone	108-10-1	Aldrich: 29,326-1
31	Dibenzoyl-L-tartaric acid	2743-38-6	Aldrich: 34,584-9
32	Ethanol	64-17-5	local vendor
33	Methanol	67-56-1	local vendor
34	Ethyl acetoacetate	141-97-9	Aldrich: 24,070-2
35	Promethazine hydrochloride	58-33-3	Aldrich: 28,411-4
36	Deoxycholic acid, sodium salt	302-95-4	Sigma: D-6750
37	MYRJ-45		ICI: A-8563
38	BRIJ-35	9002-92-0	Sigma: P-1254
39	Tetraaminopyrimidine sulfate	5392-28-9	Aldrich: T 380-7
40	N-Lauroylsarcosine, sodium salt	7631-98-3	Sigma: L-5125
41	Quinacrine	69-05-6	Sigma: Q-3251
42	Hexadecyltrimethylammonium bromide	57-09-0	Sigma: H-5882
43	Thiourea	62-56-6	Aldrich: 24,025-7
44	Dimethylbiguanide	657-24-9	Sigma: D-5035
45	Benzethonium chloride	121-54-0	Sigma: B-8879
46	Triton X-155	9010-44-0	Sigma: X-155
47	1,2,3-Trichloropropane	96-18-4	Aldrich: 11,012-4
48	Cyclohexanone	108-94-1	Aldrich: C10 218-0
49	Diacetone alcohol	123-42-2	Aldrich: H4 154-4
50	Laurylsulfobetaine	14933-08-5	Sigma: D-4516
51	Pyridine	110-86-1	Aldrich: 27,040-7
52	Triethanolamine	102-71-6	Aldrich: T5 830-0

*Chemical Abstracts Service registry no.

EEC VALIDATION STUDY ON THE BOVINE CORNEA OPACITY-PERMEABILITY ASSAY

BLIND CODE	CHEMICAL	L	OPACITY			PERMEABILITY		IN VITRO SCORE	EXP. Nr.	Re- marks	
			Su	10 min	120 min	240 min	O.D.				µg/ml
1	2-ethoxyethanol	L	62.3 ± 2.3	61.7 ± 1.9		1.515 ± 0.134	19.3	84.4 ± 1.2	5	I	
2	anthracene	So			1.4 ± 1.2	0.003 ± 0.007	0.0	1.4 ± 1.3	42	C	
3	allyl alcohol	L	97.6 ± 18.9	94.1 ± 18.9		1.948 ± 0.455	24.7	123.3 ± 14.4	5	I	
4	ethylenediaminetetraacetate DiK	So			0.8 ± 0.5	0.010 ± 0.014	0.1	0.9 ± 0.6	42	C	
5	hexane	L	1.3 ± 0.8	1.3 ± 1.8		0.002 ± 0.002	0	1.4 ± 1.8	6	I	
6	2,4-pentadione	L	54.6 ± 4.7	49.1 ± 3.4		0.084 ± 0.036	1.1	50.3 ± 3.4	6	I	
7	phenylbutazone	So			0.7 ± 0.4	-0.008 ± 0.008	0	0.5 ± 0.4	42	C	
8	1-nitropropane	L	1.5 ± 1.1	16.5 ± 1.7		0.008 ± 0.018	0.1	16.6 ± 1.9	7	I	
9	3-glycidioxypropyltrimethoxysilane	L	16.1 ± 5.2	16.6 ± 4.5		0.065 ± 0.082	0.8	17.6 ± 4.7	7	I	
10	aluminium hydroxide	So			9.7 ± 2.3	0.012 ± 0.007	0.1	9.9 ± 2.3	43	C	
11	1,2,4-trimethylbenzene	L	4.6 ± 0.9	12.5 ± 1.5		0.579 ± 0.369	7.3	21.2 ± 4.5	8	I	
12	2-mercaptopyrimidine	So			-0.2 ± 0.4	-0.004 ± 0.002	0	-0.2 ± 0.4	43	C	
13	betaine monohydrate	So			3.1 ± 2.3	0.029 ± 0.014	0.1	3.5 ± 2.2	43	C	
14	sodium oxalate	So			1.7 ± 0.9	0.103 ± 0.042	0.6	3.2 ± 1.3	22	C	
15	DL-glutamic acid	So			-0.2 ± 0.5	-0.005 ± 0.005	0	-0.2 ± 0.5	22	C	
16	petroleum ether	L	0.7 ± 1.1	1.4 ± 1.9		0.015 ± 0.011	0.2	2.1 ± 1.9	8	I	
17	butyrolactone	L	32.3 ± 3.9	34.2 ± 3.1		0.495 ± 0.199	6.3	41.6 ± 5.0	9	I	
18	2,4-dichloro-5-sulfamoyl-benzoic acid	So			19.3 ± 4.8	-0.010 ± 0.004	0	19.2 ± 4.7	25	C	
19	furan	L	15.2 ± 2.1	20.6 ± 2.5		1.970 ± 0.197	24.9	50.2 ± 4.0	9	I	
20	imidazole	So			40.3 ± 9.9	1.598 ± 0.271	9.2	64.3 ± 11.2	25	C	

EEC VALIDATION STUDY ON THE BOVINE CORNEA OPACITY-PERMEABILITY ASSAY

BLIND CODE	CHEMICAL	L	OPACITY			PERMEABILITY		IN VITRO SCORE	EXP. Nr.	Re- marks
			10 min	120 min	240 min	O.D.	µg/ml			
21	1-phenyl-3-pyrazolidone	So			11.1 ± 1.0	0.143 ± 0.052	0.8	13.2 ± 1.6	40	C
22	2-aminophenol	So			10.9 ± 1.4	0.144 ± 0.188	0.8	13.0 ± 2.5	40	C
23	gluconolactone	So			85.2 ± 5.6	0.154 ± 0.041	0.8	87.5 ± 5.3	26	C
24	2-methoxyethanol	L	46.6 ± 8.4	45.1 ± 7.1		0.800 ± 0.137	10.1	57.1 ± 8.9	10	I
25	DMSO	L	8.7 ± 2.6	6.3 ± 1.7		0.204 ± 0.056	2.6	9.4 ± 1.4	10	I
26	magnesium carbonate	So			0.5 ± 0.5	0.016 ± 0.004	0.1	0.7 ± 0.5	26	C
27	propyl-4-hydroxybenzoate	So			5.2 ± 1.7	0.066 ± 0.059	0.4	6.2 ± 1.5	27	C
28	iminodibenzyl	So			0.2 ± 0.4	-0.001 ± 0.003	0	0.2 ± 0.4	27	C
29	octanol	L	22.4 ± 2.2	27.7 ± 5.0		2.212 ± 0.377	28.0	60.9 ± 6.9	11	I
30	methyl isobutyl ketone	L	10.6 ± 1.0	11.2 ± 2.7		0.546 ± 0.244	6.8	19.4 ± 3.1	11	I
31	dibenzoyl-L-tartaric acid	So			75.2 ± 14.2	0.416 ± 0.116	2.4	81.5 ± 13.7	27	C
32	ethanol	L	23.9 ± 4.0	22.3 ± 4.1		1.560 ± 0.316	19.8	45.7 ± 6.6	12	I
33	methanol	L	81.7 ± 5.6	73.7 ± 6.0		1.698 ± 0.560	9.8	99.2 ± 12.8	13b	C
34	ethyl acetoacetate	L	30.7 ± 2.8	24.0 ± 2.9		0.117 ± 0.007	0.6	25.7 ± 3.8	14	C
35	promethazine HCl	So			134.9 ± 9.7	0.287 ± 0.216	1.6	139.2 ± 10.2	38	C
36	deoxycholic acid sodium salt	Su	10.8 ± 1.5	13.9 ± 2.6		5.718 ± 0.511	32.6	99.6 ± 8.0	17	C
37	MYRJ 45	Su	-0.3 ± 0.4	0.4 ± 1.4		0.005 ± 0.004	0	0.5 ± 1.4	17	C
38	polyoxyethylene 23 lauryl ether	Su	0.7 ± 0.0	1.1 ± 0.6		-0.002 ± 0.008	0	1.0 ± 0.7	18	C
39	tetraaminopyrimidine sulfafate	So			2.6 ± 1.4	-0.003 ± 0.006	0	2.5 ± 1.4	38	C
40	N-lauroylsarcosine sodium salt	Su	3.4 ± 1.2	7.8 ± 0.9		3.653 ± 0.496	21.0	62.6 ± 7.3	18	C

EEC VALIDATION STUDY ON THE BOVINE CORNEA OPACITY-PERMEABILITY ASSAY

BLIND CODE	CHEMICAL	L	OPACITY			PERMEABILITY		IN VITRO SCORE	EXP. Nr.	Re- marks	
			Su	So	120 min	240 min	O.D.				µg/ml
41	quinacrine	So			57.0 ± 5.4	0.063 ± 0.040	0.4	57.9 ± 5.8	38	C	
42	hexadecyltrimethylammonium bromide	Su	11.3 ± 1.8	18.3 ± 3.6		3.438 ± 0.562	19.8	69.9 ± 6.9	18	C	
43	thiourea	So			85.8 ± 9.2	4.373 ± 1.028	25.0	151.4 ± 20.7	39	C	
44	dimethyl biguanide	So			0.7 ± 1.8	0.097 ± 0.176	0.6	2.1 ± 2.6	39	C	
45	benzethonium chloride	Su	53.1 ± 3.8	84.6 ± 3.3		5.420 ± 0.949	30.9	165.9 ± 14.5	19	C	
46	Triton X-155	Su	1.4 ± 1.3	3.0 ± 1.6		0.008 ± 0.014	0	3.1 ± 1.7	19	C	
47	1,2,3-trichloropropane	L	4.1 ± 1.3	7.7 ± 1.9		5.561 ± 1.398	31.7	91.1 ± 20.0	14	C	
48	cyclohexanone	L	57.9 ± 3.4	76.6 ± 3.9		4.341 ± 0.551	24.9	141.7 ± 8.2	16	C	
49	diacetone alcohol	L	24.1 ± 3.6	31.1 ± 3.2		4.119 ± 1.341	23.6	92.2 ± 22.0	17	C	
50	laurylsulfobetaine	Su	11.8 ± 2.6	16.2 ± 4.3		5.742 ± 1.462	32.7	102.4 ± 24.8	41	C	
51	pyridine	L	39.3 ± 4.1	44.4 ± 3.3		4.015 ± 0.849	23.0	104.7 ± 15.7	16	C	
52	triethanolamine	L	0.8 ± 0.7	2.6 ± 0.9		0.025 ± 0.011	1.4	3.0 ± 1.0	16	C	

L = Liquid (100%)

Su = Surfactant (10%)

So = Solid (20%)

I = Incomplete medium (MEM with only 1% FBS) ----> Exp. Nr. 5 to 13a

C = Complete medium

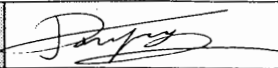
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 09 Mar 92
Experiment no. 5
Compound of the same pair no. 3

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				correc.	Permeability (OD)		In-vitro score
		C1	9	9	9.0	C1	13	13	13.0		0.003	correc.	
1	MEM	C1	9	9	9.0	C1	13	13	13.0		0.003		13.0
2		-9	C2	0	-4.5	-14	C2	0	-7.0		0.002		-7.0
3		-9	0	C3	-4.5	-14	0	C3	-7.0		0.004		-6.9
mean											0.003		-0.3
± S.D.											0.001		11.5

4	compound no.	56	65	66	62.3	51	66	66	61.0	61.3	1.447	1.444	83.0
5	1	59	68	68	65.0	54	69	68	63.7	64.0	1.502	1.498	86.5
6	concentration	54	64	64	60.7	50	64	65	59.7	60.0	1.669	1.666	85.0
7		58	68	68	64.7	54	68	69	63.7	64.0	1.307	1.304	83.6
8		100%	56	65	65	62.0	51	66	66	61.0	61.3	1.537	1.534
9		53	62	62	59.0	50	64	64	59.3	59.7	1.649	1.646	84.3
mean					62.3				61.4	61.7	1.518	1.515	84.4
± S.D.					2.3				1.9	1.9	0.134	0.134	1.2

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

4	compound no.	
5	1	
6	concentration	
7		
8		100%
9		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	71
2	B	152
	A	
3	B	223
	A	

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet


Lab. no. 09

Date: 25 Jun 92

Name: Ph. Vanparys

Experiment no. 42

Compound of the same pair no. 4 + 7

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1				
0	0	0	0.0	
-1	C2	0	-0.5	
-1	0	C3	-0.5	
				-0.3
				0.3

Permeability (OD)		in-vitro score
correc.		
0.016		0.2
0.023		-0.2
0.018		-0.2
0.019		-0.1
0.004		0.3

4	compound no.
5	2
6	concentration
7	
8	
9	
mean	
± S.D.	

2	3	3	2.7	3.0
0	0	0	0.0	0.3
1	1	2	1.3	1.7
0	0	0	0.0	0.3
2	2	3	2.3	2.7
0	0	0	0.0	0.3
			1.1	1.4
			1.2	1.2

0.020	0.001	3.0
0.010	-0.009	0.2
0.024	0.005	1.7
0.023	0.004	0.4
0.026	0.007	2.8
0.029	0.010	0.5
0.022	0.003	1.4
0.007	0.007	1.3

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-170
3	B	248
	A	-259

4	compound no.
5	2
6	concentration
7	
8	
9	
mean	
± S.D.	

pH: 8.12

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

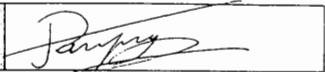
Lab. no. 09

Date: 09 Mar 92

Name: Ph. Vanparys

Experiment no. 5

Compound of the same pair no. 1

Signature: 

cor-nea	treatment	opacity at 10 min.				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	C2	C3	mean	C1	C2	C3	mean	correc.	correc.	
1	MEM	C1	9	9	9.0	C1	13	13	13.0		0.003	13.0
2		-9	C2	0	-4.5	-14	C2	0	-7.0		0.002	-7.0
3		-9	0	C3	-4.5	-14	0	C3	-7.0		0.004	-6.9
mean					0.0				-0.3		0.003	-0.3
± S.D.					7.8				11.5		0.001	11.5

cor-nea	treatment	opacity at 10 min.				opacity at 120 min				Permeability (OD)		in-vitro score		
10	compound no.	115	123	123	120.3	106	122	121	116.3	116.7	1.555		1.552	139.9
11	3	109	118	119	115.3	102	117	117	112.0	112.3	1.957	1.953	141.6	
12	concentration	88	97	97	94.0	80	95	95	90.0	90.3	1.859	1.856	118.2	
13		96	105	105	102.0	88	102	102	97.3	97.7	1.581	1.578	121.3	
14		100%	77	86	86	83.0	69	85	85	79.7	80.0	1.948	1.945	109.2
15			65	74	74	71.0	57	72	72	67.0	67.3	2.807	2.804	109.4
mean						97.6				93.7	94.1	1.951	1.948	123.3
± S.D.					18.9				18.9	18.9	0.455	0.455	14.4	

cor-nea	treatment	opacity at 10 min.				opacity at 120 min				Permeability (OD)		in-vitro score
1	MEM	C1	9	9	9.0	C1	13	13	13.0		0.003	
2		-9	C2	0	-4.5	-14	C2	0	-7.0		0.002	-7.0
3		-9	0	C3	-4.5	-14	0	C3	-7.0		0.004	-6.9
mean					0.0				-0.3		0.003	-0.3
± S.D.					7.8				11.5		0.001	11.5

cor-nea	treatment	opacity at 10 min.				opacity at 120 min				Permeability (OD)		in-vitro score		
10	compound no.	115	123	123	120.3	106	122	121	116.3	116.7	1.555		1.552	139.9
11	3	109	118	119	115.3	102	117	117	112.0	112.3	1.957	1.953	141.6	
12	concentration	88	97	97	94.0	80	95	95	90.0	90.3	1.859	1.856	118.2	
13		96	105	105	102.0	88	102	102	97.3	97.7	1.581	1.578	121.3	
14		100%	77	86	86	83.0	69	85	85	79.7	80.0	1.948	1.945	109.2
15			65	74	74	71.0	57	72	72	67.0	67.3	2.807	2.804	109.4
mean						97.6				93.7	94.1	1.951	1.948	123.3
± S.D.					18.9				18.9	18.9	0.455	0.455	14.4	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-7.1
2	B	152
	A	
3	B	223
	A	

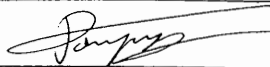
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 25 Jun 92
 Experiment no. 42
 Compound of the same pair no. 2 + 7

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
-1	C2	0	-0.5	
-1	0	C3	-0.5	
				-0.3
				0.3

Permeability (OD)	correc.	in-vitro score
0.016		0.2
0.023		-0.2
0.018		-0.2
0.019		-0.1
0.004		0.3

10	compound no.
11	4
12	
13	concentration
14	20%
15	
mean	
± S.D.	

0	0	0	0.0	0.3
0	1	1	0.7	1.0
0	0	0	0.0	0.3
0	0	0	0.0	0.3
0	1	1	0.7	1.0
1	1	2	1.3	1.7
			0.4	0.8
			0.5	0.5

0.043	0.024	0.7
0.039	0.020	1.3
0.014	-0.004	0.3
0.015	-0.004	0.3
0.043	0.024	1.4
0.019	0.000	1.7
0.029	0.010	0.9
0.014	0.014	0.6

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	4
12	
13	concentration
14	20%
15	
mean	
± S.D.	

pH: 5.2

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	-75
2	B	158
	A	-170
3	B	248
	A	-259

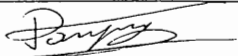
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 19 Mar 92
Experiment no. 6
Compound of the same pair no. 6

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	4	4	4.0	C1	4	4	4.0		
1	MEM	-2	C2	0	-1.0	-2	C2	0	-1.0	0.003	4.0
2		-2	0	C3	-1.0	-2	0	C3	-1.0	0.003	-1.0
3		mean								0.001	-1.0
					0.7				0.7	0.002	0.7
					± S.D.				2.9	0.001	2.9

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score	
		C1	4	4	4.0	C1	4	4	4.0			
4	compound no.	0	2	2	1.3	0	2	2	1.3	0.004	0.002	0.7
5	5	0	2	2	1.3	3	6	6	5.0	0.004	0.002	4.4
6	concentration	1	3	3	2.3	1	4	4	3.0	0.002	0.000	2.3
7		-1	1	1	0.3	-1	1	1	0.3	0.009	0.007	-0.2
8		100%	-1	1	1	0.3	-1	1	1	0.3	0.005	0.003
9		0	3	3	2.0	0	3	3	2.0	0.004	0.002	1.4
					mean				1.3	0.005	0.002	1.4
					± S.D.				0.8	0.002	0.002	1.8

cor-nea	treatment
1	MEM
2	
3	
	mean
	± S.D.

cor-nea	treatment
4	compound no.
5	5
6	concentration
7	
8	
9	
	mean
	± S.D.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-68
2	B	158
	A	-152
3	B	254
	A	-235

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 19 Mar 92

Name: Ph. Vanparys

Experiment no. 6

Compound of the same pair no. 5

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				correc.	Permeability (OD)		in-vitro score
		C1	4	4	4.0	C1	4	4	4.0		correc.		
1	MEM	C1	4	4	4.0	C1	4	4	4.0		0.003		4.0
2		-2	C2	0	-1.0	-2	C2	0	-1.0		0.003		-1.0
3		-2	0	C3	-1.0	-2	0	C3	-1.0		0.001		-1.0
mean											0.002		0.7
± S.D.											0.001		2.9

10	compound no.	47	50	49	48.7	43	46	46	45.0	44.3	0.077	0.075	45.5
11	6	51	54	54	53.0	46	49	49	48.0	47.3	0.048	0.046	48.0
12	concentration	52	55	55	54.0	50	52	52	51.3	50.7	0.135	0.133	52.7
13		50	53	53	52.0	47	50	50	49.0	48.3	0.125	0.123	50.2
14		100%	60	63	63	62.0	53	56	56	55.0	54.3	0.057	0.055
15		56	59	58	57.7	48	51	51	50.0	49.3	0.076	0.074	50.4
mean					54.6				49.7	49.1	0.086	0.084	50.3
± S.D.					4.7				3.4	3.4	0.036	0.036	3.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.	
11	6	
12	concentration	
13		
14		100%
15		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	68
2	B	158
	A	152
3	B	254
	A	235

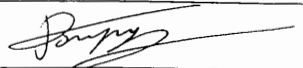
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 25 Jun 92
 Experiment no. 42
 Compound of the same pair no. 2 + 4

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
•-1	C2	0	-0.5	
-1	0	C3	-0.5	
				-0.3
				0.3

Permeability (OD)		in-vitro score
correc.		
0.016		0.2
0.023		-0.2
0.018		-0.2
0.019		-0.1
0.004		0.3

16	compound no.
17	7
18	
19	concentration
20	20%
21	
mean	
± S.D.	

0	0	0	0.0	0.3
0	0	0	0.0	0.3
0	0	0	0.0	0.3
0	1	1	0.7	1.0
0	0	1	0.3	0.7
1	1	1	1.0	1.3
				0.3
				0.7
				0.4
				0.4

0.014	-0.005	0.3
0.006	-0.012	0.1
0.003	-0.015	0.1
0.011	-0.007	0.9
0.024	0.005	0.7
0.006	-0.013	1.1
0.011	-0.008	0.5
0.008	0.008	0.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

16	compound no.
17	7
18	
19	concentration
20	20%
21	
mean	
± S.D.	

pH: not enough compound for a determination.
 Compound no. 7 was washed away 4 times instead of 3 times.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-170
3	B	248
	A	-259

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 20 Mar 92

Name: Ph. Vanparys

Experiment no. 7

Compound of the same pair no. 9

Signature:

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1				C1					
1	MEM	C1	0	-4	-2.0	C1	-2	-4	-3.0	0.004	-2.9
2		0	C2	-4	-2.0	1	C2	-2	-0.5	0.002	-0.5
3		3	3	C3	3.0	3	1	C3	2.0	0.003	2.0
mean										0.003	-0.5
± S.D.										0.001	2.5

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.		in-vitro score	
4	compound no.	3	4	0	2.3	20	18	16	18.0	18.5	0.001	-0.002	18.5
5	8	3	3	0	2.0	16	14	12	14.0	14.5	0.005	0.002	14.5
6	concentration	3	4	0	2.3	18	16	15	16.3	16.8	0.002	-0.001	16.8
7		0	1	-2	-0.3	20	18	16	18.0	18.5	0.048	0.045	19.2
8		100%	3	3	0	2.0	17	15	13	15.0	15.5	0.007	0.004
9		1	2	-1	0.7	17	14	13	14.7	15.2	0.003	0.000	15.2
mean					1.5				16.0	16.5	0.011	0.008	16.6
± S.D.					1.1				1.7	1.7	0.018	0.018	1.9

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

→ 3 very small air-bubbles

⋮

cor-nea	treatment
4	compound no.
5	8
6	concentration
7	
8	
9	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-152
3	B	254
	A	-235

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 20 Mar 92

Name: Ph. Vanparys

Experiment no. 7

Compound of the same pair no. 8

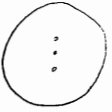
Signature:

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	In-vitro score
		C1				C1					
1	MEM	C1	0	-4	-2.0	C1	-2	-4	-3.0	0.004	-2.9
2		0	C2	-4	-2.0	• 1	C2	-2	-0.5	0.002	-0.5
3		3	3	C3	3.0	3	1	C3	2.0	0.003	2.0
mean					-0.3				-0.5	0.003	-0.5
± S.D.				2.9				2.5	0.001	2.5	

	compound no.	21	21	18	20.0	21	19	17	19.0	19.5	0.216	0.213	22.7	
10	9	20	20	17	19.0	23	20	19	20.7	21.2	0.018	0.015	21.4	
11		21	22	18	20.3	22	20	18	20.0	20.5	0.008	0.005	20.6	
12		16	16	12	14.7	14	12	10	12.0	12.5	0.114	0.111	14.2	
13	concentration	8	8	4	6.7	12	10	8	10.0	10.5	0.026	0.023	10.8	
14		100%	17	17	13	15.7	17	15	13	15.0	15.5	0.028	0.025	15.9
15		mean				16.1				16.1	16.6	0.068	0.065	17.6
	± S.D.				5.2				4.5	4.5	0.082	0.082	4.7	


cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

→ 3 very small air-bubbles



	compound no.
10	9
11	
12	
13	concentration
14	100%
15	
mean	
± S.D.	

→ small area which is not opaque



CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	158
	A	152
3	B	254
	A	235

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

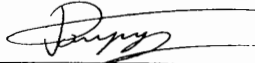
Lab. no. **09**

Date: 26 Jun 92

Name: Ph. Vanparys

Experiment no. 43

Compound of the same pair no. 12 + 13

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
• 0	C2	0	0.0	
0	0	C3	0.0	
			0.0	
			0.0	

Permeability (OD)	correc.	in-vitro score
0.012		0.2
0.010		0.2
0.022		0.3
0.015		0.2
0.006		0.1

4	compound no.
5	10
6	
7	concentration
8	20%
9	
mean	
± S.D.	

9	9	8	8.7	8.7
10	10	9	9.7	9.7
10	10	10	10.0	10.0
13	13	13	13.0	13.0
6	6	6	6.0	6.0
11	11	11	11.0	11.0
			9.7	9.7
			2.3	2.3

0.027	0.012	8.9
0.019	0.004	9.7
0.030	0.015	10.2
0.026	0.011	13.2
0.037	0.022	6.3
0.020	0.006	11.1
0.026	0.012	9.9
0.007	0.007	2.3

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

pH: not enough compound for a pH determination.

4	compound no.
5	10
6	
7	concentration
8	20%
9	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-262


EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 23 Mar 92
Experiment no. 8
Compound of the same pair no. 16

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1				C1				correc.	correc.	
1	MEM	C1	-1	0	-0.5	C1	-3	-2	-2.5			-2.5
2		0	C2	0	0.0	2	C2	0	1.0			0.9
3		0	-1	C3	-0.5	1	-1	C3	0.0			0.0
mean												-0.6
± S.D.												1.8

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score	
		C1				C1				correc.	correc.		
4	compound no.	6	6	6	6.0	14	10	11	11.7	12.2	0.337	0.340	17.3
5	11	5	4	5	4.7	15	12	13	13.3	13.8	0.529	0.532	21.8
6	concentration	4	3	4	3.7	14	11	11	12.0	12.5	0.380	0.383	18.3
7		5	4	5	4.7	14	11	12	12.3	12.8	0.783	0.786	24.6
8		100%	4	3	4	3.7	11	8	9	9.3	9.8	1.213	1.216
9		5	4	5	4.7	15	12	13	13.3	13.8	0.209	0.212	17.0
mean					4.6				12.0	12.5	0.575	0.579	21.2
± S.D.					0.9				1.5	1.5	0.369	0.369	4.5

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	
4	compound no.	
5	11	
6	concentration	
7		100%
8		
9		
mean		
± S.D.		

rinsed 4 times instead off 3 times

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	75
2	B	158
	A	168
3	B	253
	A	260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 26 Jun 92

Name: Ph. Vanparys

Experiment no. 43

Compound of the same pair no. 10 + 13

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min					Permeability (OD)		in-vitro
					correc.		score
C1	0	0	0.0		0.012		0.2
• 0	C2	0	0.0		0.010		0.2
0	0	C3	0.0		0.022		0.3
			0.0		0.015		0.2
			0.0	0.007	0.1		

10	compound no.	
11	12	
12	concentration	
13		
14		20%
15		
mean		
± S.D.		

0	0	0	0.0	0.0	0.010	-0.005	-0.1
0	0	0	0.0	0.0	0.011	-0.004	-0.1
0	0	0	0.0	0.0	0.008	-0.006	-0.1
0	0	0	0.0	0.0	0.016	0.001	0.0
0	0	0	0.0	0.0	0.010	-0.005	-0.1
-1	-1	-1	-1.0	-1.0	0.011	-0.004	-1.1
			-0.2	-0.2	0.011	-0.004	-0.2
			0.4	0.4	0.002	0.002	0.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-262

10	compound no.	
11	12	
12	concentration	
13		
14		20%
15		
mean		
± S.D.		

pH: 6.84

Compound No.12 was washed away 4 times instead of 3 times.

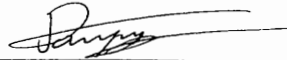
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 26 Jun 92
 Experiment no. 43
 Compound of the same pair no. 10 + 12

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
			0.0	
			0.0	

Permeability (OD)		in-vitro score
correc.		
0.012		0.2
0.010		0.2
0.022		0.3
0.015		0.2
0.006		0.1

16	compound no.	
17	13	
18	concentration	
19		20%
20		
21		
mean		
± S.D.		

7	7	6	6.7	6.7
1	1	1	1.0	1.0
1	1	1	1.0	1.0
5	5	5	5.0	5.0
2	2	1	1.7	1.7
3	3	3	3.0	3.0
			3.1	3.1
			2.3	2.3

0.030	0.015	6.9
0.041	0.026	1.4
0.041	0.027	1.4
0.034	0.020	5.3
0.070	0.055	2.5
0.043	0.029	3.4
0.043	0.029	3.5
0.014	0.014	2.2

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

16	compound no.	
17	13	
18	concentration	
19		20%
20		
21		
mean		
± S.D.		

pH: 8.24

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	170
3	B	250
	A	262

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet


Lab. no. 09

Date: 27 Apr 92

Name: Ph. Vanparys

Experiment no. 22

Compound of the same pair no. 15

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min					correc.
C1	0	2	1.0		
0	C2	1	0.5		
-3	-2	C3	-2.5		
			-0.3		
			1.9		

Permeability (OD)		In-vitro score
correc.		
0.016		1.2
0.014		0.7
0.015		-2.3
0.015		-0.1
0.001		1.9

4	compound no.
5	14
6	
7	concentration
8	20%
9	
mean	
± S.D.	

-1	0	1	0.0	0.3
0	0	2	0.7	1.0
1	1	4	2.0	2.3
0	1	3	1.3	1.7
1	1	3	1.7	2.0
1	2	4	2.3	2.7
			1.3	1.7
			0.9	0.9

0.106	0.092	1.7
0.042	0.028	1.4
0.122	0.108	3.9
0.143	0.128	3.6
0.164	0.150	4.2
0.129	0.115	4.4
0.118	0.103	3.2
0.042	0.042	1.3

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

4	compound no.
5	14
6	
7	concentration
8	20%
9	
mean	
± S.D.	

Compound 14 was warmed up to 32°C and stirred on a magnetic stirrer.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-168
3	B	248
	A	-257

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

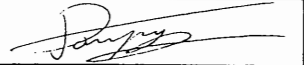
Lab. no. 09

Date: 27 Apr 92

Name: Ph. Vanparys

Experiment no. 22

Compound of the same pair no. 14

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	2	1.0	
0	C2	1	0.5	
-3	-2	C3	-2.5	
			-0.3	
			1.9	

Permeability (OD)	correc.	In-vitro score
0.016		1.2
0.014		0.7
0.015		-2.3
0.015		-0.1
0.001		1.9

10	compound no.
11	15
12	
13	concentration
14	20%
15	
mean	
± S.D.	

-1	0	1	0.0	0.3
-2	-1	0	-1.0	-0.7
-1	0	1	0.0	0.3
-2	-1	0	-1.0	-0.7
-1	0	1	0.0	0.3
-2	-1	0	-1.0	-0.7
			-0.5	-0.2
			0.5	0.5

0.011	-0.004	0.3
0.018	0.003	-0.6
0.003	-0.012	0.2
0.010	-0.005	-0.7
0.008	-0.006	0.2
0.006	-0.008	-0.8
0.009	-0.005	-0.2
0.005	0.005	0.5

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	15
12	
13	concentration
14	20%
15	
mean	
± S.D.	

Compound 15 was warmed up to 32°C and stirred on a magnetic stirrer.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-168
3	B	248
	A	-257

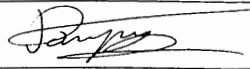
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Name: Ph. Vanparys

Date: 23 Mar 92
Experiment no. 8
Compound of the same pair no. 11

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	In-vitro score
		C1	-1	0	-0.5	C1	-3	-2	-2.5		
1	MEM	0	C2	0	0.0	2	C2	0	1.0	-0.003	-2.5
2		0	-1	C3	-0.5	1	-1	C3	0.0	-0.005	0.9
3		0	-1	C3	-0.5					-0.002	0.0
mean					-0.3				-0.5	-0.003	-0.6
± S.D.					0.3				1.8	0.002	1.8

10	compound no.	1	0	0	0.3	5	1	2	2.7	3.2	0.003	0.006	3.3
11	16	0	0	0	0.0	1	-1	0	0.0	0.5	0.017	0.020	0.8
12	concentration	3	2	3	2.7	5	2	3	3.3	3.8	0.032	0.035	4.4
13		0	0	0	0.0	4	0	1	1.7	2.2	0.005	0.008	2.3
14		100%	2	1	1	1.3	4	1	2	2.3	2.8	0.003	0.006
15		0	-1	0	-0.3	0	-3	-2	-1.7	-1.2	0.009	0.012	-1.0
mean					0.7				1.4	1.9	0.012	0.015	2.1
± S.D.					1.1				1.9	1.9	0.011	0.011	1.9

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.	
11	16	
12	concentration	
13		
14		100%
15		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	-75
2	B	158
	A	-168
3	B	253
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

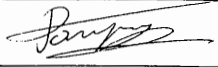
Lab. no. 09

Date: 26 Mar 92

Name: Ph. Vanparys

Experiment no. 9

Compound of the same pair no. 19

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1				C1				correc.		
1	MEM	C1	0	0	0.0	C1	-1	0	-0.5		0.000	-0.5
2		0	C2	1	0.5	1	C2	2	1.5		0.005	1.6
3		0	-1	C3	-0.5	0	-2	C3	-1.0		0.038	-0.4
mean					0.0				0.0		0.014	0.2
± S.D.					0.5				1.3		0.021	1.2

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score	
		C1				C1				correc.			
4	compound no.	31	31	32	31.3	35	34	36	35.0	35.0	0.394	0.380	40.7
5	17	32	31	32	31.7	34	32	34	33.3	33.3	0.520	0.506	40.9
6	concentration	27	26	28	27.0	31	30	32	31.0	31.0	0.305	0.291	35.4
7		32	31	32	31.7	32	30	33	31.7	31.7	0.761	0.747	42.9
8		100%	39	38	40	39.0	40	38	41	39.7	39.7	0.735	0.721
9		33	32	34	33.0	35	33	36	34.7	34.7	0.340	0.326	39.6
mean					32.3				34.2	34.2	0.509	0.495	41.6
± S.D.					3.9				3.1	3.1	0.199	0.199	5.0

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	
4	compound no.	
5	17	
6	concentration	
7		
8		100%
9		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-166
3	B	244
	A	-254

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

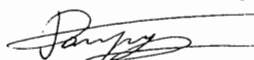
Lab. no. 09

Date: 07 May 92

Name: Ph. Vanparys

Experiment no. 25

Compound of the same pair no. 20 + 21

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
			0.0	
			0.0	

Permeability (OD)		in-vitro score
correc.		
0.021		0.3
0.012		0.2
0.010		0.1
0.014		0.2
0.006		0.1

4	compound no.
5	18
6	
7	concentration
8	20%
9	
mean	
± S.D.	

24	24	24	24.0	24.0
21	21	21	21.0	21.0
15	16	15	15.3	15.3
12	12	11	11.7	11.7
22	22	22	22.0	22.0
22	22	22	22.0	22.0
			19.3	19.3
			4.8	4.8

0.004	-0.011	23.8
0.000	-0.014	20.8
0.003	-0.011	15.2
0.011	-0.003	11.6
0.002	-0.012	21.8
0.006	-0.008	21.9
0.004	-0.010	19.2
0.004	0.004	4.7

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	170
3	B	250
	A	260

4	compound no.
5	18
6	
7	concentration
8	20%
9	
mean	
± S.D.	

Compound 18 was warmed up to 32 °C and stirred on a magnetic stirrer.


EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 26 Mar 92
Experiment no. 9
Compound of the same pair no. 17

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1								correc.		
1	MEM	C1	0	0	0.0	C1	-1	0	-0.5		0.000	-0.5
2		0	C2	1	0.5	1	C2	2	1.5		0.005	1.6
3		0	-1	C3	-0.5	0	-2	C3	-1.0		0.038	-0.4
mean					0.0				0.0		0.014	0.2
± S.D.					0.5				1.3		0.021	1.2

10	compound no.	18	17	19	18.0	24	23	25	24.0	24.0	1.900	1.886	52.3
11	19	17	16	18	17.0	23	21	24	22.7	22.7	2.288	2.274	56.8
12		15	14	15	14.7	20	18	21	19.7	19.7	1.829	1.815	46.9
13	concentration	13	13	14	13.3	20	18	20	19.3	19.3	1.785	1.771	45.9
14	100%	16	15	16	15.7	21	20	22	21.0	21.0	1.944	1.930	49.9
15		13	12	13	12.7	17	16	18	17.0	17.0	2.157	2.143	49.1
mean					15.2				20.6	20.6	1.984	1.970	50.2
± S.D.					2.1				2.5	2.5	0.197	0.197	4.0

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	19
12	
13	concentration
14	100%
15	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-166
3	B	244
	A	-254

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

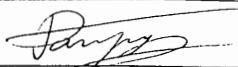
Lab. no. 09

Date: 07 May 92

Name: Ph. Vanparys

Experiment no. 25

Compound of the same pair no. 18 + 21

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
			0.0	
			0.0	

Permeability (OD)	correc.	In-vitro score
0.021		0.3
0.012		0.2
0.010		0.1
0.014		0.2
0.006		0.1

10	compound no.
11	20
12	
13	concentration
14	20%
15	
mean	
± S.D.	

43	41	41	41.7	41.7
33	33	32	32.7	32.7
28	28	27	27.7	27.7
52	53	51	52.0	52.0
37	37	36	36.7	36.7
51	52	51	51.3	51.3
			40.3	40.3
			9.9	9.9

2.110	2.096	73.1
1.430	1.416	53.9
1.427	1.412	48.9
1.400	1.386	72.8
1.694	1.680	61.9
1.612	1.597	75.3
1.612	1.598	64.3
0.271	0.271	11.2

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	20
12	
13	concentration
14	20%
15	
mean	
± S.D.	

Compound 20 was warmed up to 32 °C en stirred on a magnetic stirrer.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-260


EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 18 Jun 92
 Experiment no. 40
 Compound of the same pair no. 14 + 22

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
-1	C2	0	-0.5	
0	0	C3	0.0	
				-0.2
				0.3

Permeability (OD)		in-vitro score
correc.		
0.025		0.4
0.019		-0.2
0.018		0.3
0.020		0.1
0.004		0.3

10	compound no.
11	21
12	
13	concentration
14	20%
15	
mean	
± S.D.	

10	12	12	11.3	11.5
10	12	12	11.3	11.5
9	10	10	9.7	9.8
10	12	11	11.0	11.2
9	10	10	9.7	9.8
12	13	12	12.3	12.5
			10.9	11.1
			1.0	1.0

0.176	0.156	13.8
0.113	0.093	12.9
0.131	0.110	11.5
0.134	0.114	12.9
0.165	0.145	12.0
0.258	0.237	16.1
0.163	0.143	13.2
0.052	0.052	1.6

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	21
12	
13	concentration
14	20%
15	
mean	
± S.D.	

pH: 7.41
 Compound No. 21 was washed away 4 times instead of 3 times.

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	-75
2	B	158
	A	-170
3	B	249
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

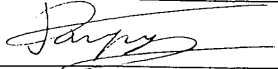
Lab. no. 09

Date: 18 Jun 92

Name: Ph. Vanparys

Experiment no. 40

Compound of the same pair no. 14 + 21

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
-1	C2	0	-0.5	
0	0	C3	0.0	
				-0.2
				0.3

Permeability (OD)		in-vitro score
correc.		
0.025		0.4
0.019		-0.2
0.018		0.3
0.020		0.1
0.004		0.3

16	compound no.
17	22
18	
19	concentration
20	20%
21	
mean	
± S.D.	

8	10	9	9.0	9.2
10	11	11	10.7	10.8
12	12	12	12.0	12.2
10	11	11	10.7	10.8
12	13	13	12.7	12.8
9	9	10	9.3	9.5
			10.7	10.9
			1.4	1.4

0.113	0.093	10.6
0.076	0.056	11.7
0.086	0.065	13.1
0.059	0.039	11.4
0.104	0.083	14.1
0.546	0.526	17.4
0.164	0.144	13.0
0.188	0.188	2.5

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	-75
2	B	158
	A	-170
3	B	249
	A	-260

16	compound no.
17	22
18	
19	concentration
20	20%
21	
mean	
± S.D.	

pH: 7.88


EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 08 May 92
Experiment no. 26
Compound of the same pair no. 22 + 26

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min					Permeability (OD)		in-vitro score
					correc.		
C1	0	0	0.0		0.017		0.3
0	C2	0	0.0		0.031		0.5
0	0	C3	0.0		0.012		0.2
				0.0	0.020		0.3
				0.0	0.010		0.1

10	compound no.
11	23
12	
13	concentration
14	20%
15	
mean	
± S.D.	

87	89	90	88.7	88.7	0.192	0.171	91.2
85	87	88	86.7	86.7	0.201	0.181	89.4
76	78	80	78.0	78.0	0.163	0.143	80.1
77	79	80	78.7	78.7	0.230	0.210	81.8
85	87	92	88.0	88.0	0.120	0.100	89.5
89	91	94	91.3	91.3	0.138	0.118	93.1
			85.2	85.2	0.174	0.154	87.5
			5.6	5.6	0.041	0.041	5.3

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

Fluorescein leakage into the waterbath

O.D. versus C1
 measured 8 min. after
 first measurement.

10	compound no.
11	23
12	
13	concentration
14	20%
15	
mean	
± S.D.	

Compound No. 23 was warmed up to 32°C
 and stirred on a magnetic stirrer.

106
 101
 92
 91
 107
 104

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	171
3	B	251
	A	260

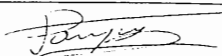
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 27 Mar 92
Experiment no. 10
Compound of the same pair no. 25

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	1	2	1.5	C1	1	1	1.0	correc.		
1	MEM	C1	1	2	1.5	C1	1	1	1.0	0.005		1.1
2		-1	C2	1	0.0	-2	C2	0	-1.0	0.001		-1.0
3		-2	0	C3	-1.0	-2	0	C3	-1.0	0.004		-0.9
mean					0.2				-0.3	0.003		-0.3
± S.D.				1.3				1.2	0.002		1.2	

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score		
		C1	1	2	1.5	C1	1	1	1.0	correc.				
4	compound no.	49	51	52	50.7	47	49	49	48.3	48.7	0.882	0.879	61.8	
5	24	40	42	43	41.7	38	40	40	39.3	39.7	0.688	0.685	49.9	
6	concentration	52	53	55	53.3	51	53	53	52.3	52.7	0.754	0.751	63.9	
7		36	38	39	37.7	36	38	38	37.3	37.7	0.735	0.732	48.6	
8		100%	56	58	59	57.7	51	53	53	52.3	52.7	1.047	1.044	68.3
9		37	39	40	38.7	37	40	39	38.7	39.0	0.716	0.713	49.7	
mean				46.6				44.7	45.1	0.804	0.800	57.1		
± S.D.				8.4				7.1	7.1	0.137	0.137	8.6		

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	
4	compound no.	
5	24	
6	concentration	
7		
8		100%
9		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-166
3	B	249
	A	-255

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 27 Mar 92
Experiment no. 10
Compound of the same pair no. 24

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	1	2	1.5	C1	1	1	1.0	correc.		
1	MEM	C1	1	2	1.5	C1	1	1	1.0	0.005		1.1
2		-1	C2	1	0.0	-2	C2	0	-1.0	0.001		-1.0
3		-2	0	C3	-1.0	-2	0	C3	-1.0	0.004		-0.9
mean					0.2				-0.3	0.003		-0.3
± S.D.					1.3				1.2	0.002		1.2

10	compound no.	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score	
		10	11	12	11.0	5	7	7	6.3	6.7	0.221		0.218
11	25	5	7	7	6.3	4	6	5	5.0	5.3	0.162	0.159	7.7
12	concentration	10	12	12	11.3	7	9	9	8.3	8.7	0.199	0.196	11.6
13		4	5	6	5.0	2	5	4	3.7	4.0	0.294	0.291	8.4
14		100%	8	10	11	9.7	4	6	6	5.3	5.7	0.233	0.230
15		8	9	10	9.0	6	8	8	7.3	7.7	0.137	0.134	9.7
mean					8.7				6.0	6.3	0.208	0.204	9.4
± S.D.					2.6				1.7	1.7	0.056	0.056	1.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.	
11	25	
12	concentration	
13		100%
14		
15		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	75
2	B	159
	A	166
3	B	249
	A	255

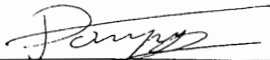
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 08 May 92
Experiment no. 26
Compound of the same pair no. 22 + 23

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
				0.0
				0.0

Permeability (OD)	correc.	In-vitro score
0.017		
0.031		
0.012		
0.020		
0.010		

16	compound no.
17	26
18	
19	concentration
20	20%
21	
mean	
± S.D.	

1	1	1	1.0	1.0
0	0	0	0.0	0.0
0	0	0	0.0	0.0
1	1	1	1.0	1.0
0	0	0	0.0	0.0
1	1	1	1.0	1.0
		0.5		0.5
		0.5		0.5

0.040	0.020	1.3
0.035	0.015	0.2
0.044	0.023	0.4
0.032	0.012	1.2
0.035	0.015	0.2
0.035	0.014	1.2
0.037	0.016	0.7
0.004	0.004	0.5

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

Fluorescein leakage into the waterbath.

16	compound no.
17	26
18	
19	concentration
20	20%
21	
mean	
± S.D.	

Compound No. 26 was warmed up to 32°C and stirred on a magnetic stirrer.
 Anterior chambers were opened for treatment and washing.
 Glass of the anterior chamber No. 17 was found to be cracked at the end of the fluorescein incubation period.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	171
3	B	251
	A	260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

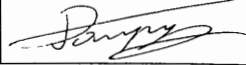
Lab. no. 09

Date: 11 May 92

Name: Ph. Vanparys

Experiment no. 27

Compound of the same pair no. 28 + 31

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
			0.0	
			0.0	

Permeability (OD)	correc.	in-vitro score
0.013		0.2
0.020		0.3
0.010		0.2
0.014		0.2
0.005		0.1

4	compound no.
5	27
6	concentration
7	
8	
9	20%
mean	
± S.D.	

8	8	8	8.0	8.0
4	4	4	4.0	4.0
6	6	7	6.3	6.3
4	4	4	4.0	4.0
4	5	5	4.7	4.7
4	4	4	4.0	4.0
			5.2	5.2
			1.7	1.7

0.023	0.008	8.1
0.183	0.169	6.5
0.077	0.063	7.3
0.028	0.014	4.2
0.103	0.089	6.0
0.067	0.053	4.8
0.080	0.066	6.2
0.059	0.059	1.5

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

Glass of the anterior chamber No. 3 was found to be cracked at the end of the fluorescein incubation period.

4	compound no.
5	27
6	concentration
7	
8	
9	20%
mean	
± S.D.	

Fluorescein leakage from chamber No. 5.
Compound No. 27 was warmed up to 32°C and stirred on a magnetic stirrer.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-171
3	B	249
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

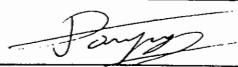
Lab. no. **09**

Date: 11 May 92

Name: Ph. Vanparys

Experiment no. 27

Compound of the same pair no. 27 + 31

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min					correc.
C1	0	0	0.0		
0	C2	0	0.0		
0	0	C3	0.0		
				0.0	
				0.0	

Permeability (OD)		in-vitro score
correc.		
0.013		0.2
0.020		0.3
0.010		0.2
0.014		0.2
0.005		0.1

10	compound no.
11	28
12	
13	concentration
14	20%
15	
mean	
± S.D.	

0	0	0	0.0	0.0
0	0	0	0.0	0.0
0	0	0	0.0	0.0
0	0	0	0.0	0.0
1	1	1	1.0	1.0
0	0	0	0.0	0.0
				0.2
				0.2
				0.4
				0.4

0.016	0.002	0.0
0.017	0.002	0.0
0.012	-0.002	0.0
0.012	-0.003	0.0
0.015	0.001	1.0
0.010	-0.004	-0.1
0.014	-0.001	0.2
0.003	0.003	0.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

Glass of the anterior chamber No. 3 was found to be cracked at the end of the fluorescein incubation period.

10	compound no.
11	28
12	
13	concentration
14	20%
15	
mean	
± S.D.	

Compound No. 28 was warmed up to 32°C and stirred on a magnetic stirrer

Fluorescein leakage from chamber No.13.

Compound No. 28 was washed away 6 times instead of 3 times

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-171
3	B	249
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 30 Mar 92
Experiment no. 11
Compound of the same pair no. 30

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	-2	-3	-2.5	C1	-2	-4	-3.0	correc.	correc.	
1	MEM	C1	-2	-3	-2.5	C1	-2	-4	-3.0		0.003	-3.0
2		C2	0		1.0	1	C2	-2	-0.5		0.002	-0.5
3		3	0	C3	1.5	3	1	C3	2.0		0.003	2.0
mean					0.0				-0.5		0.003	-0.5
±S.D.					2.2				2.5		0.001	2.5

4	compound no.	26	24	23	24.3	20	19	17	18.7	19.2	2 585	2.582	57.9
5	29	28	25	24	25.7	34	32	30	32.0	32.5	1 949	1.946	61.7
6	concentration	24	22	21	22.3	29	28	26	27.7	28.2	2.268	2.265	62.1
7		23	21	20	21.3	32	31	29	30.7	31.2	2.688	2.685	71.4
8		100%	22	20	19	20.3	32	30	28	30.0	30.5	2.094	2.091
9		22	20	19	20.3	26	24	23	24.3	24.8	1.703	1.700	50.3
mean					22.4				27.2	27.7	2.215	2.212	60.9
±S.D.					2.2				5.0	5.0	0.377	0.377	6.9

cor-nea	treatment
1	MEM
2	
3	
mean	
±S.D.	

4	compound no.	
5	29	
6	concentration	
7		
8		100%
9		
mean		
±S.D.		

the anterior compartment was rinsed 5-times instead of 3-times

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	157
	A	166
3	B	247
	A	256

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet


Lab. no. 09

Date: 30 Mar 92

Name: Ph. Vanparys

Experiment no. 11

Compound of the same pair no. 29

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				correc.	Permeability (OD)		in-vitro score
		C1	-2	-3	-2.5	C1	-2	-4	-3.0		correc.		
1	MEM	C1	-2	-3	-2.5	C1	-2	-4	-3.0		0.003		-3.0
2		2	C2	0	1.0	1	C2	-2	-0.5		0.002		-0.5
3		3	0	C3	1.5	3	1	C3	2.0		0.003		2.0
mean											0.003		-0.5
± S.D.											0.001		2.5

	compound no.	13	11	10	11.3	13	11	9	11.0	11.5	0.507	0.504	19.1	
10	30	13	11	10	11.3	13	11	9	11.0	11.5	0.507	0.504	19.1	
11		13	11	10	11.3	16	14	12	14.0	14.5	0.398	0.395	20.4	
12	concentration	11	9	8	9.3	10	8	6	8.0	8.5	0.362	0.359	13.9	
13		11	9	8	9.3	9	7	5	7.0	7.5	0.943	0.940	21.6	
14		100%	13	10	10	11.0	15	13	11	13.0	13.5	0.338	0.335	18.5
15		13	10	10	11.0	13	11	9	11.0	11.5	0.743	0.740	22.6	
mean					10.6				10.7	11.2	0.549	0.546	19.4	
± S.D.					1.0				2.7	2.7	0.244	0.244	3.1	

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

	compound no.	
10	30	
11		
12	concentration	
13		
14		100%
15		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	157
	A	166
3	B	247
	A	256


EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 11 May 92
Experiment no. 27
Compound of the same pair no. 27 +28

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
				0.0
				0.0

Permeability (OD)		In-vitro score
correc.		
0.013		0.2
0.020		0.3
0.010		0.2
0.014		0.2
0.005		0.1

16	compound no.
17	31
18	
19	concentration
20	20%
21	
mean	
± S.D.	

93	90	87	90.0	90.0
84	81	78	81.0	81.0
57	53	51	53.7	53.7
67	63	61	63.7	63.7
87	88	88	87.7	87.7
78	75	73	75.3	75.3
			75.2	75.2
			14.2	14.2

0.538	0.523	97.9
0.439	0.425	87.4
0.467	0.453	60.5
0.499	0.485	70.9
0.209	0.194	90.6
0.430	0.416	81.6
0.430	0.416	81.5
0.116	0.116	13.7

cor-nea	treatment	
1	MEM	Glass of the anterior chamber No. 3 was found to be cracked at the end of the fluorescein incubation period.
2		
3		
mean		O.D. versus C1
± S.D.		measured 4 min. after first measurement.
16	compound no.	Compound No. 31 was warmed up to 32°C
17	31	and stirred on a magnetic stirrer.
18		
19	concentration	
20	20%	
21		Compound No. 31 was washed away 6 times instead of 3 times.
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	171
3	B	249
	A	260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet


Lab. no. 09

Date: 02 Apr 92

Name: Ph. Vanparys

Experiment no. 12

Compound of the same pair no. -

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	-2	0	-1.0	C1	-2	0	-1.0	correc.		
1	MEM	C1	-2	0	-1.0	C1	-2	0	-1.0		0.001	-1.0
2		1	C2	2	1.5	1	C2	2	1.5		0.000	1.5
3		-1	-3	C3	-2.0	-2	-4	C3	-3.0		0.001	-3.0
mean											0.001	-0.8
± S.D.											0.001	2.2

	compound no.	32	30	33	31.7	29	27	31	29.0	29.8	1.628	1.627	54.2	
10	32	23	21	24	22.7	20	19	22	20.3	21.2	1.908	1.907	49.8	
11		23	22	24	23.0	21	19	22	20.7	21.5	1.687	1.686	46.8	
12		24	23	26	24.3	23	21	25	23.0	23.8	1.395	1.394	44.7	
13	concentration	21	20	22	21.0	19	17	20	18.7	19.5	1.012	1.011	34.7	
14		100%	21	19	22	20.7	17	16	19	17.3	18.2	1.731	1.730	44.1
15		mean				23.9				21.5	22.3	1.560	1.560	45.7
± S.D.					4.0				4.1	4.1	0.316	0.316	6.6	

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

	compound no.
10	32
11	
12	
13	concentration
14	100%
15	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	-75
2	B	158
	A	-167
3	B	248
	A	-256


EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 03 Apr 92
Experiment no. 13 b
Compound of the same pair no. -

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1				C1				correc.		
1	MEM with	C1	-3	-2	-2.5	C1	-2	-2	-2.0		0.002	-2.0
2	I-Glutamine	2	C2	0	1.0	0	C2	0	0.0		0.003	0.0
3	Bicarbonate	1	-1	C3	0.0	1	0	C3	0.5		0.000	0.5
mean	pH 7.4				-0.5				-0.5		0.002	-0.5
± S.D.					1.8				1.3		0.002	1.3

10	compound no.	87	83	84	84.7	77	76	76	76.3	76.8	1.554	1.552	100.1
11	33 (2)	74	71	72	72.3	65	63	64	64.0	64.5	0.919	0.917	78.3
12		83	80	80	81.0	71	70	71	70.7	71.2	2.090	2.088	102.5
13	concentration	81	77	78	78.7	71	70	70	70.3	70.8	1.797	1.795	97.8
14	100%	87	84	85	85.3	79	77	77	77.7	78.2	1.335	1.333	98.2
15		90	87	87	88.0	81	80	80	80.3	80.8	2.502	2.500	118.3
mean					81.7				73.2	73.7	1.700	1.698	99.2
± S.D.					5.6				6.0	6.0	0.560	0.560	12.8

cor-nea	treatment
1	MEM with
2	I-Glutamine
3	Bicarbonate
mean	pH 7.4
± S.D.	

10	compound no.
11	33 (2)
12	
13	concentration
14	100%
15	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
1	B	
	A	
2	B	
	A	
3	B	
	A	

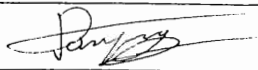
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 06 Apr 92
Experiment no. 14
Compound of the same pair no. 47

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	-1	-1	-1.0	C1	0	0	0.0	correc.		
1	MEM	C1	-1	-1	-1.0	C1	0	0	0.0	0.014		0.2
2		0	C2	0	0.0	0	C2	0	0.0	0.007		0.1
3		0	0	C3	0.0	0	0	C3	0.0	0.005		0.1
mean									0.0	0.009		0.1
± S.D.									0.0	0.005		0.1

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score	
		C1	-1	-1	-1.0	C1	0	0	0.0	correc.			
4	compound no.	34	34	35	34.3	28	29	28	28.3	28.3	0.224	0.215	31.6
5	34	33	33	33	33.0	25	26	25	25.3	25.3	0.052	0.043	26.0
6	concentration	30	30	30	30.0	20	21	21	20.7	20.7	0.069	0.060	21.6
7		28	29	29	28.7	23	24	23	23.3	23.3	0.316	0.307	27.9
8		100%	31	32	31	31.3	25	26	25	25.3	25.3	0.032	0.023
9		26	27	27	26.7	21	21	21	21.0	21.0	0.058	0.049	21.7
mean					30.7				24.0	24.0	0.125	0.117	25.7
± S.D.					2.8				2.9	2.9	0.117	0.117	3.8

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	
4	compound no.	
5	34	
6	concentration	
7		100%
8		
9		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
1	B	75
	A	75
2	B	158
	A	167
3	B	248
	A	255

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

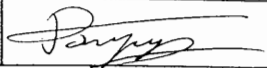
Lab. no. 09

Date: 12 Jun 92

Name: Ph. Vanparys

Experiment no. 38

Compound of the same pair no. 39 + 41

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	C2	C3		
0	0	0	0.0	
0	0	0	0.0	
0	0	0	0.0	
				0.0
				0.0

Permeability (OD)	correc.	in-vitro score
0.009		0.1
0.019		0.3
0.005		0.1
0.011		0.2
0.007		0.1

4	compound no.
5	35
6	concentration
7	
8	
9	20%
mean	
± S.D.	

118	119	120	119.0	119.0
132	134	137	134.3	134.3
142	145	145	144.0	144.0
139	140	143	140.7	140.7
141	144	144	143.0	143.0
128	128	130	128.7	128.7
			134.9	134.9
			9.7	9.7

0.272	0.261	122.9
0.575	0.564	142.8
0.062	0.051	144.8
0.550	0.539	148.8
0.190	0.179	145.7
0.139	0.128	130.6
0.298	0.287	139.2
0.216	0.216	10.2

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

4	compound no.
5	35
6	concentration
7	
8	
9	20%
mean	
± S.D.	

pH: 5.80

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 16 Apr 92

Name: Ph. Vanparys

Experiment no. 17

Compound of the same pair no. 37 + 49

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	1	0	0.5	C1	2	1	1.5	correc.		
1	MEM	C1	1	0	0.5	C1	2	1	1.5			1.6
2		-2	C2	-1	-1.5	-3	C2	-2	-2.5			-2.4
3		0	0	C3	0.0	-2	1	C3	-0.5			-0.3
mean												
± S.D.												2.0

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score		
		C1	1	0	0.5	C1	2	1	1.5	correc.				
4	compound no.	9	11	9	9.7	10	13	12	11.7	12.2			89.9	
5	36	10	12	11	11.0	13	16	14	14.3	14.8			97.2	
6	concentration	9	11	10	10.0	10	13	11	11.3	11.8			103.3	
7		12	14	13	13.0	15	18	16	16.3	16.8			94.9	
8		10%	11	13	12	12.0	14	18	16	16.0	16.5			113.2
9		8	10	9	9.0	9	12	10	10.3	10.8			99.3	
mean					10.8				13.3	13.8			99.6	
± S.D.					1.5				2.6	2.6			8.0	

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	1	0	0.5	C1	2	1	1.5	correc.		
1	MEM	C1	1	0	0.5	C1	2	1	1.5			1.6
2		-2	C2	-1	-1.5	-3	C2	-2	-2.5			-2.4
3		0	0	C3	0.0	-2	1	C3	-0.5			-0.3
mean												
± S.D.					1.0				2.0			2.0

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score		
		C1	1	0	0.5	C1	2	1	1.5	correc.				
4	compound no.	9	11	9	9.7	10	13	12	11.7	12.2			89.9	
5	36	10	12	11	11.0	13	16	14	14.3	14.8			97.2	
6	concentration	9	11	10	10.0	10	13	11	11.3	11.8			103.3	
7		12	14	13	13.0	15	18	16	16.3	16.8			94.9	
8		10%	11	13	12	12.0	14	18	16	16.0	16.5			113.2
9		8	10	9	9.0	9	12	10	10.3	10.8			99.3	
mean					10.8				13.3	13.8			99.6	
± S.D.					1.5				2.6	2.6			8.0	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-263

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 16 Apr 92

Name: Ph. Vanparys

Experiment no. 17

Compound of the same pair no. 36 + 49

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	In-vitro score
		C1				C1			correc.		
1	MEM	C1	1	0	0.5	C1	2	1	1.5	0.006	1.6
2		-2	C2	-1	-1.5	-3	C2	-2	-2.5	0.010	-2.4
3		0	0	C3	0.0	-2	1	C3	-0.5	0.015	-0.3
mean										0.010	-0.3
± S.D.										0.005	2.0

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.		In-vitro score	
		C1				C1			correc.				
10	compound no.	0	1	0	0.3	1	4	2	2.3	2.8	0.022	0.012	3.0
11	37	-2	0	-1	-1.0	-3	0	-2	-1.7	-1.2	0.012	0.001	-1.1
12	concentration	-1	0	0	-0.3	-2	1	0	-0.3	0.2	0.016	0.005	0.2
13		-1	0	0	-0.3	-2	0	-1	-1.0	-0.5	0.013	0.002	-0.5
14		10%	-1	0	0	-0.3	-1	1	0	0.0	0.5	0.011	0.001
15		-1	0	0	-0.3	-1	1	0	0.0	0.5	0.019	0.009	0.6
mean					-0.3				-0.1	0.4	0.015	0.005	0.5
± S.D.					0.4				1.4	1.4	0.004	0.004	1.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	
10	compound no.	
11	37	
12	concentration	
13		
14		10%
15		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	170
3	B	250
	A	263

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

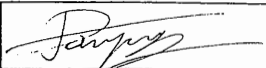
Lab. no. 09

Date: 17 Apr 92

Name: Ph. Vanparys

Experiment no. 18

Compound of the same pair no. 40 + 42

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	C2	C3	mean	C1	C2	C3	mean		
1	MEM	C1	0	0	0.0	C1	0	0	0.0	0.013	0.2
2		0	C2	0	0.0	0	C2	0	0.0	0.011	0.2
3		1	1	C3	1.0	0	0	C3	0.0	0.008	0.1
mean					0.3				0.0	0.011	0.2
± S.D.					0.6				0.0	0.003	0.0

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.		in-vitro score	
		C1	C2	C3	mean	C1	C2	C3	mean	± S.D.			
4	compound no.	1	1	0	0.7	2	2	1	1.7	1.7	0.022	0.012	1.8
5	38	1	1	0	0.7	1	1	0	0.7	0.7	0.012	0.001	0.7
6	concentration	1	1	0	0.7	1	1	0	0.7	0.7	0.011	0.000	0.7
7		1	1	0	0.7	2	2	2	2.0	2.0	0.005	-0.006	1.9
8		10%	1	1	0	0.7	1	1	0	0.7	0.7	0.003	-0.008
9		1	1	0	0.7	1	1	0	0.7	0.7	0.002	-0.009	0.5
mean					0.7				1.1	1.1	0.009	-0.002	1.0
± S.D.					0.0				0.6	0.6	0.008	0.008	0.7

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	
4	compound no.	
5	38	
6	concentration	
7		
8		10%
9		
mean		
± S.D.		

Compound No. 38 was warmed up to 32°C and stirred on a magnetic stirrer

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	158
	A	169
3	B	249
	A	258

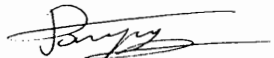
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 12 Jun 92
 Experiment no. 38
 Compound of the same pair no. 35 + 41

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
•0	C2	0	0.0	
0	0	C3	0.0	
			0.0	
			0.0	

Permeability (OD)	correc.	In-vitro score
0.009		0.1
0.019		0.3
0.005		0.1
0.011		0.2
0.007		0.1

10	compound no.
11	39
12	
13	concentration
14	20%
15	
mean	
± S.D.	

3	3	2	2.7	2.7
3	3	3	3.0	3.0
3	3	3	3.0	3.0
1	1	1	1.0	1.0
1	1	1	1.0	1.0
5	5	4	4.7	4.7
			2.6	2.6
			1.4	1.4

0.002	-0.009	2.5
0.013	0.002	3.0
0.002	-0.009	2.9
0.018	0.007	1.1
0.004	-0.007	0.9
0.007	-0.004	4.6
0.008	-0.003	2.5
0.006	0.006	1.4

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	39
12	
13	concentration
14	20%
15	
mean	
± S.D.	

pH: 2.97
 The anterior chamber was opened for washing.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 17 Apr 92

Name: Ph. Vanparys

Experiment no. 18

Compound of the same pair no. 38 + 42

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	0	0	0.0	C1	0	0	0.0	correc.		
1	MEM	C1	0	0	0.0	C1	0	0	0.0			0.2
2		0	C2	0	0.0	0	C2	0	0.0			0.2
3		1	1	C3	1.0	0	0	C3	0.0			0.1
mean												0.2
± S.D.												0.0

	compound no.	opacity at 10 min				opacity at 120 min					Permeability (OD)		in-vitro score		
10	40	3	4	3	3.3	9	9	8	8.7	8.7	3.128	3.117		55.4	
11		3	3	2	2.7	9	9	8	8.7	8.7	3.775	3.764	65.1		
12		5	5	4	4.7	8	9	8	8.3	8.3	3.992	3.981	68.1		
13		concentration	2	2	1	1.7	7	7	6	6.7	6.7	4.426	4.415	72.9	
14			10%	5	5	4	4.7	7	7	6	6.7	6.7	3.238	3.227	55.1
15				4	4	3	3.7	8	8	7	7.7	7.7	3.422	3.411	58.8
mean														62.6	
± S.D.														7.3	

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

	compound no.	
10	40	
11		
12		
13		concentration
14		10%
15		
mean		
± S.D.		

Compound No. 40 was warmed up to 32°C and stirred on a magnetic stirrer.

Membranes released from the corneas:
very small air-bubbles behind the corneas.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-169
3	B	249
	A	-258

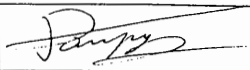
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 12 Jun 92
Experiment no. 38
Compound of the same pair no. 35 + 39

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min					correc.	Permeability (OD)		in-vitro score
C1	0	0	0.0			correc.		
0	C2	0	0.0			0.009		0.1
0	0	C3	0.0			0.019		0.3
			0.0			0.005		0.1
			0.0			0.011		0.2
			0.0			0.007		0.1

16	compound no.
17	41
18	
19	concentration
20	20%
21	
mean	
± S.D.	

53	52	52	52.3	52.3	0.035	0.024	52.7
58	58	58	58.0	58.0	0.052	0.041	58.6
64	64	64	64.0	64.0	0.108	0.097	65.4
54	53	53	53.3	53.3	0.029	0.018	53.6
52	52	51	51.7	51.7	0.096	0.085	52.9
63	63	62	62.7	62.7	0.123	0.112	64.3
			57.0	57.0	0.074	0.063	57.9
			5.4	5.4	0.040	0.040	5.8

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

16	compound no.	pH : 7.26 Compound no. 41 was washed away 4 times.
17	41	
18		
19	concentration	
20	20%	
21		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

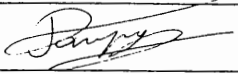
Lab. no. 09

Date: 17 Apr 92

Name: Ph. Vanparys

Experiment no. 18

Compound of the same pair no. 38 + 40

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	0	0	0.0	C1	0	0	0.0		
1	MEM	C1	0	0	0.0	C1	0	0	0.0	0.013	0.2
2		0	C2	0	0.0	0	C2	0	0.0	0.011	0.2
3		1	1	C3	1.0	0	0	C3	0.0	0.008	0.1
mean					0.3				0.0	0.011	0.2
± S.D.					0.6				0.0	0.003	0.0

	compound no.	12	12	11	11.7	18	18	17	17.7	17.7	3.170	3.159	65.1
16	42	12	12	11	11.7	18	18	17	17.7	17.7	3.170	3.159	65.1
17		13	13	12	12.7	19	19	18	18.7	18.7	3.968	3.957	78.0
18		11	12	11	11.3	25	25	24	24.7	24.7	2.638	2.627	64.1
19	concentration	8	8	7	7.7	14	14	13	13.7	13.7	3.449	3.438	65.2
20	10%	12	12	12	12.0	19	19	18	18.7	18.7	3.282	3.271	67.7
21		12	13	12	12.3	17	17	16	16.7	16.7	4.187	4.176	79.3
mean					11.3				18.3	18.3	3.449	3.438	69.9
± S.D.					1.8				3.6	3.6	0.562	0.562	6.9

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

	compound no.
16	42
17	
18	
19	concentration
20	10%
21	
mean	
± S.D.	

Compound No. 42 was warmed up to 32°C and stirred on a magnetic stirrer.

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	158
	A	169
3	B	248
	A	258

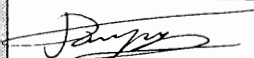
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 15 Jun 92
 Experiment no. 39
 Compound of the same pair no. 44

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min				correc.
C1	0	0	0.0	
0	C2	0	0.0	
0	0	C3	0.0	
				0.0
				0.0

Permeability (OD)		in-vitro score
correc.		
0.036		0.5
0.022		0.3
0.028		0.4
0.029		0.4
0.007		0.1

4	compound no.
5	43
6	concentration
7	
8	
9	20%
mean	
± S.D.	

86	86	86	86.0	86.0
71	71	71	71.0	71.0
79	79	79	79.0	79.0
94	94	94	94.0	94.0
91	91	91	91.0	91.0
95	93	93	93.7	93.7
			85.8	85.8
			9.2	9.2

4.402	4.373	151.6
3.408	3.379	121.7
4.386	4.357	144.4
4.370	4.342	159.1
6.292	6.263	184.9
3.553	3.524	146.5
4.402	4.373	151.4
1.028	1.028	20.7

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	75
2	B	159
	A	170
3	B	249
	A	260

4	compound no.
5	43
6	concentration
7	
8	
9	20%
mean	
± S.D.	

pH: 8.66

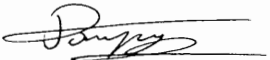
EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 15 Jun 92
Experiment no. 39
Compound of the same pair no. 43

Name: Ph. Vanparys

Signature: 

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

opacity at 240 min					correc.
C1	0	0	0.0		
0	C2	0	0.0		
0	0	C3	0.0		
			0.0		
			0.0		

Permeability (OD)		in-vitro score
correc.		
0.036		0.5
0.022		0.3
0.028		0.4
0.029		0.4
0.007		0.1

10	compound no.
11	44
12	
13	concentration
14	20%
15	
mean	
± S.D.	

0	0	0	0.0	0.0
2	2	2	2.0	2.0
1	1	1	1.0	1.0
-1	-2	-2	-1.7	-1.7
0	-1	-1	-0.7	-0.7
4	3	3	3.3	3.3
			0.7	0.7
			1.8	1.8

0.045	0.016	0.2
0.043	0.014	2.2
0.064	0.036	1.5
0.062	0.034	-1.2
0.485	0.457	6.2
0.055	0.026	3.7
0.126	0.097	2.1
0.176	0.176	2.6

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.
11	44
12	
13	concentration
14	20%
15	
mean	
± S.D.	

pH: 8.50

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	249
	A	-260

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 21 Apr 92

Name: Ph. Vanparys

Experiment no. 19

Compound of the same pair no. 46

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1								correc.	correc.	
1	MEM	C1	0	0	0.0	C1	-1	0	-0.5		0.012	-0.3
2		0	C2	0	0.0	1	C2	1	1.0		0.009	1.1
3		0	0	C3	0.0	0	-1	C3	-0.5		0.015	-0.3
mean					0.0				0.0		0.012	0.2
± S.D.					0.0				0.9		0.003	0.8

4	compound no.	52	52	54	52.7	84.	83	84	83.7	83.7	6.949	6.937	187.7
5	45	57	58	59	58.0	88	87	88	87.7	87.7	4.728	4.716	158.4
6	concentration	54	55	56	55.0	86	85	86	85.7	85.7	4.464	4.452	152.5
7		50	50	51	50.3	84	83	84	83.7	83.7	5.923	5.911	172.3
8		10%	47	47	48	47.3	79	78	80	79.0	79.0	4.781	4.769
9		54	55	56	55.0	89	87	88	88.0	88.0	5.748	5.736	174.0
mean					53.1				84.6	84.6	5.432	5.420	165.9
± S.D.					3.8				3.3	3.3	0.949	0.949	14.5

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

4	compound no.	
5	45	
6	concentration	
7		
8		10%
9		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-171
3	B	252
	A	-263

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

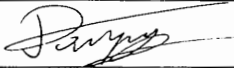
Lab. no. 09

Date: 21 Apr 92

Name: Ph. Vanparys

Experiment no. 19

Compound of the same pair no. 45

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	C2	C3	mean	C1	C2	C3	mean		
1	MEM	C1	0	0	0.0	C1	-1	0	-0.5	0.012	-0.3
2		0	C2	0	0.0	1	C2	1	1.0	0.009	1.1
3		0	0	C3	0.0	0	-1	C3	-0.5	0.015	-0.3
mean					0.0				0.0	0.012	0.2
± S.D.					0.0				0.9	0.003	0.8

10	compound no.	1	1	1	1.0	3	2	3	2.7	2.7	0.014	0.003	2.7
11	46	2	1	1	1.3	4	3	4	3.7	3.7	0.005	-0.006	3.6
12	concentration	3	3	3	3.0	5	4	5	4.7	4.7	0.011	0.000	4.7
13		0	0	0	0.0	1	0	1	0.7	0.7	0.016	0.004	0.7
14		10%	1	0	0	0.3	2	1	2	1.7	1.7	0.031	0.020
15		3	3	3	3.0	5	4	5	4.7	4.7	0.043	0.032	5.1
mean					1.4				3.0	3.0	0.020	0.008	3.1
± S.D.					1.3				1.6	1.6	0.014	0.014	1.7

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.	
11	46	
12	concentration	
13		10%
14		
15		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-171
3	B	252
	A	-263

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

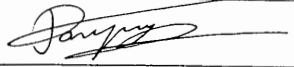
Lab. no. 09

Date: 06 Apr 92

Name: Ph. Vanparys

Experiment no. 14

Compound of the same pair no. 34

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	-1	-1	-1.0	C1	0	0	0.0		
1	MEM	C1	-1	-1	-1.0	C1	0	0	0.0	0.014	0.2
2		0	C2	0	0.0	0	C2	0	0.0	0.007	0.1
3		0	0	C3	0.0	0	0	C3	0.0	0.005	0.1
mean										0.009	0.1
± S.D.										0.005	0.1

10	compound no.	4	4	4	4.0	6	6	6	6.0	6.0	6.160	6.151	98.3
11	47	5	6	6	5.7	11	12	11	11.3	11.3	4.200	4.191	74.2
12	concentration	3	4	3	3.3	6	7	6	6.3	6.3	4.500	4.491	73.7
13		4	5	5	4.7	7	7	7	7.0	7.0	7.760	7.751	123.3
14		100%	2	2	2	2.0	8	9	8	8.3	8.3	4.520	4.511
15		4	5	5	4.7	7	8	7	7.3	7.3	6.280	6.271	101.4
mean		4.1				7.7				7.7	5.570	5.561	91.1
± S.D.		1.3				1.9				1.9	1.398	1.398	20.0

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

10	compound no.	
11	47	
12	concentration	
13		100%
14		
15		
mean		
± S.D.		

Na-fluorescein concentration in posterior compartment diluted with a factor 4. The OD values were multiplied with 4 to obtain the final OD value indicated in the table.

CALIBRATION		
Filter paper	Holder	Opacity
-		0
1	B	75
	A	75
2	B	158
	A	167
3	B	248
	A	255

EEC VALIDATION OF THE BC0-P ASSAY


Data sheet

Lab. no. 09

Date: 13 Apr 92
Experiment no. 16
Compound of the same pair no. 51 + 52

*REPEAT OF
 EXP. NR. 15*

Name: Ph. Vanparys

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	-1	0	-0.5	C1	-1	0	-0.5		
1	MEM	C1	-1	0	-0.5	C1	-1	0	-0.5	0.009	-0.4
2		0	C2	1	0.5	0	C2	1	0.5	0.009	0.6
3		0	-1	C3	-0.5	-1	-2	C3	-1.5	0.010	-1.4
mean					-0.2				-0.5	0.009	-0.4
± S.D.					0.6				1.0	0.001	1.0

16	compound no.	63	62	63	62.7	80	80	81	80.3	80.8	3.963	3.954	140.1
17	48 (2)	57	57	58	57.3	76	75	76	75.7	76.2	5.402	5.393	157.1
18	concentration	52	52	53	52.3	70	69	70	69.7	70.2	4.382	4.373	135.8
19		57	57	59	57.7	75	74	76	75.0	75.5	3.912	3.903	134.0
20		100%	59	59	60	59.3	80	79	81	80.0	80.5	4.090	4.081
21		58	57	59	58.0	76	75	77	76.0	76.5	4.350	4.341	141.6
mean					57.9				76.1	76.6	4.350	4.341	141.7
± S.D.					3.4				3.9	3.9	0.551	0.551	8.2

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

16	compound no.	
17	48 (2)	
18	concentration	
19		
20		100%
21		
mean		
± S.D.		

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-168
3	B	249
	A	-259

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. **09**

Date: 16 Apr 92
 Experiment no. 17
 Compound of the same pair no. 36 + 37

Name: Ph. Vanparys

*REPEAT OF
 EXP. NR. 15*

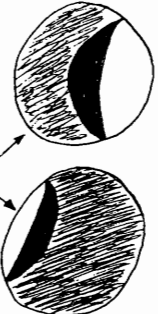
Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1				C1				correc.	correc.	
1	MEM	C1	1	0	0.5	C1	2	1	1.5		0.006	1.6
2		-2	C2	-1	-1.5	• -3	C2	-2	-2.5		0.010	-2.4
3		0	0	C3	0.0	-2	1	C3	-0.5		0.015	-0.3
mean					-0.3				-0.5		0.010	-0.3
± S.D.					1.0				2.0		0.005	2.0

	compound no.	21	24	23	22.7	30	34	32	32.0	32.5	4.517	4.507	100.1	
16	49 (2)	23	25	24	24.0	29	33	30	30.7	31.2	4.129	4.119	92.9	
17		29	31	30	30.0	33	36	34	34.3	34.8	6.519	6.509	132.5	
18		18	20	19	19.0	23	27	25	25.0	25.5	3.785	3.775	82.1	
19	concentration	24	27	26	25.7	31	35	31	32.3	32.8	3.074	3.064	78.8	
20		100%	22	24	23	23.0	28	31	29	29.3	29.8	2.750	2.740	70.9
21		mean				24.1				30.6	31.1	4.129	4.119	92.9
	± S.D.				3.6				3.2	3.2	1.341	1.341	22.0	

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

	compound no.	
16	49 (2)	
17		
18		
19	concentration	
20		100%
21		
mean		
± S.D.		



Fine opaque membrane is released from the corneas

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	159
	A	-170
3	B	250
	A	-263

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

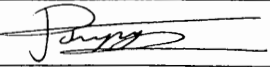
Lab. no. 09

Date: 22 Jun 92

Name: Ph. Vanparys

Experiment no. 41

Compound of the same pair no.

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD) correc.	in-vitro score
		C1	0	0	0.0	C1	0	0	0.0		
1	MEM	C1	0	0	0.0	C1	0	0	0.0	0.005	0.1
2		0	C2	0	0.0	0	C2	0	0.0	0.009	0.1
3		0	1	C3	0.5	0	0	C3	0.0	0.012	0.2
mean					0.2				0.0	0.009	0.1
± S.D.					0.3				0.0	0.004	0.1

4	compound no.	9	11	10	10.0	15	14	14	14.3	14.3	6.268	6.259	108.2
5	50	12	14	14	13.3	20	19	19	19.3	19.3	4.413	4.404	85.4
6	concentration	13	14	13	13.3	19	19	19	19.0	19.0	7.409	7.400	130.0
7		9	10	9	9.3	10	10	10	10.0	10.0	3.752	3.743	66.2
8		10%	9	10	9	9.3	14	13	13	13.3	13.3	5.552	5.543
9		15	16	16	15.7	22	21	21	21.3	21.3	7.111	7.102	127.9
mean					11.8				16.2	16.2	5.751	5.742	102.4
± S.D.					2.6				4.3	4.3	1.462	1.462	24.8

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

4	compound no.	pH: 9.06
5	50	
6	concentration	
7		Cornea no. 7 with transparant area in the middle.
8		10%
9		
mean		
± S.D.		



CALIBRATION		
Filter paper	Holder	Opacity
1	B	
	A	
2	B	
	A	
3	B	
	A	

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

Lab. no. 09

Date: 13 Apr 92

Name: Ph. Vanparys

Experiment no. 16

Compound of the same pair no. 48 + 52

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score
		C1	-1	0	-0.5	C1	-1	0	-0.5	correc.		
1	MEM	C1	-1	0	-0.5	C1	-1	0	-0.5			-0.4
2		0	C2	1	0.5	0	C2	1	0.5			0.6
3		0	-1	C3	-0.5	-1	-2	C3	-1.5			-1.4
mean												-0.4
± S.D.												1.0

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score	
		C1	-1	0	-0.5	C1	-1	0	-0.5	correc.			
4	compound no.	41	41	42	41.3	47.	46	48	47.0	47.5	5.154	5.145	124.7
5	51	37	37	38	37.3	43	43	44	43.3	43.8	3.662	3.653	98.6
6	concentration	36	35	37	36.0	40	40	41	40.3	40.8	3.053	3.044	86.5
7		36	36	37	36.3	42	41	42	41.7	42.2	3.216	3.207	90.3
8		100%	38	38	39	38.3	42	42	43	42.3	42.8	4.318	4.309
9		47	46	47	46.7	49	48	50	49.0	49.5	4.742	4.733	120.5
mean					39.3				43.9	44.4	4.024	4.015	104.7
± S.D.					4.1				3.3	3.3	0.849	0.849	15.7

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

cor-nea	treatment	opacity at 10 min				opacity at 120 min				Permeability (OD)		in-vitro score	
		C1	-1	0	-0.5	C1	-1	0	-0.5	correc.			
4	compound no.	41	41	42	41.3	47.	46	48	47.0	47.5	5.154	5.145	124.7
5	51	37	37	38	37.3	43	43	44	43.3	43.8	3.662	3.653	98.6
6	concentration	36	35	37	36.0	40	40	41	40.3	40.8	3.053	3.044	86.5
7		36	36	37	36.3	42	41	42	41.7	42.2	3.216	3.207	90.3
8		100%	38	38	39	38.3	42	42	43	42.3	42.8	4.318	4.309
9		47	46	47	46.7	49	48	50	49.0	49.5	4.742	4.733	120.5
mean					39.3				43.9	44.4	4.024	4.015	104.7
± S.D.					4.1				3.3	3.3	0.849	0.849	15.7

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-168
3	B	249
	A	-259

EEC VALIDATION OF THE BC0-P ASSAY

Data sheet

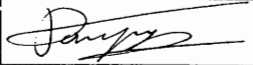
Lab. no. 09

Date: 13 Apr 92

Name: Ph. Vanparys

Experiment no. 16

Compound of the same pair no. 48 + 51

Signature: 

cor-nea	treatment	opacity at 10 min				opacity at 120 min				correc.	Permeability (OD)		in-vitro score
		C1	-1	0	-0.5	C1	-1	0	-0.5		correc.		
1	MEM	C1	-1	0	-0.5	C1	-1	0	-0.5		0.009		-0.4
2		0	C2	1	0.5	0	C2	1	0.5		0.009		0.6
3		0	-1	C3	-0.5	-1	-2	C3	-1.5		0.010		-1.4
mean					-0.2				-0.5		0.009		-0.4
± S.D.					0.6				1.0		0.001		1.0

	compound no.	1	0	2	1.0	3	2	3	2.7	3.2	0.038	0.029	3.6
10	52	1	0	2	1.0	3	2	3	2.7	3.2	0.038	0.029	3.6
11		2	1	3	2.0	3	2	3	2.7	3.2	0.039	0.030	3.6
12		0	0	1	0.3	1	1	2	1.3	1.8	0.025	0.016	2.1
13	concentration	1	0	1	0.7	3	2	4	3.0	3.5	0.052	0.043	4.1
14		1	0	1	0.7	2	2	3	2.3	2.8	0.027	0.018	3.1
15		0	0	0	0.0	1	0	1	0.7	1.2	0.025	0.016	1.4
mean					0.8				2.1	2.6	0.034	0.025	3.0
± S.D.					0.7				0.9	0.9	0.011	0.011	1.0

cor-nea	treatment
1	MEM
2	
3	
mean	
± S.D.	

	compound no.
10	52
11	
12	
13	concentration
14	100%
15	
mean	
± S.D.	

CALIBRATION		
Filter paper	Holder	Opacity
-	-	0
1	B	75
	A	-75
2	B	158
	A	-168
3	B	249
	A	-259

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Appendix G7

**Dataset Received from Johnson & Johnson Pharmaceutical Research and
Development – A Division of Janssen Pharmaceutica N.V.
(BCOP Tests With Young vs. Old Corneas)**

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The use of corneas from animals of different age in the Bovine Corneal Opacity and Permeability (BCOP) assay.

Freddy Van Goethem, Marc Sysmans and Philippe Vanparys

Johnson & Johnson Pharmaceutical Research & Development, a division of Janssen Pharmaceutica N.V.,
Genetic and In Vitro Toxicology, Turnhoutseweg 30, B-2340 Beerse, Belgium.

BCOP results obtained with corneas from:

- 1) adult animals (> 24 months)
- 2) young animals (6 - 8 months)

Methodology

After background opacity measurement, medium was removed from the anterior compartment and corneas were treated with 0.75 ml of the test solution. Corneas (3 per group) were treated for 10 minutes followed by a 120 minutes recovery period. Medium was removed from the anterior compartment and replaced by 1 ml of a 0.4% sodium-fluorescein solution. Corneas were incubated in a horizontal position for 90 minutes at 32°C in a water-bath. After incubation, medium from the posterior chamber was removed and its optical density (OD) determined with a spectrophotometer at 490 nm. In Vitro Score = opacity + [15 x permeability]

Code of each compound is recorded on each raw data sheet

>>> compound 17 (acetone) need to be repeated since results did not comply with previously collected data in our laboratory. Due to the high vapor pressure of acetone (201.57 mmHg @ 22.0 °C), a technical artefact could have occurred...

The use of corneas from animals of different age in the Bovine Corneal Opacity and Permeability (BCOP) assay.

Code	Compound	CAS No.	In vivo EU	In vivo GHS	In Vitro BCOP (>24 months)				In Vitro BCOP (6 - 8 months)			
					Opacity	Perm.	IVS	Class	Opacity	Perm.	IVS	Class
1	3,3-dimethylpentane	562-49-2	NI	NI	0.6	0.01	0.8	NON	0.0	0.02	0.3	NON
2	3-methoxy-1,2-propanediol	623-39-2	NI	NI	-0.3	0.00	0.2	NON	0.6	0.02	0.9	NON
3	polyethylene glycol 400	25322-68-3	NI	NI	-0.3	0.00	-0.3	NON	0.0	0.08	1.1	NON
4	glycerol	56-81-5	NI	NI	-1.0	0.01	-0.9	NON	-0.7	-0.01	-0.8	NON
5	methyl cyclopentane	96-37-7	NI	NI	1.0	0.43	7.5	MILD	1.3	0.26	5.2	MILD
6	tween 20	9005-64-5	NI	NI	0.0	0.01	0.1	NON	0.0	-0.01	-0.1	NON
7	methyl <i>iso</i> -butyl ketone	108-10-1	NI	NI	6.6	1.07	22.7	MILD	5.7	0.83	18.1	MILD
8	toluene	108-88-3	NI	NI	6.3	3.18	54	MOD	6.0	1.46	28.0	MOD
9	methyl amyl ketone	110-43-0	NI	NI	5.3	1.80	32.3	MOD	4.0	0.99	18.8	MILD
10	2-methyl-1-pentanol	105-30-6	NI	2B	12.0	4.30	76.6	SEV	8.6	1.94	37.7	MOD
11	ethanol	64-17-5	NI	2B	16.0	2.34	51	MOD	16.3	1.83	43.8	MOD
12	sodium hydroxide (1%)	1310-73-2	R36	2B	99.7	4.16	162	SEV	135.7	3.74	191.8	SEV
13	triton X-100 (5%)	9002-93-1	R36	2B	4.3	3.81	61.5	SEV	4.7	3.70	60.1	SEV
14	1-octanol	111-87-5	R36	2B	10.0	5.24	88.6	SEV	10.3	1.53	33.3	MOD
15	2-ethyl-1-hexanol	104-76-7	R36	2B	4.3	1.76	30.6	MOD	2.3	0.86	15.3	MILD
16	n-hexanol	111-27-3	R36	2A	15.3	3.73	71.2	SEV	14.0	3.62	68.2	SEV
17	acetone	67-64-1	R36	2A	39**	2.95	83.2	SEV	91.3	2.86	134.2	SEV
18	cyclohexanol	108-93-0	R41	1	15.3	5.04	90.7	SEV	11.6	2.13	43.6	MOD
19	cetylpyridinium bromide (6%)	140-72-7	R41	1	11.7	1.01	26.8	MOD	15.0	1.66	39.9	MOD
20	benzalkonium chloride (10%)	8001-54-5	R41	1	92.2	4.22	155.4	SEV	105.7	4.05	166.5	SEV

Prediction Model

BCOP In Vitro Score	Class
≤ 3	NON
3.1-25	MILD
25.1-55	MOD
> 55.1	SEV

** to be repeated (technical artefact probably occurred)

- Compounds 1 → 20
- Adult animals (> 24 months)

Calculation of the in vitro eye irritation score for liquids

Test article	3,3-Dimethylpentane [562-49-2]	
Batch No.	14502CN	
Concentration	100%	Treatment time: 10 min
Code	A1	
Sequence	Intern 8B	OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	2	2	0	0.006	0.1
2	MEM	1	1	0	0.012	0.2
3	100%	1	3	2	0.009	2.1
Mean ± S.D.		0.7 ± 1.2			0.009 ± 0.003	0.8 ± 1.1
					Corrected value	
4	Test article	1	3	2	0.023	1.5
5		0	1	1	0.018	0.4
6	100%	1	2	1	0.014	0.4
Mean ± S.D.		0.6 ± 0.6			0.009 ± 0.005	0.8 ± 0.6
					Corrected value	
					0.014	0.4
					0.009	0.4

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	75 B	-75
	2	154 B	-157
	3	250 B	-255

Paraph: _____

Date: 18-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	3-methoxy-1,2-propanediol 98%		
Batch No.	05307-078		
Concentration	100%	Treatment time	2 hours
Code	B1	OP-KIT	
Sequence	Intern 10A		

No. Cornea	Treatment	Opacity at			Permeability	In vitro score			
		t0	t120	t120 - t0					
1	NC	0	0	0	0.004	0.1			
2	MEM	0	0	0	0.008	0.1			
3	100%	0	1	1	0.010	1.2			
Mean ± S.D.		0.3 ± 0.6			0.007 ± 0.003	0.5 ± 0.6			
		Corrected value				Corrected value			
4	Test article	0	0	0	-0.3	0.019	0.012	-0.1	
5	100%	0	0	0	-0.3	0.066	0.059	0.6	
6		0	0	0	-0.3	0.032	0.025	0.1	
Mean ± S.D.		-0.3 ± 0.0				0.032 ± 0.024		0.2 ± 0.4	

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A	B	B
	2	A	B	B
	3	A	B	B

Paraph

Date 31-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	Polyethylene glycol 400		
Batch No.	3H0110		
Concentration	100%	Treatment time	10 min
Code	C1 (3)		
Sequence	11A	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score	
		t0	t120	t120 - t0			
1	NC	0	0	0	0.002	0.0	
2	NaCl 0.9%	0	0	0	0.003	0.0	
3	100%	1	1	0	0.001	0.0	
Mean ± S.D.		0.0 ± 0.0			0.002 ± 0.001	0.0 ± 0.0	
					Corrected value	Corrected value	
4	Test article	0	0	0	0.000	-0.002	0.0
5	100%	0	0	0	0.003	0.001	0.0
6		1	0	-1	0.010	0.008	-0.9
Mean ± S.D.		-0.3 ± 0.6			0.002 ± 0.005	-0.3 ± 0.5	

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 28-Feb-00

Calculation of the in vitro eye irritation score for liquids

Test article	Glycerol		
Batch No.	HS03116BS		
Concentration	100%	Treatment time	10 min
Code	B2 (4)		
Sequence	Intern 10A	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score		
		t0	t120	t120 - t0				
1	NC	0	0	0	0.004	0.1		
2	MEM	0	0	0	0.008	0.1		
3	100%	0	1	1	0.010	1.2		
Mean ± S.D.		0.3 ± 0.6			0.007 ± 0.003	0.5 ± 0.6		
		Corrected value				Corrected value		
7	Test article	1	0	-1	-1.3	0.017	0.010	-1.2
8	100%	1	1	0	-0.3	0.015	0.008	-0.2
9		1	0	-1	-1.3	0.017	0.010	-1.2
Mean ± S.D.		-1.0 ± 0.6				0.009 ± 0.001	-0.9 ± 0.6	

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A		B
	2	A		B
	3	A		B

Paraph

Date

Calculation of the in vitro eye irritation score for liquids

Test article	Methyl cyclopentane		
Batch No.	09817PS-089		
Concentration	100%	Treatment time	10 min
Code	D5	OP-KIT	
Sequence	12A		

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	NaCl 0.9%	1	1	0	0.006	0.1
3	100%	1	1	0	0.005	0.1
Mean ± S.D.		0.0 ± 0.0			0.005 ± 0.001	0.1 ± 0.0
					Corrected value	
16	Test article	0	1	1	1.0	4.9
17	100%	0	2	2	2.0	14.5
18		0	0	0	0.0	3.1
Mean ± S.D.		1.0 ± 1.0			0.433 ± 0.348	7.5 ± 6.1
					Corrected value	

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A		B
	2	A		B
	3	A		B

Paraph 20-Mar-00

Date

Calculation of the in vitro eye irritation score for liquids

Test article	Tween 20		
Batch No.	A010055102		
Concentration	100%	Treatment time	10 min
Code	C2 6		
Sequence	11A	OP-KIT	

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.002	0.0
2	NaCl 0.9%	0	0	0	0.003	0.0
3	100%	1	1	0	0.001	0.0
Mean ± S.D.		0.0 ± 0.0			0.002 ± 0.001	0.0 ± 0.0
					Corrected value	
7	Test article	0	0	0	0.010	0.1
8	100%	0	0	0	0.023	0.3
9		0	0	0	0.004	0.0
Mean ± S.D.		0.0 ± 0.0			0.010 ± 0.010	0.1 ± 0.2

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A		B
	2	A		B
	3	A		B

Paraph

Date

Calculation of the in vitro eye irritation score for liquids

Test article	Methyl iso-butyl ketone (4 methyl-2-pentanone) [108-10-1]		
Batch No.	CU 10369BU		
Concentration	100%	Treatment time	10 min
Code	A2 (7)		
Sequence	Intern 8B	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	2	2	0	0.006	0.1
2	MEM	1	1	0	0.012	0.2
3	100%	1	3	2	0.009	2.1
Mean ± S.D.		0.7 ± 1.2			0.009 ± 0.003	0.8 ± 1.1
					Corrected value	
7	Test article	1	8	7	6.3	34.8
8	100%	0	7	7	6.3	15.5
9		1	9	8	7.3	17.8
Mean ± S.D.		6.6 ± 0.6			1.070 ± 0.720	22.7 ± 10.5

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A		B
	2	A		B
	3	A		B

Paraph

Date 18-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	Toluene [108-88-3]		
Batch No.	990281O001		
Concentration	100%	Treatment time	
Code	D4 (8)		
Sequence	12A		OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	NaCl 0.9%	1	1	0	0.006	0.1
3	100%	1	1	0	0.005	0.1
	Mean ± S.D.	0.0 ± 0.0			0.005 ± 0.001	0.1 ± 0.0
		Corrected value			Corrected value	
13	Test article	0	6	6	6.0	58.1
14		0	7	7	7.0	49.4
15	100%	0	6	6	6.0	54.5
	Mean ± S.D.	6.3 ± 0.6			3.178 ± 0.327	54.0 ± 4.4

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 20-Mar-00

Calculation of the in vitro eye irritation score for liquids

Test article	methyl amyl ketone (2 heptanone) [110-43-0]	
Batch No.	66400-104	
Concentration	100%	Treatment time 10 min
Code	A3 (9)	
Sequence	Intern 8B	OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	2	2	0	0.006	0.1
2	MEM	1	1	0	0.012	0.2
3	100%	1	3	2	0.009	2.1
Mean ± S.D.		0.7 ± 1.2			0.009 ± 0.003	0.8 ± 1.1
		Corrected value			Corrected value	
10	Test article	1	8	7	6.3	22.6
11		0	6	6	5.3	34.0
12	100%	2	7	5	4.3	40.2
Mean ± S.D.		5.3 ± 1.0			1.799 ± 0.662	32.3 ± 8.9

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 18-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	2-methyl-1-pentanol		
Batch No.	05002PG		
Concentration	100%	Treatment time	10 min
Code	B3	(10)	
Sequence	Intern 10A	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	MEM	0	0	0	0.008	0.1
3	100%	0	1	1	0.010	1.2
Mean ± S.D.		0.3 ± 0.6			0.007 ± 0.003	0.5 ± 0.6
Corrected value					Corrected value	
10	Test article	0	10	10	9.7	59.6
11	100%	0	13	13	12.7	86.3
12		0	14	14	13.7	83.8
Mean ± S.D.		12.0 ± 2.1			4.304 ± 0.852	76.6 ± 14.7

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A		B
	2	A		B
	3	A		B

Paraph

Date 31-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	Ethanol [64-17-5]	
Batch No.	993O710002	
Concentration	100%	Treatment time 10 min
Code	D1 11	
Sequence	12A	OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	NaCl 0.9%	1	1	0	0.006	0.1
3	100%	1	1	0	0.005	0.1
Mean ± S.D.		0.0 ± 0.0			0.005 ± 0.001	0.1 ± 0.0
					Corrected value	Corrected value
4	Test article	0	16	16	2.340	51.0
5	100%	0	17	17	2.164	49.4
6		0	15	15	2.520	52.7
Mean ± S.D.		16.0 ± 1.0			2.336 ± 0.178	51.0 ± 1.7

NC: Negative Control

REMARKS	Filter		OPACITY	
	1	A	B	
	2	A	B	
	3	A	B	

Paraph

Date 20-Mar-00

RDF/BCO/18

Calculation of the in vitro eye irritation score for liquids

Test article	Sodium hydroxide 1%		
Batch No.	66H0320		
Concentration	1%	Treatment time	
Code	D3		
Sequence	12A		OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	NaCl 0.9%	1	1	0	0.006	0.1
3	100%	1	1	0	0.005	0.1
Mean ± S.D.		0.0 ± 0.0			0.005 ± 0.001	0.1 ± 0.0
					Corrected value	Corrected value
10	Test article	0	101	101	101.0	160.2
11		0	111	111	111.0	175.1
12	100%	0	87	87	87.0	150.8
Mean ± S.D.		99.7 ± 12.1			4.156 ± 0.182	162.0 ± 12.3

NC: Negative Control

REMARKS	Filter	OPACITY	
		A	B
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 20-Mar-00

Calculation of the in vitro eye irritation score for liquids

Test article	Triton X-100 (5%)	
Batch No.	28H2536	
Concentration	100%	Treatment time 10 min
Code	C4 (13)	
Sequence	11A	OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.002	0.0
2	NaCl 0.9%	0	0	0	0.003	0.0
3	100%	1	1	0	0.001	0.0
Mean ± S.D.		0.0 ± 0.0			0.002 ± 0.001	0.0 ± 0.0
		Corrected value			Corrected value	
13	Test article	1	6	5	5.0	69.0
14		0	4	4	4.0	54.7
15	100%	2	6	4	4.0	60.9
Mean ± S.D.		4.3 ± 0.6			3.813 ± 0.442	61.5 ± 7.2

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 28-Feb-00

Calculation of the in vitro eye irritation score for liquids

Test article	n-octanol		
Batch No.	27336-019		
Concentration	100%	Treatment time	10 min
Code	B4	14	
Sequence	Intern 10A	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score	
		t0	t120	t120 - t0			
1	NC	0	0	0	0.004	0.1	
2	MEM	0	0	0	0.008	0.1	
3	100%	0	1	1	0.010	1.2	
Mean ± S.D.		0.3 ± 0.6			0.007 ± 0.003	0.5 ± 0.6	
Corrected value					Corrected value		
13	Test article	1	7	6	5.180	5.173	83.3
14	100%	0	15	15	5.828	5.821	102.0
15		1	11	10	4.724	4.717	80.5
Mean ± S.D.		10.0 ± 4.5			5.237 ± 0.555		88.6 ± 11.7

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 31-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	2-ethyl-1-hexanol [107-76-7]		
Batch No.	26812-019		
Concentration	100%	Treatment time	10 min
Code	A4	OP-KIT	
Sequence	Intern 8B		

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	2	2	0	0.006	0.1
2	MEM	1	1	0	0.012	0.2
3	100%	1	3	2	0.009	2.1
Mean ± S.D.		0.7 ± 1.2			0.009 ± 0.003	0.8 ± 1.1
					Corrected value	Corrected value
13	Test article	2	6	4	3.3	29.6
14	100%	1	7	6	5.3	38.1
15		2	7	5	4.3	24.2
Mean ± S.D.		4.3 ± 1.0			1.756 ± 0.430	30.6 ± 7.0

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 18-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	1-Hexanol [111-27-3]		
Batch No.	381949/1		
Concentration	100%	Treatment time	
Code	D2		
Sequence	12A		OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	NaCl 0.9%	1	1	0	0.006	0.1
3	100%	1	1	0	0.005	0.1
Mean ± S.D.		0.0 ± 0.0			0.005 ± 0.001	0.1 ± 0.0
					Corrected value	
7	Test article	0	17	17	17.0	72.4
8	100%	0	13	13	13.0	73.8
9		0	16	16	16.0	67.5
Mean ± S.D.		15.3 ± 2.1			3.728 ± 0.311	71.2 ± 3.3
					Corrected value	
		3.700	3.695			
		4.060	4.055			
		3.440	3.435			

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 20-Mar-00

Calculation of the in vitro eye irritation score for liquids

Test article	Acetone [67-64-1]	
Batch No.	39H3430	
Concentration	100%	Treatment time 10 min
Code	A5 (17)	
Sequence	Intern 8B	OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	2	2	0	0.006	0.1
2	MEM	1	1	0	0.012	0.2
3	100%	1	3	2	0.009	2.1
Mean ± S.D.		0.7 ± 1.2			0.009 ± 0.003	0.8 ± 1.1
					Corrected value	
16	Test article	1	36	35	34.3	59.5
17		1	42	41	40.3	83.5
18	100%	1	44	43	42.3	106.7
Mean ± S.D.		39.0 ± 4.2			2.951 ± 1.309	83.2 ± 23.6
					Corrected value	
					1.688	1.679
					2.888	2.879
					4.304	4.295

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 18-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	Cyclohexanol		
Batch No.	18285-049		
Concentration	100%	Treatment time	10 min
Code	B5	(18)	
Sequence	Intern 10A	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.004	0.1
2	MEM	0	0	0	0.008	0.1
3	100%	0	1	1	0.010	1.2
Mean ± S.D.		0.3 ± 0.6			0.007 ± 0.003	0.5 ± 0.6
					Corrected value	Corrected value
16	Test article	0	16	16	6.180	108.3
17		0	16	16	3.288	64.9
18	100%	0	14	14	5.680	98.8
Mean ± S.D.		15.0 ± 1.2			5.042 ± 1.546	90.7 ± 22.8

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A _t	B
	2	A _t	B
	3	A _t	B

Paraph

Eate 31-Jan-00

Calculation of the in vitro eye irritation score for liquids

Test article	Cetylpyridinium bromide (6%)		
Batch No.	105H0915		
Concentration	100%	Treatment time	
Code	C5		
Sequence	11A		OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.002	0.0
2	NaCl 0.9%	0	0	0	0.003	0.0
3	100%	1	1	0	0.001	0.0
Mean ± S.D.		0.0 ± 0.0			0.002 ± 0.001	0.0 ± 0.0
		Corrected value			Corrected value	
16	Test article	1	15	14	14.0	38.9
17		1	12	11	11.0	20.8
18	100%	0	10	10	10.0	20.7
Mean ± S.D.		11.7 ± 2.1			1.008 ± 0.563	26.8 ± 10.5

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	B
	2	A	B
	3	A	B

Paraph

Date 28-Jan-00

Benzalkonium chloride (10%)

Exp.	Opacity	Permeability	In Vitro Score
1	88.0	4.426	154.4
2	94.6	4.148	156.9
3	87.0	4.252	150.8
4	93.0	4.278	157.2
5	98.3	3.972	157.9
mean	92.2	4.2	155.4
SD	4.7	0.17	2.9

BCOP PREVALIDATION 1997

Calculation of in vitro eye irritation score for surfactants (10% w/w)

Test article	1 (BAK)		
Batch No.	76H2520		
Concentration	10 g/g%	Treatment time	10 min
Prevalidation phase	II		
Sequence	A		

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
16	NC	1	2	1	0.005	1.1
17	0.9 % NaCl	1	2	1	0.018	1.3
18	100%	1	2	1	0.002	1.0
Mean ± S.D.		1.0 ± 0.0			0.008 ± 0.009	1.1 ± 0.2
					Corrected value	
19	Test article	1	97	96	95.0	153.8
20		1	82	81	80.0	143.6
21		10g/g%	1	91	90	89.0
Mean ± S.D.		88.0 ± 7.5			4.426 ± 0.623	154.4 ± 11.1

NC: Negative control
PC: Positive control

REMARKS	Filter		OPACITY	
	1	A	75	B -75
	2	A	153	B -159
	3	A	236	B -253

Paraph

Date 13-Feb-97

BCOP PREVALIDATION 1997

Calculation of in vitro eye irritation score for surfactants (10% w/w)

Test article	I (BAK)		
Batch No.	76H2520		
Concentration	10 g/g%	Treatment time	10 min
Prevalidation phase	II		
Sequence	D		

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
16	NC	1	1	0	0.005	0.1
17	0.9 % NaCl	1	2	1	0.007	1.1
18	100%	0	1	1	0.004	1.1
Mean ± S.D.		0.7 ± 0.6			0.005 ± 0.002	0.8 ± 0.6

No.	Test article	Opacity at			Corrected value		Corrected value		In vitro score
		t0	t120	t120 - t0					
19	10g/g%	1	108	107	106.3	4.785	4.780	178.0	
20		0	92	92	91.3	3.464	3.459	143.2	
21		0	87	87	86.3	4.210	4.205	149.4	
Mean ± S.D.		♦ 94.6 ± 10.4			4.148 ± 0.662		156.9 ± 18.6		

NC: Negative control
 PC: Positive control

REMARKS	Filter		OPACITY	
	1	A	75	B -75
	2	A	153	B -158
	3	A	235	B -252

Paraph

Date

BCOP PREVALIDATION 1997

Calculation of in vitro eye irritation score for surfactants (10% w/w)

Test article	1 (BAK)		
Batch No.	76H2520		
Concentration	10 g/g%	Treatment time	10 min
Prevalidation phase	II		
Sequence	F		

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
10	NC	0	1	1	0.009	1.1
11	0.9 % NaCl	1	2	1	0.001	1.0
12	100%	0	1	1	0.018	1.3
	Mean ± S.D.			1.0 ± 0.0	0.009 ± 0.009	1.1 ± 0.2

No.	Test article	Opacity at			Corrected value		Corrected value	In vitro score
		t0	t120	t120 - t0				
19	10g/g%	1	88	87	86.0	4.333	4.324	150.9
20		1	82	81	80.0	4.255	4.246	143.7
21		1	97	96	95.0	4.196	4.187	157.8
	Mean ± S.D.				87.0 ± 7.5		4.252 ± 0.069	150.8 ± 7.1

NC: Negative control
 PC: Positive control

REMARKS	Filter	OPACITY	
	1	A	75 B -75
	2	A	152 B -158
	3	A	234 B -252

Paraph

Date 13-Mar-97

BCOP PREVALIDATION 1997

Calculation of in vitro eye irritation score for surfactants (10% w/w)

Test article	I (BAK)		
Batch No.	76H2520		
Concentration	10 g/g%	Treatment time	10 min
Prevalidation phase	II		
Sequence	G		

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
19	NC	3	3	0	0.008	0.1
20	0.9 % NaCl	0	0	0	0.038	0.6
21	100%	1	1	0	0.012	0.2
Mean ± S.D.		0.0 ± 0.0			0.019 ± 0.016	0.3 ± 0.3
					Corrected value	Corrected value
25	Test article	0	96	96	96.0	163.7
26		0	93	93	93.0	171.0
27	10g/g%	2	92	90	90.0	136.8
Mean ± S.D.		93.0 ± 3.0			4.278 ± 1.058	157.2 ± 18.0

NC: Negative control
 PC: Positive control

REMARKS	Filter		OPACITY	
	1	A	75	B -75
	2	A	152	B -158
	3	A	231	B -249

Paraph

Date 20-Mar-97

BCOP PREVALIDATION 1997

Calculation of in vitro eye irritation score for surfactants (10% w/w)

Test article	1 (BAK)		
Batch No.	76H2520		
Concentration	10 g/g%	Treatment time	10 min
Prevalidation phase	II		
Sequence	F H		

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
10	NC	1	1	0	0.013	0.2
11	0.9 % NaCl	1	4	3	0.013	3.2
12	100%	1	1	0	0.021	0.3
Mean ± S.D.		1.0 ± 1.7			0.016 ± 0.005	1.2 ± 1.7
					Corrected value	Corrected value
19	Test article	1	99	98	97.0	157.5
20		1	99	98	97.0	161.4
21	10g/g%	1	103	102	101.0	154.8
Mean ± S.D.		98.3 ± 2.3			3.972 ± 0.360	157.9 ± 3.3

NC: Negative control

PC: Positive control

REMARKS	Filter	OPACITY		
	1	A	75	B -75
	2	A	152	B -161
	3	A	236	B -253

Paraph

Date 21-Mar-97

• Compounds 1 → 20

• young animals (6-8 months)

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	3,3 Dimethylpentane [562-49-2]		
Batch No.	14602CN		
Concentration	99%	Treatment time	10 min
Code	A1		
Sequence	2005/ Intern3 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.008	0.1
2	MEM	0	0	0	0.026	0.4
3	100%	0	0	0	0.006	0.1
Mean ± S.D.		0.0 ± 0.0			0.013 ± 0.011	0.2 ± 0.2
		Corrected value			Corrected value	
4	Test article	0	0	0	0.046	0.5
5		0	0	0	0.028	0.2
6	100%	0	0	0	0.023	0.2
Mean ± S.D.		0.0 ± 0.0			0.019 ± 0.012	0.3 ± 0.2

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 158	B -160
	3	A 256	B -258

Paraph		Filter	
		0.1	1
		0.3	15
Date	07-Mar-05	0.6	50
		0.8	90
		1	145

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	3-methoxy-1,2-propanediol [623-39-2]		
Batch No.	A0155893001		
Concentration	100%	Treatment time	10 min
Code	B1		
Sequence	2005/ intern2 kalveren		OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.084	1.3
2	NaCl 0.9%	0	2	2	0.085	3.3
3	100%	1	1	0	0.036	0.5
Mean ± S.D.		0.7 ± 1.2			0.068 ± 0.028	1.7 ± 1.4
					Corrected value	Corrected value
4	Test article	0	0	0	0.090	-0.4
5		2	6	4	0.096	3.7
6	100%	0	0	0	0.070	-0.7
Mean ± S.D.		0.6 ± 2.3			0.017 ± 0.014	0.9 ± 2.5

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 155	B -161
	3	A 259	B -261

Paraph		Filter		
		0.1	1	
		0.3	16	
Date	01-Mar-05	0.6	51	
		0.8	91	
		1	143	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	polyethylene glycol 400 [25322-68-3]		
Batch No.	S23152-394		
Concentration	100%	Treatment time	10 min
Code	C1 (3)		
Sequence	2005/ intern 1 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.023	0.3
2	NaCl 0.9%	0	0	0	0.069	1.0
3	100%	0	0	0	0.044	0.7
Mean ± S.D.		0.0 ± 0.0			0.045 ± 0.023	0.7 ± 0.4
					Corrected value	Corrected value
4	Test article	0	0	0	0.102	0.9
5		0	0	0	0.178	2.0
6	100%	0	0	0	0.080	0.5
Mean ± S.D.		0.0 ± 0.0			0.075 ± 0.051	1.1 ± 0.8

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	75 B -75
	2	A	157 B -161
	3	A	260 B -259

Paraph	Filter	0.1	1
		0.3	16
Date	28-Feb-05	0.6	50
		0.8	88
		1	140

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	glycerol [56-81-5]		
Batch No.	13574HC		
Concentration	100%	Treatment time	10 min
Code	B2 (4)		
Sequence	2005/ intern2 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.084	1.3
2	NaCl 0.9%	0	2	2	0.085	3.3
3	100%	1	1	0	0.036	0.5
Mean ± S.D.		0.7 ± 1.2			0.068 ± 0.028	1.7 ± 1.4
					Corrected value	
7	Test article	0	0	0	0.008	-1.6
8	100%	0	0	0	0.009	-1.6
9		2	2	0	0.161	0.7
Mean ± S.D.		-0.7 ± 0.0			-0.009 ± 0.088	-0.8 ± 1.3

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 155	B -161
	3	A 259	B -261

Paraph		Filter		
		0.1	1	
		0.3	16	
Date	01-Mar-05	0.6	51	
		0.8	91	
		1	143	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Methyl cyclopentane [96-37-7]		
Batch No.	1097605		
Concentration	95%	Treatment time	10 min
Code	D5 (5)		
Sequence	2005/ Intern3 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.008	0.1
2	NaCl 0.9%	0	0	0	0.026	0.4
3	100%	0	0	0	0.006	0.1
Mean ± S.D.		0.0 ± 0.0			0.013 ± 0.011	0.2 ± 0.2
					Corrected value	Corrected value
16	Test article	0	2	2	2.0	8.5
17		1	2	1	1.0	3.5
18	100%	0	1	1	1.0	3.7
Mean ± S.D.		1.3 ± 0.6			0.260 ± 0.149	5.2 ± 2.8

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75 B	-75
	2	A 158 B	-160
	3	A 256 B	-258

Paraph		Filter			
		0.1	1		
		0.3	15		
Date	07-Mar-05	0.6	50		
		0.8	90		
		1	145		

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Tween 20 {9005-64-5}		
Batch No.	094K01761		
Concentration	100%	Treatment time	10 min
Code	C2	⑥	
Sequence	2005/Intern4 kalverogen	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.045	0.7
2	NaCl 0.9%	0	0	0	0.022	0.3
3	100%	0	0	0	0.012	0.2
Mean ± S.D.		0.0 ± 0.0			0.026 ± 0.017	0.4 ± 0.3
					Corrected value	Corrected value
19	Test article	0	0	0	0.028	0.002
20		0	0	0	0.021	-0.005
21	100%	0	0	0	0.013	-0.013
Mean ± S.D.		0.0 ± 0.0			-0.005 ± 0.008	-0.1 ± 0.1

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 156	B -158
	3	A 263	B -258

Paraph		Filter		
		0.1		0
		0.3		15
Date	14-Mar-05	0.6		50
		0.8		89
		1		141

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Methyl iso-butyl ketone (4 methyl-2-pentanone) [108-10-1]		
Batch No.	1127250		
Concentration	100%	Treatment time	10 min
Code	A2 (7)		
Sequence	2005/ internI kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.023	0.3
2	NaCl 0.9%	0	0	0	0.069	1.0
3	100%	0	0	0	0.044	0.7
Mean ± S.D.		0.0 ± 0.0			0.045 ± 0.023	0.7 ± 0.4
					Corrected value	Corrected value
7	Test article	0	3	3	0.714	13.0
8	100%	0	8	8	0.861	20.2
9		0	6	6	1.059	21.2
Mean ± S.D.		5.7 ± 2.5			0.833 ± 0.173	18.1 ± 4.5

NC: Negative Control

REMARKS	Filter	OPACITY
	1	A 75 B -75
	2	A 157 B -161
	3	A 260 B -259

Paraph		Filter		
		0.1	1	
		0.3	16	
Date	28-Feb-05	0.6	50	
		0.8	88	
		1	140	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Toluene [108-88-3]		
Batch No.	A0204558001		
Concentration	100%	Treatment time	10 min
Code	D4	⑧	
Sequence	2005/ Intern3 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.008	0.1
2	NaCl 0.9%	0	0	0	0.026	0.4
3	100%	0	0	0	0.006	0.1
Mean ± S.D.		0.0 ± 0.0			0.013 ± 0.011	0.2 ± 0.2
					Corrected value	Corrected value
13	Test article	0	2	2	2.0	25.1
14	100%	0	9	9	9.0	36.6
15		0	7	7	7.0	22.3
Mean ± S.D.		6.0 ± 3.6			1.464 ± 0.416	28.0 ± 7.6

NC: Negative Control

REMARKS	Filter	A	B	OPACITY
	1	A	B	75 -75
	2	A	B	158 -160
	3	A	B	256 -258

Paraph		Filter		
		0.1	1	
		0.3	15	
Date	07-Mar-05	0.6	50	
		0.8	90	
		1	145	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	methyl amyl ketone (2 heptanone) [110-43-0]		
Batch No.	13622JC		
Concentration	100%	Treatment time	10 min
Code	A3 (9)		
Sequence	2005/ intern 1 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score		
		t0	t120	t120 - t0				
1	NC	0	0	0	0.023	0.3		
2	NaCl 0.9%	0	0	0	0.069	1.0		
3	100%	0	0	0	0.044	0.7		
Mean ± S.D.		0.0 ± 0.0			0.045 ± 0.023	0.7 ± 0.4		
		Corrected value				Corrected value		
10	Test article	0	5	5	5.0	1.065	1.020	20.3
11	100%	0	5	5	5.0	1.030	0.985	19.8
12		2	4	2	2.0	0.995	0.950	16.3
Mean ± S.D.		4.0 ± 1.7				0.985 ± 0.035		18.8 ± 2.2

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 157	B -161
	3	A 260	B -259

Paraph		Filter		
		0.1	1	
		0.3	16	
Date	28-Feb-05	0.6	50	
		0.8	88	
		1	140	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	2-methyl-1-pentanol [105-30-6]		
Batch No.	451942/1		
Concentration	100%	Treatment time	10 min
Code	B3	10	
Sequence	2005/ intern 2 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score		
		t0	t120	t120 - t0				
1	NC	0	0	0	0.084	1.3		
2	NaCl 0.9%	0	2	2	0.085	3.3		
3	100%	1	1	0	0.036	0.5		
Mean ± S.D.		0.7 ± 1.2			0.068 ± 0.028	1.7 ± 1.4		
		Corrected value				Corrected value		
10	Test article	0	11	11	10.3	1.801	1.733	36.3
11		0	8	8	7.3	2.436	2.368	42.8
12	100%	0	9	9	8.3	1.773	1.705	33.9
Mean ± S.D.		8.6 ± 1.5				1.935 ± 0.375		37.7 ± 4.6

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	75 B -75
	2	A	155 B -161
	3	A	259 B -261

Paraph		Filter			
		0.1	1		
		0.3	16		
Date	01-Mar-05	0.6	51		
		0.8	91		
		1	143		

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Ethanol [64-17-5]		
Batch No.	K33957583 448		
Concentration	100%	Treatment time	10 min
Code	D1		
Sequence	2005/ Intern3 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.008	0.1
2	NaCl0.9%	0	0	0	0.026	0.4
3	100%	0	0	0	0.006	0.1
Mean ± S.D.		0.0 ± 0.0			0.013 ± 0.011	0.2 ± 0.2
					Corrected value	Corrected value
7	Test article	0	18	18	18.0	52.4
8	100%	0	16	16	16.0	41.3
9		0	15	15	15.0	37.8
Mean ± S.D.		16.3 ± 1.5			1.834 ± 0.408	43.8 ± 7.6

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 158	B -160
	3	A 256	B -258

Paraph	Filter
	0.1 1
	0.3 15
Date 07-Mar-05	0.6 50
	0.8 90
	1 145

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Sodium hydroxide 1% [1310-73-2]		
Batch No.	014K0006	Treatment time	10 min
Concentration	1%		
Code	D3		
Sequence	2005/Intern4 kalverogen		OP-KIT

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.045	0.7
2	NaCl 0.9%	0	0	0	0.022	0.3
3	100%	0	0	0	0.012	0.2
Mean ± S.D.		0.0 ± 0.0			0.026 ± 0.017	0.4 ± 0.3
Corrected value					Corrected value	
16	Test article	0	139	139	139.0	206.7
17		0	145	145	145.0	183.6
18	100%	0	123	123	123.0	185.1
Mean ± S.D.		135.7 ± 11.4			3.742 ± 1.029	191.8 ± 12.9

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 156	B -158
	3	A 263	B -258

Paraph	Filter	
	0.1	0
	0.3	15
Date	0.6	50
	0.8	89
	1	141

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Triton X-100 (5%) [9002-93-1]		
Batch No.	A019437801		
Concentration	5%	Treatment time	10 min
Code	C4		
Sequence	2005/Intern ⁴ kalverogen		OP-KIT

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.045	0.7
2	NaCl 0.9%	0	0	0	0.022	0.3
3	100%	0	0	0	0.012	0.2
Mean ± S.D.		0.0 ± 0.0			0.026 ± 0.017	0.4 ± 0.3
Corrected value					Corrected value	
10	Test article	0	5	5	5.0	69.1
11		0	5	5	5.0	49.7
12	100%	0	4	4	4.0	61.5
Mean ± S.D.		4.7 ± 0.6			3.695 ± 0.659	60.1 ± 9.8

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 156	B -158
	3	A 263	B -258

Paraph		Filter			
			0.1	0	
			0.3	15	
Date	14-Mar-05		0.6	50	
			0.8	89	
			1	141	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	α-octanol [111-87-5]		
Batch No.	S02961-454		
Concentration	100%	Treatment time	10 min
Code	B4	(14)	
Sequence	2005/ intern2 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.084	1.3
2	NaCl 0.9%	0	2	2	0.085	3.3
3	100%	1	1	0	0.036	0.5
Mean ± S.D.		0.7 ± 1.2			0.068 ± 0.028	1.7 ± 1.4
					Corrected value	Corrected value
13	Test article	1	7	6	5.3	23.2
14		0	18	18	17.3	44.8
15	100%	0	9	9	8.3	31.8
Mean ± S.D.		10.3 ± 6.2			1.533 ± 0.322	33.3 ± 10.9

NC: Negative Control

REMARKS	Filter	A	B	OPACITY
	1	A	75	B -75
	2	A	155	B -161
	3	A	259	B -261

Paraph		Filter			
		0.1	1		
		0.3	16		
Date	01-Mar-05	0.6	51		
		0.8	91		
		1	143		

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	2-ethyl-1-hexanol [107-76-7]		
Batch No.	S01263-011	Treatment time	10 min
Concentration	100%	Code	A4 (15)
Sequence	2005/ intern I kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.023	0.3
2	NaCl 0.9%	0	0	0	0.069	1.0
3	100%	0	0	0	0.044	0.7
Mean ± S.D.		0.0 ± 0.0			0.045 ± 0.023	0.7 ± 0.4
					Corrected value	Corrected value
13	Test article	0	4	4	4.0	11.2
14		0	0	0	0.0	5.3
15	100%	0	3	3	3.0	29.4
Mean ± S.D.		2.3 ± 2.1			0.864 ± 0.777	15.3 ± 12.6

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A	75 B -75
	2	A	157 B -161
	3	A	260 B -259

Paraph		Filter			
		0.1	1		
		0.3	16		
Date	28-Feb-05	0.6	50		
		0.8	88		
		1	140		

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	1-Hexanol [111-27-3]		
Batch No.	A020123401		
Concentration	98%	Treatment time	10 min
Code	D2	16	
Sequence	2005/ Intern3 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.008	0.1
2	NaCl 0.9%	0	0	0	0.026	0.4
3	100%	0	0	0	0.006	0.1
Mean ± S.D.		0.0 ± 0.0			0.013 ± 0.011	0.2 ± 0.2
					Corrected value	Corrected value
10	Test article	0	16	16	3.624	70.2
11	100%	0	13	13	3.232	61.3
12		0	13	13	4.028	73.2
Mean ± S.D.		14.0 ± 1.7			3.615 ± 0.398	68.2 ± 6.2

NC: Negative Control

REMARKS	Filter	A	B	OPACITY
	1	A	B	75 -75
	2	A	B	158 -160
	3	A	B	256 -258

Paraph

Date 07-Mar-05

Filter		
0.1	1	
0.3	15	
0.6	50	
0.8	90	
1	145	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Acetone [67-64-1]		
Batch No.	442942/1		
Concentration	100%	Treatment time	10 min
Code	A5	17	
Sequence	2005/ intern 1 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.023	0.3
2		0	0	0	0.069	1.0
3	100%	0	0	0	0.044	0.7
Mean ± S.D.		0.0 ± 0.0			0.045 ± 0.023	0.7 ± 0.4
					Corrected value	Corrected value
16	Test article	0	101	101	101.0	142.7
17		0	92	92	92.0	128.1
18	100%	0	81	81	81.0	131.7
Mean ± S.D.		91.3 ± 10.0			2.856 ± 0.493	134.2 ± 7.6

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 157	B -161
	3	A 260	B -259

Paraph		Filter		
		0.1	1	
		0.3	16	
Date	28-Feb-05	0.6	50	
		0.8	88	
		1	140	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	cyclohexanol		
Batch No.	S05238-044		
Concentration	100%	Treatment time	10 min
Code	B5	(18)	
Sequence	2005/ intern2 kalveren	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.084	1.3
2	NaCl 0.9%	0	2	2	0.085	3.3
3	100%	1	1	0	0.036	0.5
Mean ± S.D.		0.7 ± 1.2			0.068 ± 0.028	1.7 ± 1.4
					Corrected value	Corrected value
16	Test article	1	13	12	11.3	36.8
17		0	12	12	11.3	38.7
18	100%	0	13	13	12.3	55.4
Mean ± S.D.		11.6 ± 0.6			2.132 ± 0.644	43.6 ± 10.2

NC: Negative Control

REMARKS	Filter	OPACITY	
	1	A 75	B -75
	2	A 155	B -161
	3	A 259	B -261

Paraph		Filter		
		0.1	1	
		0.3	16	
Date	01-Mar-05	0.6	51	
		0.8	91	
		1	143	

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Cetylpyridinium bromide (6%) [140-72-7]		
Batch No.	038H2509		
Concentration	6%	Treatment time	10 min
Code	C5		
Sequence	2005/Intern4 kalverogen	OP-KIT	

No.	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.045	0.7
2	NaCl 0.9%	0	0	0	0.022	0.3
3	100%	0	0	0	0.012	0.2
Mean ± S.D.		0.0 ± 0.0			0.026 ± 0.017	0.4 ± 0.3
					Corrected value	
13	Test article	0	20	20	20.0	53.4
14		0	13	13	13.0	40.8
15	100%	0	12	12	12.0	25.4
Mean ± S.D.		15.0 ± 4.4			1.657 ± 0.688	39.9 ± 14.0

NC: Negative Control

REMARKS	Filter	OPACITY	
		A	B
	1	75	-75
	2	156	-158
	3	263	-258

Paraph	Filter	0.1	0
		0.3	15
Date	14-Mar-05	0.6	50
		0.8	89
		1	141

RDF/BCO/18

VALIDATION

Calculation of the in vitro eye irritation score for liquids

Test article	Benzalkoniumchloride [8001-54-5]		
Batch No.	033K2544		
Concentration	10g/g%	Treatment time	10 min
Code	C3 20		
Sequence	2005/Intern4 kalverogen	OP-KIT	

No. Cornea	Treatment	Opacity at			Permeability	In vitro score
		t0	t120	t120 - t0		
1	NC	0	0	0	0.045	0.7
2	NaCl 0.9%	0	0	0	0.022	0.3
3	100%	0	0	0	0.012	0.2
Mean ± S.D.		0.0 ± 0.0			0.026 ± 0.017	0.4 ± 0.3
					Corrected value	
7	Test article	0	115	115	115.0	174.9
8		0	95	95	95.0	152.5
9	100%	0	107	107	107.0	172.0
Mean ± S.D.		105.7 ± 10.1			4.050 ± 0.255	166.5 ± 12.2

NC: Negative Control

REMARKS	Filter	OPACITY	
		A	B
	1	75	-75
	2	156	-158
	3	263	-258

Paraph		Filter	0.1	0
			0.3	15
Date	14-Mar-05		0.6	50
			0.8	89
			1	141

RDF/BCO/18