

Annex II-4

**Summary LLNA, Human, and Guinea Pig Data Used in the Regression and
Classification Rate Analyses**

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Chemical Name	LLNA Results			Human Results		Guinea Pig Results	
	N	GM ¹ EC3 (%)	GM ¹ EC3 (µg/cm ²)	N	GM ¹ DSA ₀₅ (µg/cm ²)	N	Overall ² GHS Category
Abietic acid	5	12	2909	NA	NA	6	Cat 1B
Acetyl isovaleryl	1	26	6450	2	3258	NA	NA
AE F016382 00 TK71 A101	1	NC	NC	NA	NA	1	Unclassified
alpha-Amylcinnamyl alcohol	2	NC	NC	1	12308	NA	NA
alpha-Methyl cinnamic aldehyde	1	4.5	1125	2	-	1	Cat 1B
Aluminum chloride	1	NC	NC	NA	-	1	Unclassified
p-Aminobenzoic acid	1	NC	NC	1	-	2	Cat 1B
3-Aminophenol	2	2.4	600	NA	NA	1	Cat 1A
Amylcinnamic aldehyde	5	11	2699	1	-	2	Cat 1B
Aniline	5	33	8129	1	2463	2	Cat 1B
Anisyl alcohol	1	5.9	1475	1	-	NA	NA
A SC600	1	NC	NC	NA	NA	1	Unclassified
Atrazine	2	36	8989	NA	NA	1	Unclassified
Basil oil	1	6.2	1550	1	-	NA	NA
Benzalkonium chloride	1	0.07	17	2	-	1	Unclassified
Benzocaine	7	7.8	1948	4	10140	7	Cat 1B
Benzoic acid	1	NC	NC	1	-	2	Unclassified
Benzoisothiazolione	4	7.79	1948	1	50	NA	NA
Benzoquinone	1	0.01	2.475	NA	NA	1	Cat 1A
Benzoyl peroxide	6	0.07	17	5	1283	1	Cat 1B
Benzyl alcohol	1	NC	NC	1	48670	1	Unclassified
Benzylbenzoate	1	17	4250	2	-	NA	NA
Benzyl cinnamate	1	18	4600	2	-	1	Cat 1B
Benzylidene acetone	1	3.70	925	2	299	NA	NA
Benzyl salicylate	1	2.9	725	2	-	1	Unclassified
Beryllium sulfate	1	0.68	170	1	11	NA	NA
Bourgeonal	1	4.3	1075	1	1541	NA	NA

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Butanol	1	NC	NC	NA	-	NA	NA
Butyl acrylate	1	11	2750	NA	NA	1	Cat 1B
Butyl glycidyl ether	1	30.9	7725	1	437	1	Cat 1B
C.I. Reactive Red 231	1	0.6	150	NA	NA	3	Cat 1B
C.I. Reactive Yellow 174	1	0.3	75	NA	NA	1	Unclassified
Carvone	4	10	2514	1	19284	NA	NA
Chloramine T	1	0.40	100	NA	NA	2	Cat 1A
4-Chloroaniline	2	NC	NC	NA	NA	1	Cat 1B
(Chloro)methylisothiazolinone	13	0.01	2.8	5	5.0	16	Cat 1A
Chorpromazine	2	5.8	1455	1	1149	NA	NA
Cinnamic aldehyde	27	1.0	254	5	382	4	Cat 1A
Cinnamyl alcohol	2	20	5007	6	3002	2	Cat 1B
Cinnamyl nitrile	1	NC	NC	1	1828	NA	NA
Citral	16	5.0	1246	5	915	1	Cat 1B
Citronella oil	1	NC	NC	1	-	NA	NA
dl-Citronellol	1	44	10875	1	1429	NA	NA
Clove oils	3	7.1	1775	3	-	NA	NA
Cobalt (II) salts	2	0.57	141	2	279	1	Cat 1A
Copper (II) chloride	1	0.40	100	NA	-	NA	NA
Coumarin	2	30	7395	2	14523	NA	NA
Cyclamen aldehyde	1	22	5575	1	-	NA	NA
Damascone	2	1.2	307	1	-	NA	NA
t-alpha Damascone	1	3.3	825	1	-	NA	NA
trans beta Damascone	1	2.4	600	2	-	NA	NA
delta Damascone	3	3.51	877	1	193	NA	NA
D EC25	1	NC	NC	NA	NA	1	Unclassified
D EW 15	1	NC	NC	NA	NA	1	Unclassified

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<i>d</i> -Limonene	6	32	32	2	-	1	Cat 1B
Dextran	1	NC	NC	NA	NA	1	Unclassified
Dibromodicyanobutane	6	1.9	480	NA	NA	2	Unclassified
Diethyl phthalate	1	NC	NC	1	-	1	Unclassified
Diethylenetriamine	1	3.3	825	1	411	NA	NA
Diethylmaleate	4	3.27	818	2	400	NA	NA
Dihydrocoumarin	2	4.3	1067	2	759	1	Cat 1B
1,4-Dihydroquinone	11	0.12	30	NA	NA	3	Cat 1B
5,5-Dimethyl-3-methylenedihydro-2(3H)-furanone	1	1.8	450	NA	NA	1	Unclassified
Dimethyl sulfoxide	1	72	18000	1	-	1	Unclassified
2,4-Dinitrochlorobenzene	24	0.04	11	2	3.4	13	Cat 1A
Dinocap EC	5	1.2	311	NA	NA	1	Cat 1B
Ethyl acrylate	2	32	8125	3	818	1	Unclassified
Ethyl vanillin	1	NC	NC	NA	-	NA	NA
Ethylene glycol dimethacrylate	3	33	8237	NA	NA	1	Unclassified
Ethylenediamine	2	2.7	684	1	732	5	Cat 1A
Eugenol	23	11	2743	1	5926	5	Cat 1A
EXP 10810 A	1	2.1	527	NA	NA	2	Cat 1A
EXP 11120 A	1	65	16223	NA	NA	1	Unclassified
F & Fo WG 50 + 25	1	0.003	0.78	NA	NA	3	Unclassified
FAR01042-00	1	NC	NC	NA	NA	1	Unclassified
FAR01060-00	1	88	22115	NA	NA	1	Unclassified
Farnesol	2	4.7	1187	1	2593	NA	NA
Fatty acid glutamate	1	75	18750	NA	NA	1	Unclassified
Fatty alcohol #1	1	7.6	1899	NA	NA	1	Unclassified
Fatty alcohol #2	1	8.6	2140	NA	NA	1	Unclassified
Formaldehyde	21	1.4	344	2	191	16	Cat 1B

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Fumaric acid	1	NC	NC	NA	NA	1	Unclassified
Fx + Me EW 69	1	25	6306	NA	NA	1	Unclassified
Geraniol	7	18	4474	2	1265	1	Cat 1B
Geranium oil	1	NC	NC	1	-	NA	NA
Glutaraldehyde	8	0.16	41	1	1073	1	Cat 1B
Glycerol	1	NC	NC	1	-	2	Unclassified
Glyceryl thioglycolate	1	4.7	1165	NA	NA	1	Unclassified
Glyoxal	3	0.75	187	1	345	NA	NA
Gold chloride	1	0.48	120	1	98.5	NA	NA
Hexane	1	NC	NC	1	-	NA	NA
Hexyl cinnamic aldehyde	27	8.9	2233	1	-	3	Cat 1A
2-Hexylidene cyclopentanone	1	2.4	600	1	255	NA	NA
Hexyl salicylate	1	0.18	45	2	-	NA	NA
Hydrocortisone	1	NC	NC	1	-	NA	NA
4-Hydroxybenzoic acid	4	NC	NC	NA	NA	2	Cat 1B
Hydroxycitronellal	13	23	5764	8	5237	8	Cat 1B
2-Hydroxyethyl acrylate	3	2.4	597	NA	NA	1	Cat 1A
2-Hydroxypropyl methacrylate	4	NC	NC	NA	NA	1	Unclassified
Imidazolidinyl urea	1	24	6000	1	3846	1	Cat 1B
Isocyclemone E	1	25	6285	1	-	NA	NA
Isocyclocitral	1	7.4	1838	2	-	NA	NA
Isocyclogeraniol	1	NC	NC	1	6250	NA	NA
Isoeugenol	66	1.4	342	2.0	1016	2	Cat 1A
Isomethylionone	1	21.8	5450	1	-	NA	NA
Isopropanol	1	NC	NC	1	-	1	Unclassified
Isopropyl myristate	1	44	11000	1	-	NA	NA
Jasmine absolute (grandiflorum)	1	5.9	1475	1	967	NA	NA

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Jasmine absolute (sambac)	1	36	9100	1	-	NA	NA
Kanamycin	1	NC	NC	1	1874	NA	NA
Lead acetate	1	NC	NC	NA	-	NA	NA
Lemongrass oil	1	6.5	1625	1	-	NA	NA
Lilial	6	8.8	2194	1	335545	NA	NA
Linalool	1	55	13750	3	-	NA	NA
Linoleic acid	1	14	3523	NA	NA	1	Unclassified
Linolenic acid	1	9.9	2463	NA	NA	1	Unclassified
Litsea cubeba oil	1	8.4	2100	1	-	NA	NA
Lyrar HMPCC	2	17	4262	2	-	NA	NA
Majantal	1	NC	NC	1	-	NA	NA
Maleic acid	1	7.0	1743	NA	NA	1	Unclassified
Manganese chloride	1	NC	NC	NA	-	NA	NA
Menthadiene-7-methyl formate	2	NC	NC	1	3406	NA	NA
2-Mercaptobenzothiazole	6	2.6	645	2	1930	4	Cat 1A
Mercuric (II) chloride	1	0.39	98	2	225	1	Cat 1A
4-Methoxyacetophenone	1	NC	NC	1	-	NA	NA
Methoxy dicyclopentadiene carboxaldehyde	1	NC	NC	1	-	NA	NA
2-Methoxy-4-methylphenol	1	5.8	1450	1	-	NA	NA
4-Methylaminophenol sulfate	1	0.80	200	NA	NA	1	Cat 1A
Methylanisylidene acetone	1	9.30	2325	1	412	NA	NA
6-Methylcoumarin	2	NC	NC	1	-	NA	NA
Methyl dodecanesulfonate	1	0.39	98	NA	NA	1	Cat 1A
Methylhexanedione	1	26	6500	2	3595	NA	NA
Methylhydrocinnamal	4	18	4417	1	2378	NA	NA
Methylisothiazolinone	2	0.87	218	2	223.5	NA	NA
Methyl methacrylate	2	73	18371	NA	NA	8	Cat 1B

Chemical Name	LLNA Results			Human Results		Guinea Pig Results	
	N	GM ¹ EC3 (%)	GM ¹ EC3 (µg/cm ²)	N	GM ¹ DSA ₀₅ (µg/cm ²)	N	Overall ² GHS Category
Methyl 2-nonynoate	1	2.5	625	1	79	1	Cat 1B
Methyl 2-octynoate	1	0.50	125	1	388	1	Cat 1B
Methyl salicylate	2	17	4239	1	-	2	Unclassified
NAVY 14 08 723	1	0.49	123	NA	NA	3	Cat 1B
Neomycin sulfate	1	NC	NC	5	3466	1	Cat 1B
Nickel (II) salts	8	NC	NC	3	27	10	Cat 1B
Oakmoss	1	3.8	950	1	3374	NA	NA
Octanoic acid	1	NC	NC	1	-	NA	NA
1-Octen-3-yl acetate	1	NC	NC	1	6712	NA	NA
Octinol	1	4.7	1187	NA	NA	1	Unclassified
Oleic acid	1	10	2622	NA	NA	1	Unclassified
Oxalic acid	2	4	958	NA	NA	1	Unclassified
Oxazolone	8	0.002	0.59	NA	NA	1	Cat 1A
Oxyfluorfen EC	3	22	5471	NA	NA	1	Unclassified
Palmarosa oil	1	9.6	2400	1	-	NA	NA
Penicillin G	11	17	4338	4	634	4	Cat 1A
Pentachlorophenol	1	20	5000	1	2155	NA	NA
Pentaerythritol triacrylate	1	NC	NC	1	576	4	Cat 1A
Perillaldehyde	3	7.9	1987	1	1484	NA	NA
Peru balsam absolute	1	2.5	625	1	862	NA	NA
Phenyl benzoate	4	9.5	2366	1	52489	NA	NA
Phenylacetaldehyde	3	4.99	1247	5	329	NA	NA
4-Phenylenediamine	17	0.12	29.7	4	30	5	Cat 1A
Phenylpropionaldehyde	1	6.3	1575	1	692	NA	NA
Phthalic anhydride	1	0.36	90	NA	NA	3	Cat 1A
Potassium dichromate	19	0.12	30	3	106	5	Cat 1A
Produkt P-4G	1	NC	NC	NA	NA	1	Cat 1B

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	N	GM ¹ EC3 (%)	GM ¹ EC3 (µg/cm ²)	N	GM ¹ DSA ₀₅ (µg/cm ²)	N	Overall ² GHS Category
Propyl gallate	1	0.32	80	NA	NA	1	Cat 1A
Propylene glycol	1	NC	NC	2	-	1	Unclassified
Propylidene phthalate	1	3.7	925	1	1150	NA	NA
Propylparaben	1	NC	NC	NA	NA	1	Unclassified
Pyridine	1	72	17975	1	41051	NA	NA
Quinoxifen SC	1	NC	NC	NA	NA	1	Unclassified
Quinoxifen/cyproconazole	6	21	5223	NA	NA	1	Cat 1B
Resorcinol	2	5.9	1481	1	-	NA	NA
Salicylic acid	1	12	3056	1	-	1	Unclassified
Sodium lauryl sulfate	10	4.0	1001	1	-	2	Unclassified
Spearmint oil	1	8.2	2050	1	-	NA	NA
Squalene	1	7.9	1975	NA	NA	1	Unclassified
Streptomycin	4	NC	NC	6	245	1	Cat 1B
Succinic acid	1	NC	NC	NA	NA	1	Unclassified
Sulfanilamide	1	NC	NC	1	4310	1	Unclassified
Sulfanilic acid	4	NC	NC	NA	-	2	Cat 1A
Tartaric acid	1	NC	NC	NA	-	1	Unclassified
Tea leaf absolute	1	NC	NC	1	-	NA	NA
Tetrachlorosalicylanilide	2	0.04	8.8	4	27	2	Cat 1A
Tetramethylthiuramdisulphide	2	5.6	1396	2	4544	NA	NA
Thioglycerol	1	3.6	895	3	1232	2	Cat 1A
Toluene-2,4-diisocyanate	1	0.11	27.5	NA	NA	2	Cat 1A
trans-2-Hexenal	2	3.78	945	1	49	NA	NA
Treemoss	1	NC	NC	1	3423	NA	NA
Trifluralin EC	5	9.6	2412	NA	NA	1	Unclassified
Trimellitic anhydride	1	0.22	55	NA	NA	2	Cat 1A
Tween 80	1	NC	NC	1	-	2	Unclassified

Chemical Name	LLNA Results			Human Results		Guinea Pig Results	
	N	GM ¹ EC3 (%)	GM ¹ EC3 (µg/cm ²)	N	GM ¹ DSA ₀₅ (µg/cm ²)	N	Overall ² GHS Category
Undec-10-enal	1	6.8	1700	NA	NA	1	Unclassified
Undecylenic acid	1	19	4844	NA	NA	1	Cat 1B
Vanillin	1	NC	NC	NA	NA	3	Cat 1B
Xylene	1	96	23950	1	-	NA	NA
Yellow E-JD 3442	1	NC	NC	NA	NA	3	Unclassified
Ylang ylang	1	6.8	1700	1	16150	NA	NA
Zinc sulfate	1	NC	NC	NA	-	NA	NA

Abbreviations: Cat = subcategory of the GHS classification for skin sensitizers; DSA₀₅ = induction dose per skin area, in µg/cm², in a human repeat-insult patch test or human maximization test that produces a positive response in 5% of the tested population; EC3 = estimated concentration of a substance expected to produce a stimulation index of 3, which is the threshold value for a substance to be considered a sensitizer in the LLNA; GHS = Globally Harmonized System of Classification and Labelling of Chemicals (UN 2009); GM = geometric mean; LLNA = murine local lymph node assay; N = number of studies; NA = not available; NC = not calculated.

¹ For substances with >1 study.

² Based on the most prevalent results for substances with multiple studies.