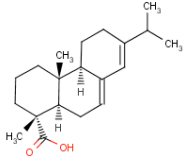
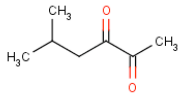

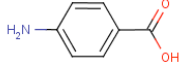
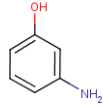
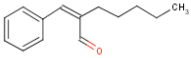
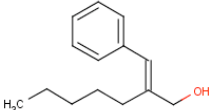
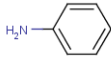


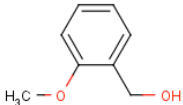
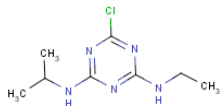
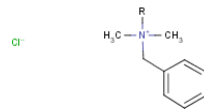
Annex III

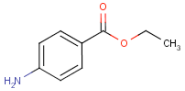
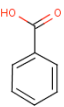
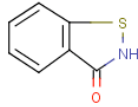
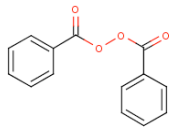
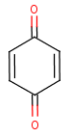
Physicochemical Properties of Substances Evaluated

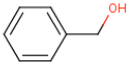
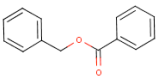
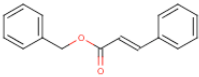
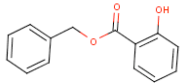
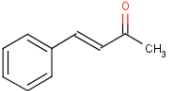
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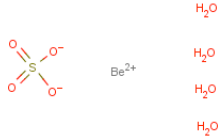
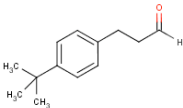
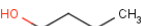
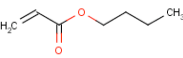
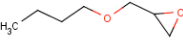
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Abietic acid	Sylvic acid	514-10-3	302.46	4.61	Solid	NA	Hydrocarbons, cyclic; Polycyclic compounds	Manufacturing	
Acetyl isovaleryl	5-Methyl-2,3-hexanedione	13706-86-0	128.17	1.42	Liquid	NA	NA	Fragrance agent	
AE F016382 00 TK71 A101	NA	NA	NA	NA	NA	NA	Formulations	Pesticide	NA
Aluminum chloride	Aluminum chloride; anhydrous; Aluminum trichloride	7446-70-0	133.34	NA	Solid	NA	Aluminum compounds; Inorganic chemicals	Intermediate in chemical synthesis; Household products; Manufacturing	
p-Aminobenzoic acid	4-Aminobenzoic acid; PABA	150-13-0	137.14	0.68	Solid	NA	Carboxylic acids	Cosmetics; Food additive; Pharmaceutical	

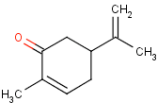
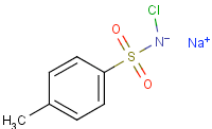
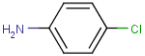
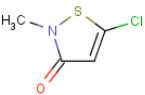
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
3-Aminophenol	m-Aminophenol; 3-Hydroxyaniline	591-27-5	109.13	1.17	Solid	Minimal	Amines; Phenols	Cosmetics; Pharmaceuticals	
Amylcinnamic aldehyde	Amyl cinnamic aldehyde; Amylcinnamal; 2-Benzylideneheptanal; 2-Pentyl cinnamaldehyde	122-40-7	202.30	4.33	Liquid	Minimal	Aldehydes	Food additive	
alpha-Amylcinnamyl alcohol	Amyl cinnamic alcohol; Amylcinnamol; 2-Pentylcinnamic alcohol; 2-Amyl-3-phenyl-2-propen-1-ol; 2-Benzylidene heptanol; Buxinol	101-85-9	204.31	4.35	Liquid	NA	Alcohols	Food additive	
Aniline	Benzenamine	62-53-3	93.13	1.56	Liquid	NA	Amines	Food additive; Manufacturing; Personal care products; Pesticides; Pharmaceuticals	

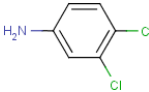
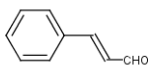
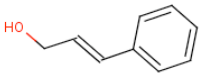
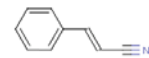
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Anisyl alcohol	Benzenemethanol, ar-methoxy-	1331-81-3	138.17	1.16	NA	NA	Ethers; Phenols	Food additive; Fragrance agent; Manufacturing	
A SC600	NA	NA	NA	NA	NA	NA	Formulations	Pesticides	NA
Atrazine	Atrazine SC; 1-Chloro-3-ethylamino-5-isopropylamino-2,4,6-triazine	1912-24-9	215.69	2.82	Solid	NA	Formulations; Heterocyclic compounds	Herbicide	
Basil oil	Ocimum basilicum herb oil	8015-73-4	NA	NA	Liquid	NA	Lipids; Natural complex substances	Food additive; Fragrance agent	NA
Benzalkonium chloride	Alkyl dimethylbenzyl ammonium chloride	8001-54-5	NA	NA	Solid	NA	Amines; Onium compounds	Cosmetics; Manufacturing; Household products; Pharmaceuticals	

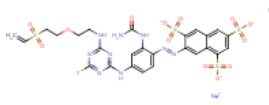
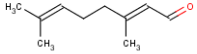
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Benzocaine	Benzoic acid, 4-amino-, ethyl ester; Ethyl 4-aminobenzoate; Ethyl p-aminobenzoate	94-09-7	165.19	1.52	Solid	NA	Carboxylic acids	Pharmaceuticals	
Benzoic acid	Benzenecarboxylic acid; Benzeneformic acid; Benzenemethanoic acid; Benzoate	65-85-0	212.20	1.87	Solid	NA	Carboxylic acids	Food additive; Manufacturing; Pharmaceuticals	
Benzoisothiazolinone	1,2-Benzisothiazol-3(2H)-one; 1,2-Benzisothiazolin-3-one	2634-33-5	151.19	0.64	Solid	High	Sulfur compounds; Heterocyclic compounds	Biocide; Disinfectant; Manufacturing	
Benzoyl peroxide	Dibenzoyl peroxide	94-36-0	242.23	3.46	Solid	High	Carboxylic acids	Manufacturing; Household products	
Benzoquinone	p-Quinone; 1,4-Cyclohexadienedione	106-51-4	108.10	1.17	Solid	High	Quinones	Manufacturing; Pesticides; Pharmaceuticals	

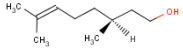
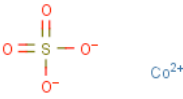
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K_{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Benzyl alcohol	Benzenemethanol	100-51-6	108.14	1.1	Liquid	NA	Hydrocarbons, cyclic	Food additive; Fragrance agent; Manufacturing; Pharmaceuticals	
Benzyl benzoate	Benylate; Benzoic acid benzyl ester	120-51-4	212.25	3.14	Liquid	Minimal	Carboxylic acids	Food additive; Fragrance agent; Manufacturing; Pharmaceuticals	
Benzyl cinnamate	2-Propenoic acid, 3-phenyl-phenylmethyl ester; Phenylmethyl 3-phenyl-2-propenoate; Cinnamein	103-41-3	238.29	4.06	Solid	NA	Esters	Food additive; Fragrance agent	
Benzyl salicylate	Phenylmethyl-2-hydroxybenzoate	118-58-1	228.25	4.31	Liquid	NA	Carboxylic acids	Fragrance agent	
Benzylidene acetone	4-Phenyl-3-buten-2-one; Methyl styryl ketone	122-57-6	146.19	2.54	Solid	High	Ketones	Food additive; Manufacturing	

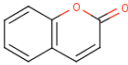
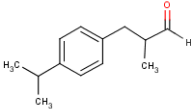
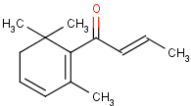
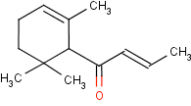
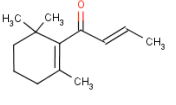
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Beryllium sulfate	Beryllium sulfate tetrahydrate	7787-56-6	177.14	NA	Solid	NA	Inorganic chemicals; Metals	Manufacturing	
Bourgenol	p-t-Butyl-dihydrocinnamaldehyde	18127-01-0	190.28	3.34	Liquid	NA	Aldehydes	Fragrance agent	
1-Butanol	NA	71-36-3	74.12	1.06	Liquid	Minimal	Alcohols; Lipids	Intermediate in chemical synthesis; Household products; Manufacturing; Pharmaceuticals	
Butyl acrylate	n-Butyl acrylate; n-Butyl propenoate; 2-Propenoic acid; Butyl ester	141-32-2	128.17	2.20	Liquid	NA	Carboxylic acids	Intermediate in chemical synthesis; Manufacturing	
Butyl glycidyl ether	NA	2426-08-6	130.19	1.42	Liquid	NA	Ethers	Intermediate in chemical synthesis; Manufacturing	

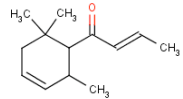
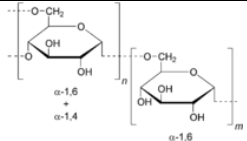
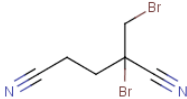
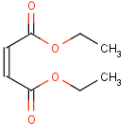
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Carvone	2-Cyclohexen-1-one; 2-Methyl-5-(1-methylethenyl)-; p-Mentha-6,8-dien-2-one	99-49-0; 2244-16-8; 6485-40-2	150.22	3.07	Liquid	NA	Hydrocarbons, other	Food additive; Fragrance agent	
Chloramine T	(N-Chloro-p-toluenesulfonamido) sodium	127-65-1	227.65	0.84	Solid	NA	Amides; Hydrocarbons, cyclic; Sulfur compounds	Pesticide; Pharmaceuticals	
4-Chloroaniline	p-Chloroaniline; 1-Amino-4-chlorobenzene; 4-Chloro-1-aminobenzene; 4-Chlorobenzamine; 4-Chlorophenylamine	106-47-8	127.57	1.83	Liquid	NA	Amines	Intermediate in chemical synthesis; Manufacturing; Pesticides; Pharmaceuticals	
(Chloro)methylisothiazolinone	CMI; MCI/MI; Kathon CG; 5-Chloro-2-methylisothiazolinone /2-methylisothiazolinone; 5 Chloro-2-methyl-3(2H)-isothiazolone and 2-methyl-2H-isothiazolone; Methyl/chloromethylisothiazolinone	26172-55-4	149.60	-0.34	Liquid	High	Heterocyclic compounds; Sulfur compounds	Biocide; Household products	

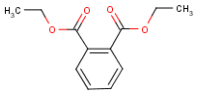
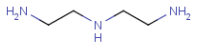
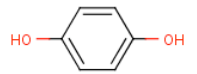
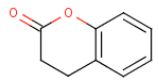
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Chlorpromazine	3,4-Dichloroaniline	95-76-1	162.02	2.60	Solid	NA	Amines	Intermediate in chemical synthesis; Manufacturing	
Cinnamic aldehyde	Cinnamaldehyde	104-55-2	132.16	2.29	Liquid	High	Aldehydes	Cosmetics; Food additive; Fragrance agent; Intermediate in chemical synthesis; Personal care products; Pesticides	
Cinnamyl alcohol	3-Phenyl-2-propen-1-ol	104-54-1	134.18	2.29	Solid	NA	Alcohols	Cosmetics; Food additive; Fragrance agent; Intermediate in chemical synthesis; Personal care products	
Cinnamyl nitrile	Cinnamionitrile; 1-Cyano-2-phenylethylene; 2-Propenenitrile, 3-phenyl-; Styryl cyanide; beta-Cyanostyrene; beta-Phenylacrylonitrile	4360-47-8	129.16	1.84	Liquid	NA	Nitriles	Fragrance agent	


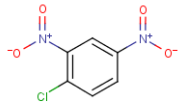
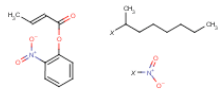
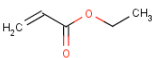
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
C.I. Reactive Red 231	Potassium/sodium-5-(4-chlor-6(N4-(4-chlor-6-(5-hydroxy-2,7-disulfonato-6-(2-sulfonato-phenylazo)-4-naphthylamino)-1,3,5-triazin-2-ylamino)-phenyl-N-methylamino)-1,3,5-triazin-2-ylamino)-4-hydroxy-3-(2-sulfonatophenylazo)-naphthalen-2,7-disulfonate	NA	NA	NA	Solid	NA	NA	Dye	NA
C.I. Reactive Yellow 174	1,3,6-Naphthalene-trisulfonic acid, 7-(2-(2-((aminocarbonyl)amino)-4-((4-((2-(2-(ethenyl sulfonyl)ethoxy)ethyl)amino)-6-fluoro-1,3,5-triazin-2-yl) amino) phenyl)diazenyl)-, sodium salt (1:3)	106359-91-5	885.75	NA	Solid	NA	NA	Dye	
Citral	3,7-Dimethyl-2,6-octadienal; Geranial-Neral mixture	5392-40-5	152.23	2.54/ 3.45	Liquid	High	Hydrocarbons, other	Fragrance agent	

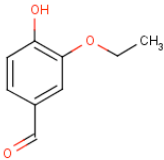
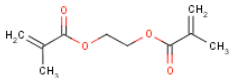
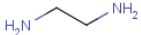
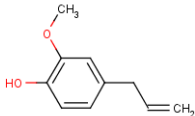
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Citronella oil	NA	8000-29-1	NA	NA	Liquid	NA	Lipids; Natural complex substances	NA	NA
dl-Citronellol	3,7-Dimethyl-6-octen-1-ol, (+)-	26489-01-0	156.27	3.56	Liquid	NA	Hydrocarbons	Fragrance agent	
Clove oil	NA	8000-34-8	NA	NA	Liquid	NA	Natural complex substances	Pharmaceutical	NA
Cobalt chloride	Cobaltous chloride; Cobalt chloride hexahydrate; Cobalt (II) salts	7646-79-9	129.84	0.85	Solid	NA	Elements; Inorganic chemicals; Metals	Manufacturing; Pesticides	$[Co^{2+}] [Cl^{-}]_2$
Cobalt sulfate	Cobaltous sulfate; Cobalt (II) salts	10124-43-3	155.00	0.63	Solid	NA	Elements; Inorganic chemicals; Metals	Manufacturing; Pesticides	
Copper (II) chloride	NA	1344-67-8	99.00	NA	Solid	NA	Inorganic chemicals; Metals	Manufacturing	Cu-Cl

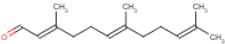
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Coumarin	1,2-Benzopyrone	91-64-5	146.15	1.91	Solid	Minimal	Heterocyclic compounds	Fragrance agent; Manufacturing; Pharmaceuticals	
Cyclamen aldehyde	3-(4-Isopropylphenyl)isobutyraldehyde	103-95-7	190.29	3.28	Liquid	Low	Carboxylic acids	Food additive; Fragrance agent	
Damascenone	1-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-2-buten-1-one; Rose dihydroketone;	23696-85-7	190.28	4.21	Liquid	NA	Hydrocarbons, acyclic	Food additive; Fragrance agent	
trans-alpha-Damascone	(E)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one	24720-09-0	192.30	4.29	Liquid	NA	Hydrocarbons, acyclic	Food additive; Fragrance agent	
trans-beta-Damascone	(2E)-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one	23726-91-2	192.30	4.42	Liquid	NA	Hydrocarbons, acyclic	Food additive; Fragrance agent	


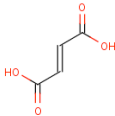
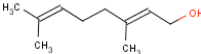

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
delta-Damascone	delta-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one	57378-68-4	192.30	4.16	Liquid	NA	NA	Food additive; Fragrance agent	
D EC25\	NA	NA	NA	NA	NA	NA	Formulations	Pesticide	NA
D EW 15	NA	NA	NA	NA	NA	NA	Formulations	Pesticide	NA
Dextran	NA	9004-54-0	Various	Various	Solid	NA	Carbohydrates	Pharmaceuticals	
1,2-Dibromo-2,4-dicyanobutane	2-Bromo-2-(bromomethyl) glutaronitrile; 2-Bromo-2-(bromomethyl) pentanedinitrile; Bromothalonil; Glutaronitrile, Methyl dibromo glutaronitrile	35691-65-7	265.93	1.91	Solid	NA	Nitriles	Manufacturing; Personal care products	
Diethyl maleate	Ethyl maleate	141-05-9	172.18	0.89	Liquid	High	Carboxylic acids	Food additive; Intermediate in chemical synthesis	

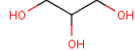
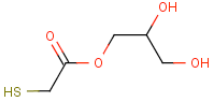

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Diethyl phthalate	NA	84-66-2	222.24	1.87	Liquid	Minimal	Carboxylic acids	Household products; Manufacturing	
Diethylenetriamine	1,2-Ethanediamine, N-(2-aminoethyl)-; 1,4,7-Triazaheptane; 1,5-Diamino-3-azapentane; 2,2'-Diaminodiethylamine; 2,2'-Iminobis(ethanamine); 2-(2-Aminoethylamino)ethylamine; 3-Azapentane-1,5-diamine	111-40-0	103.17	0.29	Liquid	NA	Amines	Intermediate in chemical synthesis	
1,4-Dihydroquinone	1,4-Benzenediol; Hydroquinone p-Hydroxyphenol	123-31-9	110.11	1.17	Solid	NA	Phenols	Manufacturing; Personal care products	
Dihydrocoumarin	1,2-Benzodihydropyrone; 3,4-Dihydrocoumarin; Hydroxydihydrocinnamic acid lactone; Melilotin	119-84-6	148.16	0.97	Liquid	NA	Heterocyclic compounds	Food additive; Fragrance agent; Pharmaceuticals	

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
5,5-Dimethyl-3-methylenedihydro-2(3H)-furanone	NA	29043-97-8	126.16	1.42	NA	NA	Heterocyclic compounds; Lactones; Sulfur compounds	NA	NA
Dimethyl sulfoxide	NA	67-68-5	78.13	0.57	Liquid	NA	Sulfur compounds	Manufacturing; Pharmaceuticals	
2,4-Dinitrochlorobenzene	1-Chloro-2,4-dinitrobenzene; DNCB	97-00-7	202.55	-0.05	Solid	High	Hydrocarbons, halogenated; Nitro compounds; Hydrocarbons, cyclic	Manufacturing; Pesticides	
Dinocap EC	NA	39300-45-3	364.39	5.76	Liquid	NA	Formulations; Hydrocarbons, cyclic; Nitro compounds	Fungicide	
Ethyl acrylate	NA	140-88-5	100.12	0.92/1.22	Liquid	High	Carboxylic acids	Manufacturing	

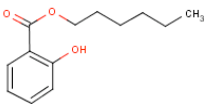
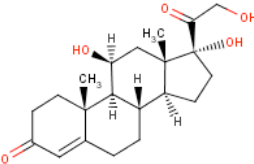
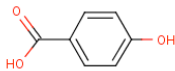
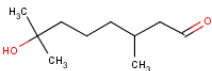
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Ethyl vanillin	3-Ethoxy-4-hydroxybenzaldehyde; 2-Ethoxy-4-formylphenol	121-32-4	166.18	1.52	Solid	Minimal	Aldehydes	Food additive; Fragrance agent; Manufacturing	
Ethylene glycol dimethacrylate	EGDMA	97-90-5	198.22	1.38	Liquid	High	Carboxylic acids	Manufacturing	
Ethylenediamine	NA	107-15-3	60.10	0.19	Liquid	NA	Amines	Manufacturing	
Eugenol	2-Methoxy-4-(2-propenyl)phenol; 4-Allyl-2-methoxyphenol; 4-Allylguaiacol	97-53-0	164.20	2.15/ 2.73	Liquid	NA	Carboxylic acids	Cosmetics; Food additive; Intermediate in chemical synthesis; Manufacturing; Personal care products; Pharmaceuticals	
EXP 10810 A	NA	NA	NA	NA	NA	NA	Formulations	Pesticides	NA

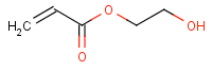
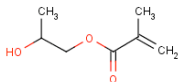
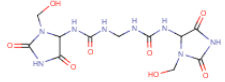
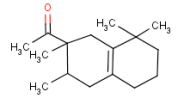
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
EXP 11120 A	NA	NA	NA	NA	NA	NA	Formulations	Pesticides	NA
F & Fo WG 50 + 25	NA	NA	NA	NA	NA	NA	Formulations	Pesticides	NA
FAR01042-00	NA	NA	NA	NA	NA	NA	Formulations	Pesticides	NA
FAR01060-00	NA	NA	NA	NA	NA	NA	Formulations	Pesticides	NA
Fatty acid glutamate	NA	NA	NA	NA	NA	NA	NA	NA	NA
Fatty alcohol #1	NA	NA	NA	NA	NA	NA	NA	NA	NA
Fatty alcohol #2	NA	NA	NA	NA	NA	NA	NA	NA	NA
Farnesal	2,6,10-Dodecatrienal, 3,7,11-trimethyl-, (2E,6E)-	4602-84-0	220.36	3.77	Liquid	Low	Alcohols; Hydrocarbons	Food additive; Fragrance agent; Manufacturing	


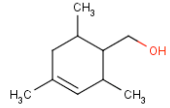
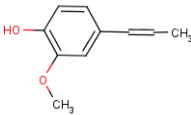
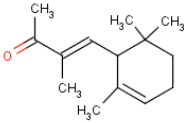
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Formaldehyde	NA	50-00-0	30.03	0.33/ 0.35	Liquid	Moderate	Aldehydes	Disinfectant; Manufacturing	
Fumaric acid	Ethylenedicarboxylic acid; 2-Butenedioic acid; Allomaleic acid; Boletic acid; Lichenic acid	110-17-8	116.00	0.03	Solid	NA	Carboxylic acids	Food additive; Household products; Manufacturing	
Geraniol	Rhodinol	106-24-1	154.25	2.54/ 3.47	Liquid	NA	Hydrocarbons, other	Cosmetics; Fragrance agent; Personal care products	
Geranium oil	Pelargonium oil	8000-46-2	NA	NA	Liquid	NA	Natural complex substances	Cosmetics; Fragrance agent; Personal care products; Pesticides	NA
Glutaraldehyde	Glutaral; Pentanedial	111-30-8	100.12	0.92	Liquid	High	Aldehydes	Cosmetics; Disinfectant; Manufacturing; Pesticides	


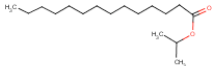
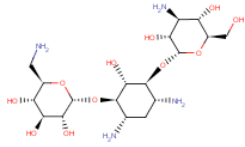
Chemical Name	Synonyms	CASRN	Mol. Weight	Log $K_{ow}^{1,2}$	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Glycerol	1,2,3-Propanetriol	56-81-5	92.09	0.05	Liquid	Minimal	Alcohols; Carbohydrates	Cosmetics; Food additive; Intermediate in chemical synthesis; Manufacturing; Personal care products; Pharmaceuticals; Solvent	
Glyceryl thioglycolate	Acetic acid, mercapto, monoester with 1,2,3-propanetriol; Glycerol monomercaptoacetate; Glyceryl monothioglycolate; Mercaptoacetic acid, monoester with 1,2,3-propanetriol	30618-84-9	166.19	-1.29	NA	NA	Lipids	Personal care products	
Glyoxal	Oxaldehyde; Ethanediol; Biformyl	107-22-2	58.04	0.19	Liquid	High	Aldehydes	Intermediate in chemical synthesis; Manufacturing; Pharmaceuticals	


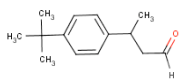
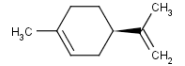
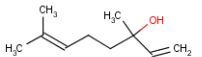
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Gold chloride	Chloroauric acid; Gold tetrachloride	16903-35-8	339.79	0.16	Solid	NA	Gold compounds; Inorganic chemicals	Manufacturing	
Hexane	NA	110-54-3	86.18	1.94	Liquid	Minimal	Hydrocarbons, acyclic	Manufacturing; Solvent	
<i>trans</i> -2-Hexenal	NA	6728-26-3	98.15	1.56	Liquid	High	Heterocyclic compounds	Fragrance agent	
Hexyl cinnamic aldehyde	HCA; alpha- Hexylcinnamaldehyde; 2-(Phenylmethylene) octanal	101-86-0	216.32	3.77/ 4.82	Liquid	Minimal	Aldehydes	Food additive; Fragrance agent	
2-Hexylidene cyclopentanone	NA	17373-89-6	166.27	3.71	Liquid	NA	NA	Cosmetics; Fragrance agent	

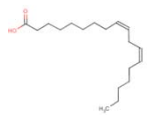

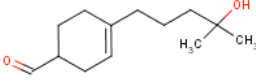
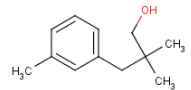
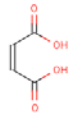
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Hexyl salicylate	Benzoic acid, 2-hydroxy-, hexyl ester	6259-76-3	222.29	5.06	Liquid	NA	NA	Food additive	
Hydrocortisone	11-beta-Hydrocortisone	50-23-7	362.46	1.16	Solid	NA	Polycyclic compounds	Pharmaceuticals	
4-Hydroxybenzoic acid	4-Carboxyphenol p-Hydroxybenzoic acid p-Salicylic acid	99-96-7	138.12	1.03	Solid	Minimal	Phenols; Carboxylic acids	Intermediate in chemical synthesis; Manufacturing; Pesticides	
Hydroxy-citronellal	NA	107-75-5	172.26	2.15	Liquid	Low	Hydrocarbons, other	Food additive; Fragrance agent; Personal care products	


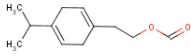
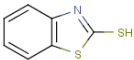

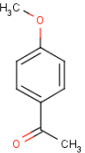
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
2-Hydroxyethyl acrylate	HEA	818-61-1	116.12	0.54	Liquid	High	Carboxylic acids	Intermediate in chemical synthesis; Manufacturing;	
2-Hydroxypropyl methacrylate	2-HPMA	923-26-2	144.17	1.03	Solid	Low	Carboxylic acids	Manufacturing: Plastics; Rubber	
Imidazolidinyl urea	Germall 115; Imidurea	39236-46-9	388.30	-3	Solid	Moderate	Ureas	Cometics; Personal care products; Pesticides	
Isocyclemone E	1-(1,2,3,4,5,6,7,8-Octahydro-2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one; OTNE; Boisvelone	54464-57-2	234.38	5.18	Liquid	NA	Hydrocarbons, cyclic; Polycyclic compounds	Food additive; Fragrance agent; Household products	

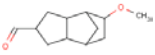
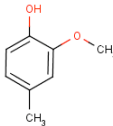
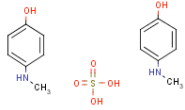
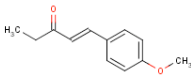
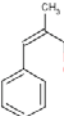

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Isocyclocitral	1-Formyl-3,5,6-trimethyl-3-cyclohexene and 1-formyl-2,4,6-trimethyl-3-cyclohexene; 2,4,6-Trimethyl-3-cyclohexen-1-carboxaldehyde	1335-66-6	152.44	3.27	NA	NA	NA	Food additive; Fragrance agent	
Isocyclogeraniol	3-Cyclohexene-1-methanol, 2,4,6-trimethyl-	68527-77-5	154.25	NA	Liquid	NA	Alcohols	Fragrance agent	
Isoeugenol	2-Methoxy-4-propenylphenol; 4-Propenylguaiacol	97-54-1	164.20	2.15	Liquid	NA	Carboxylic acids	Food additive; Fragrance agent	
Isomethyl ionone	3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	127-51-5	206.33	NA	NA	NA	Hydrocarbons, acyclic	Food additive; Fragrance agent; Personal care products	

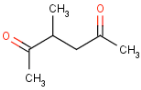
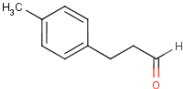
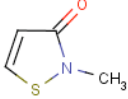
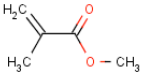
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Isopropanol	Isopropyl alcohol; 2-Propanol	67-63-0	60.10	0.82	Liquid	Minimal	Alcohols	Cosmetics; Disinfectant; Food additive; Intermediate in chemical synthesis; Manufacturing; Personal care products; Pharmaceuticals; Solvent	
Isopropyl myristate	Tetradecanoic acid, 1-methylethyl ester; Myristic acid isopropyl ester	110-27-0	270.46	3.88	Liquid	Minimal	Lipids	Cosmetics; Personal care products; Pharmaceuticals	
Jasmine absolute (grandiflorum)	NA	8022-96-6; 8024-43-9; 90045-94-6; 84776-64-7	NA	NA	NA	NA	Natural complex substances	Food additive; Fragrance agent	NA
Jasmine absolute (sambac)	NA	91770-14-8	NA	NA	NA	NA	Natural complex substances	Food additive; Fragrance agent	NA
Kanamycin	NA	59-01-8; 8063-07-8	484.50	-0.9	Solid	NA	Carbohydrates	Pharmaceuticals	

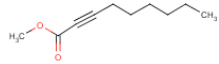
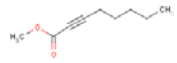
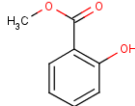
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Lead acetate	Acetic acid, lead salt	15347-57-6	325.29	-0.08	Solid	NA	Inorganic chemicals; Metals	Cosmetics; Personal care products	
Lemongrass oil	Citral terpenes; Indian melissa oil; Indian oil of verbena; Cymbopogon citratus oil	8007-02-1	NA	NA	Liquid	NA	Lipids; Hydrocarbons, other Natural complex substances	Food additive; Fragrance agent	NA
Lilial	p-tert-Butyl-a-ethyl-hydrocinnamal	80-54-6	204.31	3.52	Liquid	Low	Aldehydes	Fragrance agent	
d-Limonene	1-Methyl-4-(1-methylenethenyl)cyclohexene; Dipentene; Limonene	5989-27-5	136.24	2.93	Liquid	NA	Hydrocarbons, cyclic	Cosmetics; Food additive; Fragrance agent; Manufacturing	
Linalool	3,7-Dimethyl-2,6-octadienal; Geranial-Neral mixture	78-70-6	154.25	2.54	Liquid	NA	Hydrocarbons	Cosmetics; Food additive; Manufacturing; Personal care products; Pharmaceuticals	

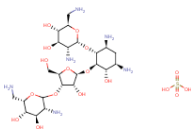


Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Linoleic acid	9,12-Octadecadienoic acid; Grape seed oil	60-33-3	280.50	7.51	Liquid	NA	Lipids	Food additive; Household products; Manufacturing	
Linolenic acid	(Z,Z,Z)-Octadeca-9,12,15-trienoic acid	463-40-1	278.40	7.30	Liquid	NA	Lipids	Food additive	
Litsea cubeba oil	NA	68855-99-2	NA	NA	Liquid	NA	Natural complex substances	Fragrance agent	NA
Lyral HMPCC	3 and 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexane-1-carboxaldehyde	31906-04-4	210.32	2.89	Liquid	NA	Aldehydes; Hydrocarbons, cyclic	Fragrance agent	
Majantal	Benzenepropanol, beta,beta,3-trimethyl-	103694-68-4	178.27	3.48	NA	NA	NA	Fragrance agent	
Maleic acid	1,2-Ethylene-dicarboxylic acid, (Z); 2-Butenedioic acid, (Z)-; Maleinic acid; Malenic acid; Toxic acid	110-16-7	116.10	0.05	Solid	NA	Carboxylic acids	Food additive; Intermediate in chemical synthesis; Manufacturing	

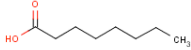
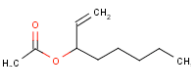
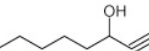
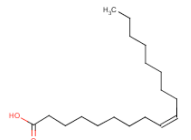

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Manganese chloride	Maganese chloride, anhydrous	7773-01-5	125.84	0.85	Solid	NA	Inorganic chemicals; Manganese compounds	Manufacturing	
Menthadiene-7-methyl formate	Menthadienyl formate; Isobergamate	68683-20-5	194.28	4.23	NA	NA	NA	Fragrance agent	
2-Mercapto-benzothiazole	Captax	149-30-4	167.25	1.80	Solid	High	Heterocyclic compounds	Manufacturing; Pesticides	
Mercuric (II) chloride	Mercuric chloride	7487-94-7	271.50	0.15	Solid	NA	Inorganic chemicals; Mercury compounds	Fungicide; Insecticide; Intermediate in chemical synthesis; Manufacturing	
4'-Methoxy-acetophenone	4-Acetylanisole; Ethanone, 1-(4-methoxyphenyl)-	100-06-1	150.18	1.91	Solid	Minimal	Ethers; Phenols	Intermediate in chemical synthesis	

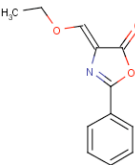
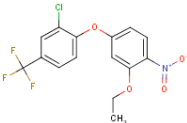
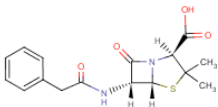
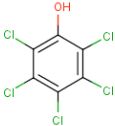
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Methoxy dicyclopentadiene carboxaldehyde	Octahydro-5-methoxy-4,7-methano-1H-indene-2-carboxaldehyde; Scentenal	86803-90-9	194.27	2.63	NA	NA	NA	Fragrance agent	
2-Methoxy-4-methylphenol	Creosol	93-51-6	138.17	1.88	Liquid	NA	Phenols	Pharmaceuticals	
4-Methyl-aminophenol sulfate	Metol; Paramethylamino-phenol sulfate	55-55-0	344.39	-0.13	Solid	High	Amines; Phenols	Household products	
Methylanisylidene acetone	alpha-Methylanisylidene-acetone; 1-Penten-3-one, 1-(p-methoxyphenyl)-	104-27-8	190.24	2.3	Solid	NA	Ethers	Food additive; Pharmaceuticals	
alpha-Methyl cinnamic aldehyde	2-Propenal, 2-methyl-3-phenyl-	101-39-3	146.19	2.37	NA	NA	DNF	Fragrance agent	
Methyl dodecane-sulfonate	1-Dodecanesulfonic acid, methyl ester	2374-65-4	264.43	2.51	NA	NA	Esters; Sulfur compounds	NA	

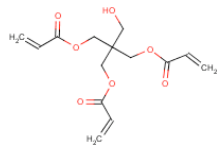
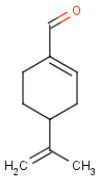
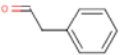
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Methylhexanedione	3-Methyl-2,5-hexanedione	13706-86-0	128.17	-0.39	Liquid	Low	Ketones	NA	
Methylhydrocinnamal	Benzenepropanal, 4-methyl-	5406-12-2	148.20	2.58	Liquid	NA	NA	NA	
Methylisothiazolinone	-Methyl-3(2H)-isothiazolone; 2-Methyl-4-isothiazolin-3-one; 3(2H)-Isothiazolone, 2-methyl-; MI	2682-20-4	115.16	-0.83	NA	High	Heterocyclic compounds; Sulfur compounds	Biocide; Household products	
Methyl methacrylate	MMA	80-62-6	100.12	0.70	Liquid	NA	Carboxylic acids	Manufacturing	

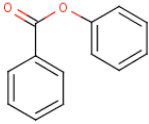
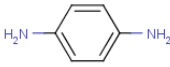
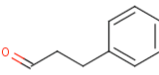
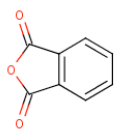

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Methyl 2-nonynoate	2-Nonynoic acid methyl ester; Methyl octine carbonate	111-80-8	168.24	2.15	Liquid	High	Lipids	Food additive; Fragrance agent	
Methyl 2-octynoate	Methyl heptene carbonate	111-12-6	154.21	3.30	NA	NA	Carboxylic acids; Lipids	Cosmetics; Food additive; Fragrance agent; Personal care products	
Methyl salicylate	Oil of wintergreen; 2-Hydroxybenzoic acid methyl ester	119-36-8	152.15	1.28/ 2.60	Liquid	Minimal	Carboxylic acids; Phenols	Cosmetics; Disinfectant; Food additive; Fragrance agent; Personal care products; Pharmaceuticals; Solvent	

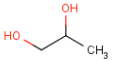
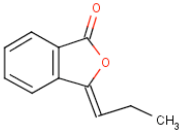
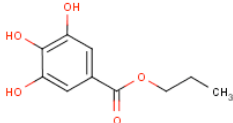
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
NAVY 14 08 723	Mixture of Sodium/potassium-(3-(4-(5-(5-chlor-2,6-difluor-pyrimidin-4-ylamino)-2-methoxy-3-sulfonatophenylazo)-2-oxido phenylazo)-2,5,7-trisulfonato-4-naphtholato)copper(II) and Sodium/potassium-(3-(4-(5-(5-chlor-4,6-difluor-pyrimidin-2-ylamino)-2-methoxy-3-sulfonatophenylazo)-2,5,7-trisulfonato-4-naphtholato)copper(II)	NA	NA	NA	Solid	NA	NA	Dye	NA
Neomycin sulfate	NA	1405-10-3	712.72	NA	Solid	NA	Carbohydrates	Pharmaceuticals	
Nickel chloride	Nickelous chloride	7718-54-9	129.60	0.05	Solid	NA	Inorganic chemicals; Metals	Manufacturing	
Nickel sulfate	Nickelous sulfate	7786-81-4	154.76	-0.17	Solid	NA	Inorganic chemicals; Metals	Manufacturing	

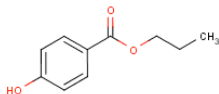

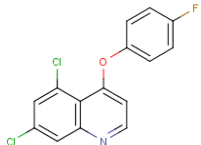
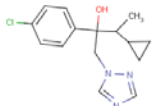
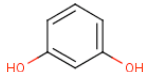
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Oakmoss	NA	68917-10-2	NA	NA	NA	NA	Natural complex substances	Fragrance agent	NA
Octanoic acid	Caprylic acid; 1-Heptanecarboxylic acid	124-07-2	144.21	1.66	Liquid	Minimal	Carboxylic acids; Lipids	Cosmetics; Disinfectant; Food additive; Pesticides	
1-Octen-3-yl acetate	Amyl crotonyl acetate; Amyl vinyl carbinol acetate; Amyl vinyl carbinyll; Octenyl acetate	2442-10-6	170.25	3.60	Liquid	NA	NA	Food additive; Fragrance agent	
Octinol	1-Octin-3-ol; 1-Octyn-3-ol	818-72-4	128.20	1.96	Liquid	NA	NA	Food additive; Flavor ingredient	
Oleic acid	9-Octadecenoic acid	112-80-1	282.47	7.73	Liquid	NA	Lipids	Food additive; Household products; Manufacturing	
Oxalic Acid	Ethanedioic acid	144-62-7	90.03	-2.22	Solid	Minimal	Carboxylic acids	Household products; Intermediate in chemical synthesis; Manufacturing	

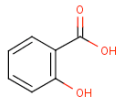
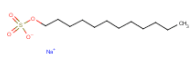

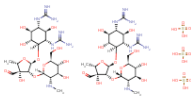
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Oxazolone	4-Ethoxymethylene-2-phenyloxazol-5-one	15646-46-5	217.22	1.87	Solid	High	Heterocyclic compounds	NA	
Oxyfluorfen EC	2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-trifluoromethylbenzene; 2-Chloro-alpha,alpha,alpha-trifluoro-p-tolyl-3-ethoxy-4-nitrophenyl ether	42874-03-3	361.70	5.21	Solid	NA	Ethers Formulations	Herbicide	
Palmarosa oil	Cymbopogon martini oil; Geranium oil, East Indian	8014-19-5	NA	NA	Liquid	NA	Natural complex substances	Fragrance agent	NA
Penicillin G	NA	61-33-6	334.39	2.09	Solid	NA	Amides; Sulfur compounds; Heterocyclic compounds	Pharmaceuticals	
Pentachlorophenol	Penta; PCP	87-86-5	266.34	2.79	Solid	NA	Phenols	Pesticides	

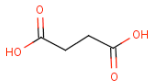
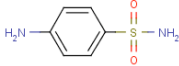
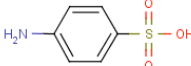
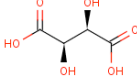
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Pentaerythritol triacrylate	2-(Hydroxymethyl)-2-(((1-oxoallyl)oxy)methyl)-1,3-propanediyl diacrylate; 2-Propenoic acid, 1,1'-(2-(hydroxymethyl)-2-(((1-oxo-2-propen-1-yl)oxy)methyl)-1,3-propanediyl) ester	3524-68-3	298.29	0.91	NA	NA	Alcohols; Carboxylic acids	Manufacturing	
Perillaldehyde	p-Mentha-1,8-dien-7-al	2111-75-3	150.22	3.34	Liquid	Moderate	Hydrocarbons	Fragrance agent	
Peru balsam absolute	Myroxylon pereirae oleoresin; Peruvian balsam	8007-00-9	NA	NA	NA	NA	Natural complex substances	Food additive; Fragrance agent; Pharmaceutical	NA
Phenylacet-aldehyde	1-Oxo-2-phenylethane; 2-Phenylethanal; Benzeneacetaldehyde; Benzylcarbox-aldehyde; Hyacinthin; Oxophenylethane; Phenylacetic aldehyde; Phenylethanal; alpha-Tolualdehyde	122-78-1	120.20	2.05	Liquid	Moderate	Aldehydes	Food additive; Fragrance agent	

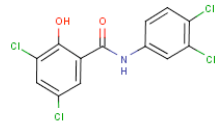
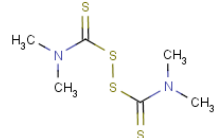
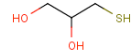
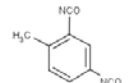
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Phenyl benzoate	NA	93-99-2	198.22	2.89	Solid	NA	Carboxylic acids	Manufacturing; Pesticides	
4-Phenylene-diamine	p-PDA; p-Phenylenediamine	106-50-3	108.14	1.17	Solid	NA	Amines	Manufacturing; Personal care products	
Phenylpropion-aldehyde	Hydrocinnamaldehyde; Propanal, phenyl-; 3-Phenylpropanal	1335-10-0	134.18	2	NA	Moderate	Aldehydes	Food additive; Fragrance agent	
Phthalic anhydride	1,2-Benzene-dicarboxylic acid anhydride; 1,3-Dioxophthalan; 1,3-Benzofurandione; 1,3 Phthalandione	85-44-9	148.12	1.6	Solid	Moderate	Anhydrides	Intermediate in chemical synthesis; Manufacturing	
Potassium dichromate	PDC	7778-50-9	294.18	0.62	Solid	NA	Chromium compounds; Inorganic chemicals; Potassium compounds	Manufacturing	

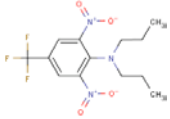
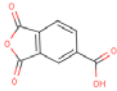
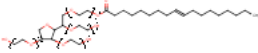
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Produkt P-4G	Lithium/sodium 4-(5-(4-chloro-6-(3-sulfonatophenylamino)-1,3,5-triazine-2yl-amino)-2-sulfonatophenylazo)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate	NA	NA	NA	Solid	NA	NA	Dye	NA
Propylene glycol	1,2-Dihydroxypropane; 1,2-Propanediol	57-55-6	76.10	0.43	Liquid	Minimal	Alcohols	Cosmetics; Food additive; Intermediate in chemical synthesis; Personal care products; Pharmaceuticals; Solvent	
Propylidene phthalate	1(3H)-Isobenzofuranone, 3-propylidene-	17369-59-4	174.20	3.10	Liquid	NA	Ketones	NA	
Propyl gallate	3,4,5-Trihydroxybenzoic acid, propyl ester; Benzoic acid, 3,4,5-trihydroxy-, propyl ester	121-79-9	212.20	1.80	Solid	High	Carboxylic acids	Food additive	


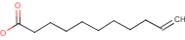
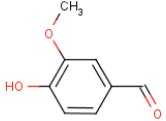
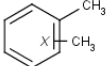
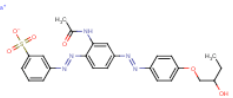
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Propylparaben	Propyl 4-hydroxybenzoate	94-13-3	180.20	1.77	Solid	Minimal	Carboxylic acids; Phenols	Cosmetics; Food additive Household products; Pharmaceuticals	
Pyridine	NA	110-86-1	79.10	1.31	Liquid	NA	Heterocyclic compounds	Food additive; Intermediate in chemical synthesis	
Quinoxifen SC	5,7-dichloro-4-(4-fluorophenoxy)quinoline	124495-18-7	308.10	5.69	Liquid	NA	Formulations; Heterocyclic compounds	Herbicide	
Quinoxifen/cyproconazole ⁶	5,7-dichloro-4-(4-fluorophenoxy)quinoline/1H-1,2,4-Triazole-1-ethanol, alpha-(4-chlorophenyl)-alpha-(1-cyclopropylethyl)-	124495-18-7/ 113096-99-4	308.10 291.80	5.69/ 3.25	Liquid	NA	Formulations Heterocyclic compounds	Herbicide	
Resorcinol	1,3-Dihydroxybenzene	108-46-3	110.11	1.17	Solid	Minimal	Phenols	Cosmetics; Manufacturing; Personal care products; Pharmaceuticals	

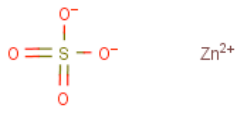
Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Salicylic acid	2-Hydroxybenzoic acid	69-72-7	138.12	1.03	Solid	NA	Carboxylic acids; Phenols	Food additive; Manufacturing; Pharmaceuticals	
Sodium lauryl sulfate	Sodium dodecyl sulfate; SLS; SDS; Irium	151-21-3	288.38	1.87/ 1.69	Solid	NA	Alcohols; Lipids; Sulfur compounds	Cosmetics; Food additive; Manufacturing; Personal care products; Pesticides; Pharmaceuticals	
Spearmint oil	Mentha spicata oil	8008-79-5	NA	NA	Liquid	NA	Natural complex substances	Food additive; Fragrance agent	NA
Squalene	2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene	111-02-4	410.73	14.12	Liquid	NA	Hydrocarbons	Food additive	
Streptomycin	D-Streptamine, O-2-deoxy-2-(methylamino)-alpha-L-glucopyranosyl-(1-2)-O-5-deoxy-3-C-formyl-alpha-L-lyxofuranosyl-(1-4)-N,N'-bis(aminoimino-methyl)-, sulfate (2:3) (salt)	3810-74-0	1457.39	-8.50	Solid	NA	Carbohydrates	Pharmaceuticals	

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Succinic acid	1,2-Ethanedicarboxylic acid; 1,4-Butanedioic acid	110-15-6	118.09	-0.59	Solid	NA	Carboxylic acids	Food additive; Intermediate in chemical synthesis; Manufacturing	
Sulfanilamide	4-Aminobenzene-sulfonamide, p-Anilinesulfonamide; p-Sulfamidoaniline	63-74-1	172.21	-0.62	Solid	Minimal	Amides; Amines; Sulfur compounds	Pharmaceuticals	
Sulfanilic acid	p-Aminobenzene-sulfonic acid; p-Anilinesulfonic acid	121-57-3	173.19	0.4	Solid	Minimal	Hydrocarbons, cyclic; Sulfur compounds	Pharmaceuticals	
Tartaric acid	[R-(R*,R*)]-2,3-Dihydroxybutanedioic acid; L-Tartaric acid	87-69-4	150.09	0.87	Solid	NA	Alcohols; Carboxylic acids	Food additive	
Tea leaf absolute	Camelia oleifera extract	84650-60-2	NA	NA	Liquid	NA	Natural complex substances	Cosmetics; Household products	NA

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Tetrachloro-salicylanilide	3,5-Dichloro-N-(3,4-dichlorophenyl)-2-hydroxybenzamide; TCS	1154-59-2	351.02	5.87	NA	Moderate	Amides Amines	Antifungal	
Tetramethyl thiuram disulfide	Thiram; Bis(dimethylthio-carbamoyl) disulfide; TMTD	137-26-8	240.44	1.17	Solid	NA	Carboxylic acids; Sulfur compounds	Fungicide	
Thioglycerol	1-Mercaptoglycerol; 1-Monothioglycerol; 1,2-Propanediol, 3-mercapto-; 1-Mercapto-2,3-propanediol	96-27-5	108.16	-8.40	Liquid	NA	Alcohols; Carbohydrates ; Sulfur compounds	Manufacturing; Pharmaceuticals	
Toluene 2,4-disocyanate	2,4-Diisocyanato-1-methylbenzene; 2,4-Diisocyanatotoluene; 2,4-TDI; 2,4-Toluene diisocyanate	584-84-9	174.16	3.74	Liquid	NA	Hydrocarbons, cyclic; Cyanates	Manufacturing	
Treemoss	Cedar moss extract; Tree moss absolute; Lichen concrete; Treemoss concrete; Treemoss concrete extract; Hyperabsolute	68648-41-9	NA	NA	Liquid	NA	Natural complex substances	Fragrance agent	NA

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Triflualin EC	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	1582-09-8	335.28	5.34	Solid	NA	Amines; Formulations; Hydrocarbons	Herbicide	
Trimellitic anhydride	1,2,4-Benzene-tricarboxylic acid, cyclic 1,2-anhydride (8CI); 1,3-Dihydro-1,3-dioxo-5-isobenzofuran-carboxylic acid; 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1,3-dioxo-; Benzene-1,2,4-tricarboxylic acid 1,2-anhydride	552-30-7	192.10	1.95	Solid	Low	Anhydrides; Carboxylic acids	Intermediate in chemical synthesis; Manufacturing	
Tween 80	Polyethylene glycol sorbitan monooleate; Polyoxyethylene-sorbitan monooleate; Polysorbate 80	9005-65-6	3968.85	NA	Liquid	NA	Alcohols	Food additive; Household products; Pharmaceuticals	

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K _{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Undec-10-enal	10-Undecylenaldehyde	112-45-8	168.28	2.79	Liquid	NA	Aldehydes	Food additive	
Undecylenic acid	10-Undecenoic acid	112-38-9	184.38	3.86	Liquid	NA	Lipids	Cosmetics; Fungicide; Pharmaceutical	
Vanillin	NA	121-33-5	152.15	1.28	Solid	Minimal	Aldehydes	Food additive; Fragrance agent	
Xylene	Dimethylbenzene	1330-20-7	107.18	3.16	Liquid	NA	Hydrocarbons, cyclic	Herbicide; Intermediate in chemical synthesis; Manufacturing	
YELLOW E-JD 3442	Benzenesulfonic acid, 3-(2-(2-(acetylamino)-4-(2-(4-(2-hydroxybutoxy)phenyl)diazenyl)phenyl)diazenyl)-, sodium salt (1:1)	147703-65-9	NA	NA	Solid	NA	NA	Dye	

Chemical Name	Synonyms	CASRN	Mol. Weight	Log K_{ow} ^{1,2}	Physical Form	Peptide Reactivity ³	Chemical Class ⁴	Product Use ⁵	Structure
Ylang Ylang	Cananga oil; Canangium odoratum genuina oil	8006-81-3; 68606-83-7; 83863-30-3	NA	NA	Liquid	NA	Natural complex substances	Fragrance agent	NA
Zinc sulfate	NA	7733-02-0	161.46	-0.07	Solid	NA	Inorganic chemicals; Sulfur compounds; Zinc compounds	Intermediate in chemical synthesis; Manufacturing; Pharmaceuticals	

Abbreviation: CASRN = Chemical Abstracts Service Registry Number; Mol. = molecular; NA = not available.

¹ K_{ow} represents the estimated octanol-water partition coefficient (expressed on log scale).

² When two numbers are shown for K_{ow} , the first number is the value calculated by the method of Moriguchi et al. (1994 Chem Pharm Bull 42:976-978) and provided in Gerberick et al. (2005 Dermatitis 16:157-202). The second number was calculated by the method of Meylan and Howard (1995 J Pharm Science 84:83-92). LogP (log K_{ow}) values for GSK chemicals were calculated using the method provided by Daylight Chemical Information Systems (see <http://www.daylight.com/dayhtml/doc/clogp/index.html>).

³ Peptide reactivity based on Cys (1:10) and Lys (1:50) data as reported in Gerberick et al. 2004 and Gerberick et al. 2007.

⁴ Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs as developed by the National Library of Medicine at <http://www.nlm.nih.gov/mesh/meshhome.html>. Chemical classification of pharmaceutical chemicals for the GSK chemicals was suggested by Dr. Michael Olson of GSK, which in spirit captures three types of pharmaceutical active substances (actives, intermediates, and starting materials).

⁵ Information gathered from the following databases: The Good Scents Company (<http://www.thegoodscentscompany.com/>); Hazardous Substances Database (<http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>); Haz-Map (<http://hazmap.nlm.nih.gov/>); Household Products Database (<http://hpd.nlm.nih.gov/index.htm>); International Programme on Chemical Safety INCHEM database (<http://www.inchem.org/>); National Library of Medicine Drug Information Portal (http://druginfo.nlm.nih.gov/drugportal/drugportal.jsp?APPLICATION_NAME=drugportal); National Toxicology Program (<http://ntp.niehs.nih.gov/>).

⁶ Structure in this row is cyproconazole. For quinoxyfen structure, see the preceding row.