

# Evaluation of the Global Performance of Eight *In Silico* Skin Sensitization Models Using Human Data

## Supplementary Data

Tab. S1: Basketter et al. (2014) data set

Number	CAS number	Chemical name	SMILES string	Potency category	Binary sensitization status
1	526-37-4	Atranol	<chem>Cc1cc(c(c1)O)C=O</chem> O	Human Class 1	Sensitizer
2	7787-56-6	Beryllium sulfate	<chem>S(=O)(=O)([O-])[O-].O.O.O.O.[Be+2]</chem>	Human Class 1	Sensitizer
3	57074-21-2	Chloroatranol	n/a	Human Class 1	Sensitizer
4	624-49-7	Dimethyl fumarate	<chem>C(\C=C\C(OC)=O)(OC)=O</chem>	Human Class 1	Sensitizer
5	97-00-7	Dinitrochlorobenzene	<chem>c1(cc(cc1Cl)[N+](=O)[O-])[N+](=O)[O-]</chem>	Human Class 1	Sensitizer
6	886-38-4	Diphenylcyclopropenone	<chem>C1(C(c2ccccc2)=C1c1ccccc1)=O</chem>	Human Class 1	Sensitizer
7	302-01-2	Hydrazine	NN	Human Class 1	Sensitizer
8*	55965-84-9/ 96118-96-6	MCI/MI	<chem>c1(Cl)cc(=O)n(s1)C.c1(n(scc1)C)=O</chem>	Human Class 1	Sensitizer
9	7487-94-7	Mercuric chloride	<chem>[Hg](Cl)Cl</chem>	Human Class 1	Sensitizer
10	2682-20-4	MI	<chem>Cn1c(=O)ccs1</chem>	Human Class 1	Sensitizer
11	106-50-3	p-Phenylenedimaine	<chem>c1cc(ccc1N)N</chem>	Human Class 1	Sensitizer
12	492-89-7	Pentadecylcatechol	<chem>CCCCCCCCCCCCCc1c(O)c(O)ccc1</chem>	Human Class 1	Sensitizer
13	7778-50-9	Potassium dichromate	<chem>[Cr](O[Cr](=O)(=O)[O-])(=O)(=O)[O-].[K+].[K+]</chem>	Human Class 1	Sensitizer
14	2892-62-8	Squaric acid dibutylester	<chem>C1(=O)C(OCCCC)=C(OCCCC)C1=O</chem>	Human Class 1	Sensitizer
15	1154-59-2	Tetrachlorosalicylanilide	<chem>c1(C(Nc2cc(c(Cl)cc2)Cl)=O)c(cc(c1)Cl)Cl)O</chem>	Human Class 1	Sensitizer
16	95-55-6	2-Aminophenol	<chem>c1(c(ccc1)O)N</chem>	Human Class 2	Sensitizer
17	2634-33-5	Benzisothiazolinone	<chem>c1ccc2c(c1)c(=O)[nH]s2</chem>	Human Class 2	Sensitizer
18	104-55-2	Cinnamal	<chem>c1(ccccc1)/C=C/C=O</chem>	Human Class 2	Sensitizer
19	10124-43-3	Cobalt sulfate	<chem>S(=O)(=O)([O-])[O-].[Co+2]</chem>	Human Class 2	Sensitizer
20	141-05-9	Diethyl maleate	<chem>C(=C/C(=O)OCC)C(OCC)=O</chem>	Human Class 2	Sensitizer
21	109-55-7	Dimethylaminopropylamine	<chem>C(N(C)C)CCN</chem>	Human Class 2	Sensitizer
22	50-00-0	Formaldehyde	<chem>C=O</chem>	Human Class 2	Sensitizer
23	111-30-8	Glutaraldehyde	<chem>C(CC=O)CC=O</chem>	Human Class 2	Sensitizer
24	107-22-2	Glyoxal	<chem>C(=O)C=O</chem>	Human Class 2	Sensitizer
25	13453-07-1	Gold chloride	<chem>[Au](Cl)(Cl)Cl</chem>	Human Class 2	Sensitizer
26	31906-04-4	Hydroxyisohexyl-3-cyclohexene carboxaldehyde	<chem>CC(C)(CCCC1=CCC(CC1)C=O)O</chem>	Human Class 2	Sensitizer
27	97-54-1	Isoeugenol	<chem>C/C=C/c1ccc(c1)OC)O</chem>	Human Class 2	Sensitizer
28	1166-52-5	Lauryl gallate	<chem>c1(cc(c(O)c(c1)O)O)C(OCCCCC)CCCCC=O</chem>	Human Class 2	Sensitizer
29	111-12-6	Methyl heptine carbonate	<chem>C(#CC(OC)=O)CCCCC</chem>	Human Class 2	Sensitizer
30	35691-65-7	Methyldibromoglutaronitrile	<chem>C(CCC#N)(C#N)(CBr)Br</chem>	Human Class 2	Sensitizer
31	7440-02-0	Nickel	<chem>[Ni]</chem>	Human Class 2	Sensitizer
32	5307-14-2	Nitro-4-phenylenediamine	<chem>c1(c(ccc1)N)N[N+](=O)[O-]</chem>	Human Class 2	Sensitizer
33	8007-00-9	Peru balsam	n/a	Human Class 2	Sensitizer
34	121-79-9	Propyl gallate	<chem>c1(cc(c(c1)O)O)O)C(=O)OCCC</chem>	Human Class 2	Sensitizer
35	4080-31-3	Quaternium-15	<chem>[N+]12(CN3CN(C1)CN(C2)C3)C\C=C\Cl.[ClH-]</chem>	Human Class 2	Sensitizer

Number	CAS number	Chemical name	SMILES string	Potency category	Binary sensitization status
36	54-64-8	Thimerosal	<chem>c1(c(cccc1)C(=O)[O-])S[Hg]CC.[Na+]</chem>	Human Class 2	Sensitizer
37	96-27-5	Thioglycerol	<chem>C([C@@H](CS)O)O</chem>	Human Class 2	Sensitizer
38	615-50-9	Toluene diamine sulfate	<chem>Cc1cc(ccc1N)N.OS(=O)(=O)O</chem>	Human Class 2	Sensitizer
39	514-10-3	Abietic acid (colophony)	<chem>C1[C@@H]2[C@@]([C@@H]3C(C=C(C(C)C)CC3)=C1)(CCC[C@]2(C(O)=O)C)C</chem>	Human Class 3	Sensitizer
40	1405-87-4	Bacitracin	<chem>CC[C@H](C)[C@H](N)C1=N[C@@H](CS1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](CCC(=O)O)C(=O)N[C@@H]([C@H](C)CC)C(=O)N[C@H]2CCCCNC(=O)[C@H](CC(=O)N)NC(=O)[C@@H](CC(=O)O)NC(=O)[C@H](Cc3c[nH]cn3)NC(=O)[C@@H](NC(=O)[C@@H](CCCNC2=O)[C@@H](C)CC</chem>	Human Class 3	Sensitizer
41	94-36-0	Benzoyl peroxide	<chem>c1(C(OOC(c2ccccc2)=O)=O)ccccc1</chem>	Human Class 3	Sensitizer
42	1675-54-3	Bisphenol A glycidyl ether	<chem>C(c1ccc(cc1)OCC1CO1)(c1ccc(cc1)OCC1CO1)(C)C</chem>	Human Class 3	Sensitizer
43	2426-08-6	Butylglycidylether	<chem>C1[C@@H](O1)COCCCC</chem>	Human Class 3	Sensitizer
44	50-53-3	Chlorpromazine	<chem>CN(C)CCCN1c2ccccc2Sc3c1cc(c3)Cl</chem>	Human Class 3	Sensitizer
45	104-54-1	Cinnamic alcohol	<chem>c1(ccccc1)/C=C/CO</chem>	Human Class 3	Sensitizer
46	5392-40-5	Citral	<chem>C(=C\C=O)/CC/C=C(/C)C)C</chem>	Human Class 3	Sensitizer
47	91-64-5	Coumarin	<chem>c12c(ccc(o1)=O)cccc2</chem>	Human Class 3	Sensitizer
48	107-15-3	Ethylenediamine	<chem>C(N)N</chem>	Human Class 3	Sensitizer
49	97-53-0	Eugenol	<chem>COc1cc(ccc1O)CC=C</chem>	Human Class 3	Sensitizer
50	4602-84-0	Farnesol	<chem>C(=C\C\C=C(C\CO)C)(\CC\C=C(\C)C)C</chem>	Human Class 3	Sensitizer
51	30618-84-9	Glycerylmonothioglycolate	<chem>C(C(COC(=O)CS)O)O</chem>	Human Class 3	Sensitizer
52	123-31-9	Hydroquinone	<chem>c1(ccc(cc1)O)O</chem>	Human Class 3	Sensitizer
53	818-61-1	Hydroxyethyl acrylate	<chem>C(OCCO)(C=C)=O</chem>	Human Class 3	Sensitizer
54	39236-46-9	Imidazolidinyl urea	<chem>N1([C@@H](C(NC1=O)=O)NC(NCNC(N[C@@H]1N(C(=O)NC1=O)CO)=O)CO</chem>	Human Class 3	Sensitizer
55	149-30-4	Mercaptobenzothiazole	<chem>c1ccc2c(c1)nc(s2)S</chem>	Human Class 3	Sensitizer
56	13706-86-0	Methyl-2,3-hexanedione	<chem>CC(C)CC(=O)C(=O)C</chem>	Human Class 3	Sensitizer
57	55-55-0	Metol	<chem>CNc1ccc(cc1)O.CNc1ccc(cc1)O.O S(=O)(=O)O</chem>	Human Class 3	Sensitizer
58	61-33-6	Penicillin	<chem>CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)Cc3ccccc3)C(=O)O)C</chem>	Human Class 3	Sensitizer
59	93-99-2	Phenyl benzoate	<chem>c1(C(Oc2ccccc2)=O)ccccc1</chem>	Human Class 3	Sensitizer
60	137-26-8	Tetramethylthiuram disulfide	<chem>CN(C)C(=S)SSC(=S)N(C)C</chem>	Human Class 3	Sensitizer
61	122-40-7	Amylcinnamal	<chem>c1(\C=C(\CCCC)C=O)ccccc1</chem>	Human Class 4	Sensitizer
62	101-85-9	Amylcinnamal alcohol	<chem>c1(\C=C(\CCCC)CO)ccccc1</chem>	Human Class 4	Sensitizer
63	62-53-3	Aniline	<chem>c1ccc(cc1)N</chem>	Human Class 4	Sensitizer
64	94-09-7	Benzocaine	<chem>c1cc(C(OCC)=O)ccc1N</chem>	Human Class 4	Sensitizer
65	52-51-7	Bronopol	<chem>C(C(O)([N+](=O)[O-])Br)O</chem>	Human Class 4	Sensitizer
66	99-49-0	Carvone	<chem>CC(=C)C1CC=C(C)C(=O)C1</chem>	Human Class 4	Sensitizer
67	55-56-1	Chlorhexidine gluconate	<chem>c1(NC(NC(NCCCCCNC(NC(Nc2ccc(Cl)cc2)=N)=N)=N)ccc(Cl)c1</chem>	Human Class 4	Sensitizer
68	9003-32-1	Ethyl acrylate	<chem>CCOC(C=C)=O</chem>	Human Class 4	Sensitizer
69	97-90-5	Ethyleneglycol dimethacrylate	<chem>C(OCCOC(C(C)=C)=O)(C(C)=C)=O</chem>	Human Class 4	Sensitizer
70	106-24-1	Geraniol	<chem>C(\CC\C=C(\C)C)(=C\CO)C</chem>	Human Class 4	Sensitizer
71	6259-76-3	Hexyl salicylate	<chem>c1(c(cccc1)O)C(OCCCCC)=O</chem>	Human Class 4	Sensitizer
72	107-75-5	Hydroxycitronellal	<chem>CC(CCCC(C)(C)O)CC=O</chem>	Human Class 4	Sensitizer
73	55406-53-6	Iodopropynyl butyl carbamate	<chem>N(C(OCC#C)I)=O)CCCC</chem>	Human Class 4	Sensitizer
74	8063-07-8	Kanamycin	n/a	Human Class 4	Sensitizer

Number	CAS number	Chemical name	SMILES string	Potency category	Binary sensitization status
75	80-54-6	p-tert-butyl-a-methylhydrocinnamal	<chem>CC(Cc1ccc(cc1)C(C)(C)C)C=O</chem>	Human Class 4	Sensitizer
76	78-70-6	Linalool	<chem>C([C@@H](C=C)(C)O)C\C=C(\C)C</chem>	Human Class 4	Sensitizer
77	80-62-6	Methylmethacrylate	<chem>C(C(C)=C)(OC)=O</chem>	Human Class 4	Sensitizer
78	1404-04-2	Neomycin sulfate	<chem>O1[C@H](O[C@H]2[C@H](O[C@H]3[C@@H]([C@@H]([C@H](O3)CO)O[C@@H]3[C@@H]([C@H]([C@@H]([C@@H](O3)CN)O)O)N)O)[C@H]([C@@H](C[C@@H]2N)N)O[C@@H]([C@H]([C@@H](O)[C@H]1CN)O)N</chem>	Human Class 4	Sensitizer
79	108-46-3	Resorcinol	<chem>c1c(ccc1O)O</chem>	Human Class 4	Sensitizer
80	104-46-1	Anethole	<chem>c1(ccc(cc1)OC)/C=C/C</chem>	Human Class 5	Sensitizer
81	150-13-0	4-Aminobenzoic acid	<chem>c1cc(ccc1C(=O)O)N</chem>	Human Class 5	Sensitizer
82	105-13-5	Anisyl alcohol	<chem>c1(ccc(OC)cc1)CO</chem>	Human Class 5	Sensitizer
83	100-52-7	Benzaldehyde	<chem>c1ccc(cc1)C=O</chem>	Human Class 5	Sensitizer
84	8001-54-5	Benzalkonium chloride	<chem>c1([N+](C)(C)*)cccc1.[ClH-]</chem>	Human Class 5	Sensitizer
85	120-51-4	Benzyl benzoate	<chem>c1(C(=O)OCc2ccccc2)ccccc1</chem>	Human Class 5	Sensitizer
86	118-58-1	Benzyl salicylate	<chem>c1(C(OCc2ccccc2)=O)c(ccc1)O</chem>	Human Class 5	Sensitizer
87	128-37-0	Butylated hydroxytoluene	<chem>c1(c(O)c(C(C)(C)C)cc(c1)C(C)(C)C</chem>	Human Class 5	Sensitizer
88	107-88-0	Butylene glycol	<chem>C([C@@H](C)O)CO</chem>	Human Class 5	Sensitizer
89	57-09-0	Cetrimide	<chem>C(CCCCCCCCCCCC)CC[N+](C)(C)C.[BrH-]</chem>	Human Class 5	Sensitizer
90	773-52-6	Cetylpyridinium chloride	n/a	Human Class 5	Sensitizer
91	106-22-9	Citronellol	<chem>C(CC/C=C(C)C)(CCO)C</chem>	Human Class 5	Sensitizer
92	111-42-2	Diethanolamine	<chem>N(CCO)CCO</chem>	Human Class 5	Sensitizer
93	101-86-0	Hexylcinnamal	<chem>CCCCCC/C(=C/c1ccccc1)/C=O</chem>	Human Class 5	Sensitizer
94	50-23-7	Hydrocortisone	<chem>C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2[C@H](C[C@@]4([C@H]3CC[C@@]4(C(=O)CO)O)C)O</chem>	Human Class 5	Sensitizer
95	67-63-0	Isopropanol	<chem>C(C)(C)O</chem>	Human Class 5	Sensitizer
96	110-27-0	Isopropyl myristate	<chem>C(CCCCCCCCCCCC)C(=O)OC(C)C</chem>	Human Class 5	Sensitizer
97**	138-86-3/ 5989-27-5	Limonene (not oxidized)	<chem>C([C@@H]1CCC(C)=CC1)(C)=C</chem>	Human Class 5	Sensitizer
98	119-36-8	Methyl salicylate	<chem>c1(c(ccc1)O)C(OC)=O</chem>	Human Class 5	Sensitizer
99	87-86-5	Pentachlorophenol	<chem>c1(c(c(c(Cl)c(Cl)Cl)Cl)Cl)O</chem>	Human Class 5	Sensitizer
100	122-99-6	Phenoxyethanol	<chem>c1(cccc1)OCCO</chem>	Human Class 5	Sensitizer
101	94-13-3	Propyl paraben	<chem>c1(c(O)ccc(C(OCC)=O)c1</chem>	Human Class 5	Sensitizer
102	57-55-6	Propylene glycol	<chem>C([C@@H](C)O)O</chem>	Human Class 5	Sensitizer
103	110-86-1	Pyridine	<chem>c1ccncc1</chem>	Human Class 5	Sensitizer
104	110-44-1	Sorbic acid	<chem>C(=C\C=C\C)C(O)=O</chem>	Human Class 5	Sensitizer
105	3380-34-5	Triclosan	<chem>c1(Oc2c(cc(Cl)cc2)Cl)c(cc(Cl)cc1)O</chem>	Human Class 5	Sensitizer
106	102-71-6	Triethanolamine	<chem>N(CCO)(CCO)CCO</chem>	Human Class 5	Sensitizer
107	121-33-5	Vanillin	<chem>c1(cc(ccc1O)C=O)OC</chem>	Human Class 5	Sensitizer
108	7446-70-0	Aluminum chloride	<chem>[Al](Cl)(Cl)Cl</chem>	Human Class 6	Non-sensitizer
109	50-81-7	Ascorbic acid	<chem>[C@H]1(C(=C(C(=O)O1)O)O)[C@H](CO)O</chem>	Human Class 6	Non-sensitizer
110	71-43-2	Benzene	<chem>c1ccccc1</chem>	Human Class 6	Non-sensitizer
111	71-36-3	Butanol	<chem>C(CC)CO</chem>	Human Class 6	Non-sensitizer
112	9004-54-0	Dextran	n/a	Human Class 6	Non-sensitizer
113	84-66-2	Diethyl phthalate	<chem>CCOC(=O)c1ccccc1C(=O)OCC</chem>	Human Class 6	Non-sensitizer
114	94271-03-1	Diethyl toluamide	<chem>c1(C(=O)N(CC)CC)cc(ccc1)C</chem>	Human Class 6	Non-sensitizer
115	67-68-5	Dimethylsulfoxide	<chem>CS(=O)C</chem>	Human Class 6	Non-sensitizer
116	50-99-7	Glucose	<chem>OC[C@H]([C@H]([C@@H]([C@H]([C@H]([C@H](O)O)O)O)O)O)O</chem>	Human Class 6	Non-sensitizer
117	56-81-5	Glycerol	<chem>C(O)(CO)O</chem>	Human Class 6	Non-sensitizer
118	70-30-4	Hexachlorophene	<chem>c1(Cc2c(c(cc2Cl)Cl)Cl)O)c(c(cc(c1Cl)Cl)Cl)O</chem>	Human Class 6	Non-sensitizer
119	110-54-3	Hexane	<chem>C(CCC)CC</chem>	Human Class 6	Non-sensitizer
120	50-21-5	Lactic acid	<chem>C([C@@H](C)O)(O)=O</chem>	Human Class 6	Non-sensitizer
121	124-07-2	Octanoic acid	<chem>C(CCCCC)CC(O)=O</chem>	Human Class 6	Non-sensitizer
122	8009-03-8	Petrolatum	n/a	Human Class 6	Non-sensitizer
123	108-95-2	Phenol	<chem>c1(ccccc1)O</chem>	Human Class 6	Non-sensitizer

124	302-79-4	Retinoic acid	<chem>C=1(C(CCCC1C)(C)C)C=C\C(=C\C=C\C(=C\C(O)=O)C)C</chem>	Human Class 6	Non-sensitizer
125	69-72-7	Salicylic acid	<chem>c1(c(cccc1)O)C(=O)O</chem>	Human Class 6	Non-sensitizer
126	151-21-3	Sodium lauryl sulfate	<chem>C(CCCCCCCCC)COS(=O)(=O)[O-].[Na+]</chem>	Human Class 6	Non-sensitizer
127	50-70-4	Sorbitol	<chem>O[C@@H]([C@@H]([C@H](CO)O)O)[C@@H](CO)O</chem>	Human Class 6	Non-sensitizer
128	59-02-9	Tocopherol	<chem>CC(C)CCC[C@@H](C)CCC[C@@H](C)CCC[C@]1(C)CCc2c(C)c(O)c(C)c(C)c2O1</chem>	Human Class 6	Non-sensitizer
129	9005-65-6	Tween 80	n/a	Human Class 6	Non-sensitizer
130	1330-20-7	Xylene	n/a	Human Class 6	Non-sensitizer
131	1314-13-2	Zinc oxide	<chem>O=[Zn]</chem>	Human Class 6	Non-sensitizer

\*CASRN 55965-84-9 was used when model input required CASRN. The SMILES string associated with this CASRN was used when model input required a SMILES string.

\*\*CASRN 138-86-3 was used when model input required CASRN. Although there are two CASRN for this chemical, the SMILES string for each CASRN is identical to the other; therefore, this SMILES string was used to represent both CASRN.

Tab. S2: HSDB data set

Number	CAS number	Chemical name	SMILES string	Binary sensitization status
1	9003-01-4	Carbomer	<chem>C(C=C)(O)=O</chem>	Non-sensitizer
2	111-30-8	Glutaraldehyde	<chem>C(CC=O)CC=O</chem>	Sensitizer
3	85-44-9	Phthalic anhydride	<chem>c12c(C(=O)OC1=O)cccc2</chem>	Sensitizer
4	79-07-2	Chloroacetamide	<chem>C(CCl)(N)=O</chem>	Sensitizer
5	94-26-8	Butylparaben	<chem>c1(ccc(cc1)O)C(=O)OCCCC</chem>	Non-sensitizer
6	1163-19-5	Decabromodiphenyl ether	<chem>Brc1c(Br)c(Br)c(Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c1Br</chem>	Non-sensitizer
7	101-20-2	Triclocarban	<chem>c1cc(ccc1NC(=O)Nc2ccc(c(c2)Cl)Cl)Cl</chem>	Non-sensitizer
8	141-78-6	Ethyl acetate	<chem>O(C(=O)C)CC</chem>	Non-sensitizer
9	50-00-0	Formaldehyde	<chem>C=O</chem>	Sensitizer
10	156052-68-5	Zoxamide	<chem>CCC(C)(C(=O)CC)NC(=O)C1=CC(=C(C(=C1)Cl)C)Cl</chem>	Sensitizer
11	80-62-6	Methyl methacrylate	<chem>C(C(C)=C)(OC)=O</chem>	Sensitizer
12	120-47-8	Ethylparaben	<chem>c1(C(OCC)=O)ccc(O)cc1</chem>	Non-sensitizer
13	141-32-2	Butyl acrylate	<chem>C(=O)(OCCCC)C=C</chem>	Sensitizer
14	96-33-3	Methyl acrylate	<chem>C(=O)(C=C)OC</chem>	Sensitizer
15	1861-40-1	Benfluralin	<chem>c1(cc(cc(F)(F)F)cc1[N+](=O)[O-])[N+](=O)[O-]N(CCC)CC</chem>	Sensitizer
16	5124-30-1	Methylene bis(4-cyclohexylisocyanate)	<chem>C1CC(CCC1CC2CCC(CC2)N=C=O)N=C=O</chem>	Sensitizer
17	2425-06-1	Captafol	<chem>CiC(Cl)C(Cl)(Cl)SN1C(=O)[C@H]2CC=CC[C@H]2C1=O</chem>	Sensitizer
18	2634-33-5	1,2-Benzisothiazolin-3-one	<chem>c1ccc2c(c1)c(=O)[nH]s2</chem>	Sensitizer
19	123-54-6	Acetyl acetone	<chem>C(CC(C)=O)(C)=O</chem>	Sensitizer
20	529-20-4	2-Methylbenzaldehyde	<chem>Cc1ccccc1C=O</chem>	Non-sensitizer
21	133-06-2	Captan	<chem>CiC(Cl)(Cl)SN1C(=O)[C@H]2CC=CC[C@H]2C1=O</chem>	Sensitizer
22	87-66-1	Pyrogallol	<chem>c1(c(cccc1O)O)O</chem>	Sensitizer
23	122-60-1	Phenyl glycidyl ether	<chem>c1(OC[C@@H]2CO2)cccc1</chem>	Sensitizer
24	120-61-6	Dimethyl terephthalate	<chem>c1(C(OC)=O)ccc(C(OC)=O)cc1</chem>	Non-sensitizer
25	111-02-4	Squalene	<chem>C=C\CC\C=C\C\CC\C=C\C\CC\C=C\C\CC\C=C\C(C)C)C)C\CC\C=C\C(C)C)C</chem>	Non-sensitizer
26	164650-44-6	Efinaconazole	<chem>C[C@H]([C@](Cn1cncn1)(c2ccc(cc2F)F)O)N3CCC(=C)CC3</chem>	Non-sensitizer
27	94-96-2	2-Ethyl-1,3-hexanediol	<chem>CCCC(C)CCO</chem>	Non-sensitizer
28	106-89-8	Epichlorohydrin	<chem>C1[C@@H](O1)CCl</chem>	Sensitizer
29	88-89-1	Picric acid	<chem>c1(c(cc(c1)[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]</chem>	Sensitizer
30	4697-36-3	Carbenicillin	<chem>CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)C(c3ccccc3)C(=O)O)C(=O)O)C</chem>	Sensitizer
31	51630-58-1	Fenvalerate	<chem>c1(C(C(=O)OC(c2cc(Oc3ccccc3)ccc2)C#N)C(C)C)ccc(cc1)Cl</chem>	Sensitizer
32	2426-08-6	n-Butyl glycidyl ether	<chem>C1[C@@H](O1)COCCCC</chem>	Sensitizer
33	57-55-6	Propylene glycol	<chem>C([C@@H](C)O)O</chem>	Non-sensitizer
34	100-43-6	4-Vinylpyridine	<chem>c1(ccnc1)C=C</chem>	Sensitizer
35	101-68-8	4,4'-Methylenediphenyl diisocyanate	<chem>c1cc(ccc1Cc2ccc(cc2)N=C=O)N=C=O</chem>	Sensitizer

Number	CAS number	Chemical name	SMILES string	Binary sensitization status
36	479-45-8	Tetryl	<chem>c1(c(cc([N+](=O)[O-])cc1[N+](=O)[O-])[N+](=O)[O-])N([N+](=O)[O-])C</chem>	Sensitizer
37	68694-11-1	Triflumizole	<chem>C(OCCC)/C(=Nc1c(C(F)(F)F)cc(Cl)cc1)n1cncc1</chem>	Sensitizer
38	61-72-3	Cloxacillin	<chem>Cc1c(c(no1)c2ccccc2Cl)C(=O)N[C@H]3[C@@H]4N(C3=O)[C@H](C(S4)(C)C)C(=O)O</chem>	Sensitizer
39	7696-12-0	Tetramethrin	<chem>CC(=CC1C(C(=O)OCN2C(=O)C3=C(CCCC3)C2=O)C1(C)C)C</chem>	Non-sensitizer
40	35691-65-7	1,2-Dibromo-2,4-dicyanobutane	<chem>C(CCC#N)(C#N)(CBr)Br</chem>	Sensitizer
41	1675-54-3	Bisphenol A Diglycidyl Ether	<chem>C(c1ccc(cc1)OCC1CO1)(c1ccc(cc1)OCC1CO1)(C)C</chem>	Sensitizer
42	10124-43-3	Cobaltous sulfate	<chem>S(=O)(=O)([O-])[O-].[Co+2]</chem>	Sensitizer
43	85-43-8	Tetrahydrophthalic anhydride	<chem>C1([C@@H]2[C@@H](C(=O)O1)CC=CC2)=O</chem>	Sensitizer
44	7778-50-9	Potassium dichromate	<chem>[Cr](O[Cr](=O)(=O)[O-])(=O)(=O)[O-].[K+].[K+]</chem>	Sensitizer
45	82-05-3	Benzanthrone	<chem>c12c3c4c(cccc4)C(c1cccc2ccc3)=O</chem>	Sensitizer
46	99-76-3	Methylparaben	<chem>COC(=O)c1ccc(cc1)O</chem>	Non-sensitizer
47	101-84-8	Diphenyl ether	<chem>c1(Oc2ccccc2)ccccc1</chem>	Non-sensitizer
48	142-59-6	Nabam	<chem>C(CNC(=S)[S-])NC(=S)[S-].[Na+].[Na+]</chem>	Sensitizer
49	100-69-6	2-Vinylpyridine	<chem>c1(cccn1)C=C</chem>	Sensitizer
50	140-88-5	Ethyl acrylate	<chem>C(=O)(OCC)C=C</chem>	Sensitizer
51	79622-59-6	Fluazinam	<chem>n1cc(C(F)(F)F)cc(Cl)c1Nc1c([N+](O-)=O)c(Cl)c(C(F)(F)F)cc1[N+](O-)=O</chem>	Sensitizer
52	131-11-3	Dimethyl phthalate	<chem>COC(=O)c1cccc1C(=O)OC</chem>	Sensitizer
53	11051-71-1	Avilamycin	<chem>O1[C@@H]([C@]([C@H]2[C@H]([C@@]31O[C@H]1)[C@@H](OC(C(C)C)=O)[C@@H](O[C@H]4[C@H]([C@@H]([C@H](O[C@H]5[C@H](O)[C@@H](O[C@H]6[C@@]7([C@@H]([C@H](O6)C)O[C@@]6(O[C@@H]([C@@H]([C@@H](C6)O)O[C@@H]6O[C@H]([C@@H]([C@@H](C6)O)OC(=O)c6c(c(c(Cl)c6C)O)Cl)OC)C)O7)C)[C@@H](OC)[C@H](C)O5)[C@H](O4)COC)O)OC)[C@H]1O3)OCO2)(C(=O)C)O)C</chem>	Sensitizer
54	94-13-3	Propylparaben	<chem>c1c(O)ccc(C(OCC)=O)c1</chem>	Non-sensitizer
55	10141-05-6	Cobaltous nitrate	<chem>[N+](O-)([O-])O.[N+](=O)([O-])[O-].[Co+2]</chem>	Sensitizer
56	60-09-3	Aniline Yellow	<chem>c1(N=Nc2ccccc2)ccc(N)cc1</chem>	Sensitizer
57	34590-94-8	Dipropylene glycol monomethyl ether	<chem>COCC(C)OCC(C)O</chem>	Non-sensitizer
58	8003-22-3	D&C Yellow No. 11	<chem>O=C1C(C(=O)c2ccccc12)c3ccc4cccc4n3</chem>	Sensitizer
59	25013-16-5	Butylated hydroxyanisole	<chem>[*]C(C)(C)C.COC1ccc(O)cc1</chem>	Sensitizer
60	111-40-0	Diethylenetriamine	<chem>N(CCN)CCN</chem>	Sensitizer
61	108-23-6	Isopropyl chloroformate	<chem>C(OC(=O)Cl)(C)C</chem>	Sensitizer
62	71-48-7	Cobaltous acetate	<chem>[Co+2].CC(=O)[O-].CC(=O)[O-]</chem>	Sensitizer
63	106-92-3	Allyl glycidyl ether	<chem>C1[C@@H](O1)COCC=C</chem>	Sensitizer
64	107-22-2	Glyoxal	<chem>C(=O)C=O</chem>	Sensitizer
65	112-53-8	1-Dodecanol	<chem>C(CCCCC)CCCCCO</chem>	Non-sensitizer
66	1404-04-02	Neomycin	<chem>O1[C@H](O[C@H]2[C@H](O[C@H]3[C@@H]([C@@H]([C@@H]([C@H](O3)CO)O[C@@H]3[C@@H]([C@@H]([C@@H]([C@@H](O3)CN)O)N)O)[C@H]([C@@H]([C@@H]2N)N)O)[C@@H]([C@H]([C@@H](O)[C@H]1CN)O)N</chem>	Sensitizer
67	4170-30-3	Crotonaldehyde	<chem>C(=C)/C=O</chem>	Sensitizer
68	141-43-5	2-Aminoethanol	<chem>C(O)NC</chem>	Sensitizer
69	78-18-2	Cyclohexanone peroxide	<chem>OOC1(CCCCC1)OOC2(O)CCCC2</chem>	Sensitizer
70	2698-41-1	2-Chlorobenzalmalononitrile	<chem>c1(\C=C(C#N)C#N)c(cccc1)Cl</chem>	Sensitizer
71	624-83-9	Methyl isocyanate	<chem>CN=C=O</chem>	Sensitizer
72	12427-38-2	Maneb	<chem>[S-]C(NCCNC([S-])=S)=S.[Mn+2]</chem>	Sensitizer
73	107-02-8	Acrolein	<chem>C=CC=O</chem>	Sensitizer
74	88-73-3	1-Chloro-2-nitrobenzene	<chem>c1(c(cccc1)Cl)[N+](=O)[O-]</chem>	Sensitizer
75	1334-78-7	Methylbenzaldehydes	<chem>c1(ccccc1)C=O.C[*]</chem>	Non-sensitizer
76	77-90-7	Acetyl tributyl citrate	<chem>CCCCOC(=O)CC(CC(=O)OCCCC)(C(=O)OCCCC)OC(=O)C</chem>	Non-sensitizer
77	18454-12-1	Lead chromate oxide	<chem>[Cr](=O)(=O)([O-])[O-].O=[Pb].[Pb+2]</chem>	Sensitizer
78	5307-02-8	2-Methoxy-1,4-benzenediamine	<chem>c1(c(ccc(c1)N)N)OC</chem>	Sensitizer
79	5421-46-5	Ammonium thioglycolate	<chem>C(S)(=O)[O-].[NH4+]</chem>	Sensitizer

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80	7446-08-4	Selenium dioxide	[Se](=O)=O	Sensitizer
81	586-62-9	Terpinolene	C1(=C(C)C)CCC(C)=CC1	Non-sensitizer
82	4680-78-8	C.I. Acid Green	[Na+].CCN(Cc1cccc(c1)S(=O)(=O)[O-])c2ccc(cc2)C(=C3C=CC(=[N+](CC)Cc4cccc(c4)S(=O)(=O)[O-])C=C3)c5cccc5	Sensitizer
83	507-70-0	Borneol	CC1(C)[C@@H]2CC[C@@]1(C)[C@@H](O)C2	Non-sensitizer
84	7488-56-4	Selenium disulfide	[Se](=S)=S	Sensitizer
85	112-55-0	1-Dodecanethiol	C(CCCCC)CCCCCS	Sensitizer
86	123-30-8	4-Aminophenol	c1(ccc(O)cc1)N	Sensitizer
87	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	CN1SC(=CC1=O)Cl	Sensitizer
88	66230-04-4	Esfenvalerate	CC(C)[C@H](C(=O)O)[C@H](C#N)c1cccc(Oc2ccccc2)c1c3ccc(Cl)cc3	Sensitizer
89	7646-79-9	Cobaltous chloride	[Cl-].[Cl-].[Co+2]	Sensitizer
90	108-32-7	Propylene carbonate	O1[C@@H](COC1=O)C	Non-sensitizer
91	101200-48-0	Tribenuron-methyl	Cc1nc(nc(n1)OC)N(C)C(=O)NS(=O)(=O)c2ccccc2C(=O)OC	Sensitizer
92	7664-93-9	Sulfuric acid	S(=O)(=O)(O)O	Non-sensitizer
93	57-11-4	Stearic acid	C(CCCCCCCCCC)CCCCC(=O)O	Non-sensitizer
94	137-26-8	Thiram	CN(C)C(=S)SSC(=S)N(C)C	Sensitizer
95	55297-95-5	Tiamulin	CCN(CC)CCSCC(=O)O[C@@H]1C[C@@](C)(C=C)[C@@H](O)[C@H](C)[C@@]23CC[C@@H](C)[C@@]1(C)[C@@H]2C(=O)CC3	Non-sensitizer
96	63449-39-8	Chlorinated paraffins	CCCC(C)CCCC(C)CCC(C)CCC(C)CCC(C)CCCC(C)CCC	Non-sensitizer
97	4016-14-2	Isopropyl glycidyl ether	C1[C@@H](O1)COC(C)C	Sensitizer
98	97-88-1	n-Butyl methacrylate	C(=O)(OCCCC)C=C(C)C	Sensitizer
99	29973-13-5	Ethiofencarb	c1(c(ccc1)OC(=O)NC)CSCC	Sensitizer
100	52-51-7	Bronopol	C(C(O)([N+](=O)[O-])Br)O	Sensitizer
101	620-23-5	3-Methylbenzaldehyde	c1(cc(ccc1)C)C=O	Non-sensitizer
102	141517-21-7	Trifloxystrobin	C/C(=N)OCc1cccc1/C(=N/OC)/C(=O)OC/c2ccccc2)C(F)(F)F	Sensitizer
103	108-91-8	Cyclohexylamine	C1(CCCCC1)N	Sensitizer
104	104-87-0	4-Methylbenzaldehyde	c1(ccc(cc1)C)C=O	Non-sensitizer
105	75-15-0	Carbon disulfide	C(=S)=S	Sensitizer
106	111-42-2	Diethanolamine	N(CCO)CCO	Sensitizer
107	85-42-7	Hexhydrophthalic anhydride	O1C([C@@H]2CCCC[C@@H]2C1=O)=O	Sensitizer
108	7727-54-0	Ammonium peroxydisulfate	S(OOS(=O)(=O)[O-])(=O)(=O)[O-].[NH4+].[NH4+]	Sensitizer
109	137-66-6	Ascorbyl palmitate	[C@@H]1(OC(=O)C(=C1O)O)[C@H](COC(=O)CCCCCCCCCCCCO)O	Non-sensitizer
110	104-55-2	Cinnamaldehyde	c1(ccccc1)/C=C/C=O	Sensitizer
111	96-09-3	Styrene-7,8-oxide	c1([C@@H]2CO2)cccc1	Sensitizer
112	420-04-2	Cyanamide	C(N)#N	Sensitizer
113	14901-07-6	beta-Ionone	C=1(C(CCCC1C)(C)C)\C=C\C(C)=O	Non-sensitizer
114	5392-40-5	Citral	C(=C/C=O)/(CC/C=C/C)C	Sensitizer
115	126-72-7	Tris(2,3-dibromo-1-propyl)phosphate	P(=O)(OCC(CBr)Br)(OCC(CBr)Br)OCC(CBr)Br	Sensitizer
116	79-10-7	Acrylic acid	C(C=C)(O)=O	Sensitizer
117	129-40-8	1-Chloro-5-nitroanthraquinone	c12c(C(c3c(ccc3C1=O)Cl)=O)cccc2[N+](=O)[O-]	Sensitizer
118	98-86-2	Acetophenone	c1(ccccc1)C(=O)C	Non-sensitizer
119	101-21-3	Chlorpropham	c1(NC(OC(C)C)=O)cc(ccc1)Cl	Sensitizer
120	2655-19-8	Butacarb	CNC(=O)Oc1cc(ccc1)C(C)(C)C(C)C	Sensitizer
121	106-24-1	Geraniol	C(\CC\C=C\C)C(=C)CO	Non-sensitizer
122	75-07-0	Acetaldehyde	CC=O	Sensitizer
123	99-56-9	4-Nitro-1,2-diaminobenzene	c1(cc(c(N)cc1)N)[N+](=O)[O-]	Sensitizer
124	115-27-5	Chlorendic anhydride	C1([C@@]2[C@@H]3[C@@H](C(=O)OC3=O)[C@@]1(C)C(=C2Cl)Cl)Cl	Sensitizer
125	108-24-7	Acetic anhydride	C(OC(=O)C)(C)=O	Sensitizer
126	15972-60-8	Alachlor	c1(N(C(CCl)=O)COC)c(CC)cccc1CC	Sensitizer
127	123-86-4	n-Butyl acetate	O(CCCC)C(C)=O	Non-sensitizer
128	111-70-6	1-Heptanol	C(CCCO)CCC	Non-sensitizer
129	112-92-5	1-Octadecanol	C(CCCCCCCC)CCCCCCCCO	Sensitizer

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130	110-85-0	Piperazine	C1CNCCN1	Sensitizer
131	123-77-3	1,1'-Azobis(formamide)	C(=O)/(N=N/C(=O)N)N	Sensitizer
132	541-73-1	1,3-Dichlorobenzene	c1c(ccc1Cl)Cl	Non-sensitizer
133	22967-92-6	Methylmercury cation	[CH3-][Hg+2]	Sensitizer
134	79-22-1	Methyl chloroformate	C(OC)(=O)Cl	Sensitizer
135	92-52-4	Biphenyl	c1(c2ccccc2)ccccc1	Sensitizer
136	26447-14-3	Cresyl glycidyl ether	c1(OC[C@H]2CO2)ccccc1.C*	Sensitizer
137	129-35-1	1-Chloro-2-methylantraquinone	c12c(C(c3ccccc3C1=O)=O)ccc(c2Cl)C	Sensitizer
138	103-11-7	2-Ethylhexyl acrylate	C([C@H](CCCC)CC)OC(C=C)=O	Non-sensitizer
139	142-91-6	Isopropyl palmitate	C(=O)(OC(C)C)CCCCCCCCCCCCC	Non-sensitizer
140	133-07-3	Flopet	c1ccc2c(c1)C(=O)N(C2=O)SC(Cl)(Cl)Cl	Sensitizer
141	26523-78-4	Tris(nonylphenyl)phosphite	CCCCCCCCCc1cccc1OP(Oc2ccccc2CCCCCCCC)Oc3ccccc3CCCCCCCC	Sensitizer
142	334-48-5	Decanoic acid	C(CCCCC)CCC(=O)O	Non-sensitizer
143	174671-46-6	Tavaborole	c1c(ccc2B(OCc12)O)F	Non-sensitizer
144	110-43-0	2-Heptanone	C(CCCC)C(C)=O	Non-sensitizer
145	818-61-1	2-Hydroxyethyl acrylate	C(OCCO)(C=C)=O	Sensitizer
146	5989-27-5	D-Limonene	C([C@H]1CCC(C)=CC1)(C)=C	Sensitizer
147	107-41-5	2-Methyl-2,4-pentanediol	C(C)[C@H](C)(O)(C)C(O)	Non-sensitizer
148	75-21-8	Ethylene oxide	C1CO1	Sensitizer
149	3761-53-3	Ponceau MX	Cc1ccc(c(c1)C)/N=N/c2c3ccc(cc3cc(c2O)S(=O)(=O)[O-])S(=O)(=O)[O-].[Na+].[Na+]	Sensitizer
150	100-47-0	Benzonitrile	c1(ccccc1)C#N	Non-sensitizer
151	123-15-9	2-Methylpentanaldehyde	C(CCC)(C=O)C	Sensitizer
152	5323-95-5	Sodium ricinoleate	[Na+].CCCCC[C@H](O)C\C=C/CCCCCCCC(=O)[O-]	Sensitizer
153	1918-02-1	Picloram	c1(c(c(c(Cl)c(n1)Cl)N)Cl)C(O)=O	Non-sensitizer
154	1403-66-3	Gentamicin	O([C@H]1[C@H]([C@H]([C@H](O[C@H]2O[C@H]([C@H]([C@H]2N)C)C)C)C)C)C([C@H]1N)O)[C@H]1[C@H]([C@H]([C@H]([C@H]([C@H](O)C(O)C(O)N)C)O)	Non-sensitizer
155	98-01-1	Furfural	c1(ccco1)C=O	Sensitizer
156	150-75-4	N-Methyl-4-aminophenol	c1(ccc(O)cc1)NC	Sensitizer
157	302-01-2	Hydrazine	NN	Sensitizer
158	2425-85-6	C.I. Pigment Red 3	c12c(\N=N\c3c(cc(C)cc3)[N+](=O)[O-])c(ccc1cccc2)O	Sensitizer
159	10124-48-8	Mercuric ammonium chloride	[NH2-].[Cl-].[Hg+2]	Sensitizer
160	142-64-3	Piperazine hydrochloride	C1CNCCN1.Cl.Cl	Sensitizer
161	100-97-0	Methenamine	C1N2CN3CN(CN1C3)C2	Sensitizer
162	30525-89-4	Paraformaldehyde	C=O	Sensitizer
163	128-66-5	C.I. Vat Yellow 4	c12c3c4c5c(cccc5)C(c3ccc1c1c(cccc1)C(c2cc4)=O)=O	Sensitizer
164	2832-40-8	C.I. Disperse Yellow 3	c1(\N=N\c2ccc(NC(C)=O)cc2)c(ccc(c1)C)O	Sensitizer
165	842-07-9	C.I. Solvent Yellow 14	c12c(\N=N\c3ccccc3)c(ccc1cccc2)O	Sensitizer
166	101-90-6	Diglycidyl resorcinol ether	c1cc(cc(c1)OCC2CO2)OCC3CO3	Sensitizer
167	111-27-3	1-Hexanol	CCCCCCO	Non-sensitizer
168	765-34-4	Glycidaldehyde	C1(CO1)C=O	Sensitizer
169	590-00-1	Potassium sorbate	C(=C\C=C\C)\C(=O)[O-].[K+]	Non-sensitizer
170	123-31-9	Hydroquinone	c1(ccc(cc1)O)O	Sensitizer
171	79-94-7	2,2',6,6'-Tetrabromobisphenol A	C(c1cc(c(O)c(c1)Br)Br)(c1cc(c(O)c(c1)Br)Br)(C)C	Non-sensitizer
172	81-88-9	Rhodamine B	c1(c2c(oc3c1ccc(\c3)=[N+](/CC)CC)cc(N(CC)CC)cc2)c1c(cccc1)C(O)=O.[Cl-]	Sensitizer
173	78-93-3	Methyl ethyl ketone	C(CC)(C)=O	Non-sensitizer
174	7789-00-6	Potassium chromate	[Cr](=O)(=O)([O-])[O-].[K+].[K+]	Sensitizer
175	25322-69-4	Polypropylene glycol	O([C@H](CO)C)C[C@H](C)O	Non-sensitizer
176	7647-10-1	Palladium(2+) chloride	[Pd](Cl)Cl	Sensitizer
177	72-14-0	Sulfathiazole	Nc1ccc(cc1)S(=O)(=O)Nc2nccs2	Sensitizer
178	60-12-8	2-Phenylethanol	c1(ccccc1)CCO	Non-sensitizer
179	107-21-1	Ethylene glycol	C(CO)O	Sensitizer
180	16071-86-6	C.I. Direct Brown 95	c1(c2ccc(\N=N\c3cc(c(O)cc3)C(=O)[O-])cc2)ccc(\N=N\c2c(c(\N=N\c3cc(ccc3[O-])S(=O)(=O)[O-])ccc2O)[O-])c1.[Cu+2].[Na+].[Na+]	Sensitizer
181	121-73-3	1-Chloro-3-nitrobenzene	c1(cc(ccc1Cl)[N+](=O)[O-]	Sensitizer
182	101-99-5	Ethyl-n-phenylcarbamate	CCOC(=O)Nc1ccccc1	Sensitizer

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183	25584-83-2	Hydroxypropyl acrylate	<chem>C(=O)(OCCCO)C=C</chem>	Sensitizer
184	104-91-6	4-Nitrosophenol	<chem>c1(ccc(O)cc1)N=O</chem>	Sensitizer
185	106-68-3	3-Octanone	<chem>C(CCCC)C(=O)CC</chem>	Non-sensitizer
186	97-63-2	Ethyl methacrylate	<chem>C(OCC)(C(C)=O)=O</chem>	Sensitizer
187	93-58-3	Methyl benzoate	<chem>COC(=O)c1ccccc1</chem>	Non-sensitizer
188	127-91-3	beta-Pinene	<chem>CC1(C)[C@H]2CCC(=C)[C@@H]1C2</chem>	Sensitizer
189	78-70-6	Linalool	<chem>C([C@@](C=C)(C)O)C\C=C(\C)C</chem>	Non-sensitizer
190	120-80-9	Catechol	<chem>c1(c(ccc1)O)O</chem>	Sensitizer
191	107-96-0	2-Mercaptopropionic acid	<chem>C(C(=O)O)CS</chem>	Non-sensitizer
192	112-05-0	Nonanoic acid	<chem>C(CCCCC)CCC(=O)O</chem>	Non-sensitizer
193	111-54-6	Ethylenebisdithiocarbamic acid	<chem>C(CNC(=S)S)NC(=S)S</chem>	Sensitizer
194	99-49-0	Carvone	<chem>CC(=C)C1CC=C(C)C(=O)C1</chem>	Sensitizer
195	8003-34-7	Pyrethrum	n/a	Non-sensitizer
196	121-21-1	Pyrethrin I	<chem>CC(=C[C@@H]1[C@@H]1[C@@H](C(=O)O[C@H]2CC(=O)C(=C2)C\C=C/C=C)C1(C)C)C</chem>	Non-sensitizer
197	78-11-5	Pentaerythritol tetranitrate	<chem>C(CO[N+](=O)[O-])(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-]</chem>	Non-sensitizer
198	78-94-4	Methyl vinyl ketone	<chem>C(C=C)C(=O)</chem>	Sensitizer
199	3319-31-1	Tri(2-ethylhexyl) trimelliate	<chem>CCCCC(CC)COC(=O)c1ccc(c(c1)C(=O)OCC(CC)CCC)C(=O)OCC(CC)CCCC</chem>	Non-sensitizer
200	2238-07-5	Diglycidyl ether	<chem>C([C@@H]1CO1)OC[C@@H]1CO1</chem>	Sensitizer
201	95-70-5	2-Methyl-1,4-benzenediamine	<chem>Cc1cc(ccc1N)N</chem>	Non-sensitizer
202	3118-97-6	C.I. Solvent Orange 7	<chem>Cc1ccc(N=Nc2c(O)ccc3ccccc23)c(C)c1</chem>	Sensitizer
203	121-29-9	Pyrethrin II	<chem>COC(=O)C(=C[C@@H]1[C@@H]1[C@@H](C(=O)O[C@H]2CC(=O)C(=C2)C\C=C/C=C)C1(C)C)C</chem>	Non-sensitizer
204	334-88-3	Diazomethane	<chem>[N+](=C)=[N-]</chem>	Sensitizer
205	64-00-6	Phenol,3(1-methylethyl)-, methyl carbamate	<chem>c1(cc(ccc1)C(C)C)OC(=O)NC</chem>	Sensitizer
206	10588-01-9	Sodium dichromate	<chem>[Cr](O[Cr])(=O)(=O)[O-])(=O)(=O)[O-].[Na+].[Na+]</chem>	Sensitizer
207	533-74-4	Dazomet	<chem>CN1CN(C=S)SC1C</chem>	Sensitizer
208	23135-22-0	Oxamyl	<chem>CNC(=O)ON=C(SC)C(=O)N(C)C</chem>	Sensitizer
209	14484-64-1	Ferbam	<chem>CN(C)C1=S[Fe+3]23([SH]C(=S2)N(C)C)([SH]C(=S3)N(C)C)[SH]-1</chem>	Sensitizer
210	25155-30-0	Sodium dodecylbenzenesulfonate	<chem>c1(c(cccc1)CCCCCCCCCCCC)S(=O)(=O)[O-].[Na+]</chem>	Sensitizer
211	64-18-6	Formic acid	<chem>C(=O)O</chem>	Sensitizer
212	34681-10-2	Butocarboxim	<chem>CNC(=O)ON=C(C)C(C)SC</chem>	Sensitizer
213	26248-24-8	Sodium tridecylbenzene sulfonate	<chem>c1(ccc(S(=O)(=O)[O-])cc1)CCCCCCCCCCCC.[Na+]</chem>	Sensitizer
214	65907-30-4	Furathiocarb	<chem>c12c(OC(=O)N(SN(C(=O)OCCCC)C)C)cccc1CC(O2)(C)C</chem>	Sensitizer
215	1338-41-6	Sorbitan monostearate	<chem>CCCCCCCCCCCCCCCC(=O)OC[C@@H](O)[C@H]1OC[C@H](O)[C@H]1O</chem>	Sensitizer
216	51218-45-2	Metolachlor	<chem>c1(N([C@@H](COC)C)C(CCl)=O)c(cccc1C)CC</chem>	Sensitizer
217	1967-16-4	Chlorbufam	<chem>c1(NC(O[C@@H](C#C)C)=O)cc(ccc1)Cl</chem>	Sensitizer
218	82-68-8	Pentachloronitrobenzene	<chem>c1(c(c(c(Cl)c(Cl)Cl)Cl)Cl)[N+](=O)[O-]</chem>	Sensitizer
219	26644-46-2	Triforine	<chem>C(N1CCN(CC1)C(C(Cl)(Cl)Cl)NC=O)(Cl)(Cl)Cl)NC=O</chem>	Sensitizer
220	90-43-7	o-Phenylphenol	<chem>c1(c2c(cccc2)O)ccccc1</chem>	Non-sensitizer
221	1918-18-9	Swep	<chem>c1(cc(c(Cl)cc1)Cl)NC(OC)=O</chem>	Sensitizer
222	12122-67-7	Zineb	<chem>C(CNC(=S)[S-])NC1=S[Zn+2][SH]-1</chem>	Non-sensitizer
223	75-02-5	Vinyl fluoride	<chem>C=C(F)</chem>	Non-sensitizer
224	25402-06-6	Cinerin I	<chem>C\C=C/CC1=C(C)[C@H](CC1=O)OC(=O)[C@@H]2[C@@H]1(C=C(C)C)C2(C)C</chem>	Non-sensitizer
225	121-20-0	Cinerin II	<chem>COC(=O)C(=C[C@@H]1[C@@H]1[C@@H](C(=O)O[C@H]2CC(=O)C(=C2)C\C=C/C)C1(C)C)C</chem>	Non-sensitizer
226	90982-32-4	Chlorimuron-ethyl	<chem>CCOC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc2nc(cc(n2)Cl)OC</chem>	Non-sensitizer
227	138-86-3	Limonene	<chem>C([C@@H]1CCC(C)=CC1)(C)=C</chem>	Non-sensitizer
228	112-60-7	Tetraethylene glycol	<chem>O(CCOCCO)CCOCCO</chem>	Non-sensitizer
229	7787-47-5	Beryllium chloride	<chem>[Be](Cl)Cl</chem>	Sensitizer
230	19044-88-3	Oryzalin	<chem>c1(c(cc(S(N)(=O)=O)cc1[N+](=O)[O-])[N+](=O)[O-])N(CCC)CCC</chem>	Sensitizer
231	556-52-5	Glycidol	<chem>C1(CO1)CO</chem>	Sensitizer



Number	CAS number	Chemical name	SMILES string	Binary sensitization status
232	89-32-7	Pyromellitic dianhydride	<chem>c12c(c(=O)oc1=O)cc1c(=O)oc(c1c2)=O</chem>	Sensitizer
233	503-38-8	Diphosgene	<chem>C(OC(=O)Cl)(Cl)(Cl)Cl</chem>	Sensitizer
234	110-02-1	Thiophene	<chem>c1ccsc1</chem>	Sensitizer
235	9003-73-0	Polylimonene	<chem>C([C@@H]1CCC(C)=CC1)(C)=C</chem>	Sensitizer
236	81-48-1	Alizuroil purple	<chem>c12c(C(=O)c3c(C2=O)cccc3)c(ccc1Nc1ccc(cc1)C)O</chem>	Sensitizer
237	94-36-0	Benzoyl peroxide	<chem>c1(C(OOC(c2cccc2)=O)=O)cccc1</chem>	Sensitizer
238	34681-23-7	Butoxycarboxim	<chem>CNC(=O)ON=C(C)C(S(=O)(=O)C</chem>	Sensitizer
239	12108-13-3	Methylcyclopentadienyl manganese tricarbonyl	<chem>[C-]1(C=CC=C1)C.[O+]#[C-].[O+]#[C-].[O+]#[C-].[Mn+]</chem>	Non-sensitizer
240	2451-62-9	Triglycidyl isocyanurate	<chem>n1(c(n(c(=O)n(c1=O)C)[C@@H]1CO1)C[C@@H]1CO1)=O)C[C@@H]1CO1</chem>	Sensitizer
241	80-48-8	Methyl p-methylbenzenesulfonate	<chem>S(c1ccc(C)cc1)(OC)(=O)=O</chem>	Sensitizer
242	94-09-7	Benzocaine	<chem>c1cc(C(OCC)=O)ccc1N</chem>	Sensitizer
243	87-56-9	Mucochloric acid	<chem>C(=O)/C(=C(\C(=O)O)/Cl)/Cl</chem>	Sensitizer
244	84-65-1	Anthraquinone	<chem>c12c(C(c3cccc3C1=O)=O)cccc2</chem>	Sensitizer
245	461-58-5	Cyanoguanidine	<chem>NC(=N)NC#N</chem>	Non-sensitizer
246	5466-77-3	Octinoxate	<chem>CCCCC(CC)COC(=O)C=Cc1ccc(OC)cc1</chem>	Non-sensitizer
247	51-78-5	4-Aminophenol hydrochloride	<chem>c1(ccc(O)cc1)N.Cl</chem>	Sensitizer
248	541-41-3	Ethyl chloroformate	<chem>O(C(=O)Cl)CC</chem>	Sensitizer
249	106-50-3	1,4-Benzenediamine	<chem>c1cc(ccc1N)N</chem>	Sensitizer
250	624-49-7	Dimethyl fumarate	<chem>C(\C=C\C(OC)=O)(OC)=O</chem>	Sensitizer
251	89-61-2	1,4-Dichloro-2-nitrobenzene	<chem>c1(c(ccc(c1)Cl)Cl)[N+](=O)[O-]</chem>	Sensitizer
252	6846-50-0	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	<chem>C([C@@H](OC(C(C)C)=O)C(C)C)(COC(C(C)C)=O)(C)C</chem>	Non-sensitizer
253	79-11-8	Chloroacetic acid	<chem>C(CCl)(O)=O</chem>	Sensitizer
254	1303-28-2	Arsenic pentoxide	<chem>[As](=O)(=O)O[As](=O)=O</chem>	Sensitizer
255	78-51-3	Tris(2-butoxyethyl) phosphate	<chem>P(=O)(OCCOCCCC)(OCCOCCCC)OCCOCCCC</chem>	Non-sensitizer
256	82-44-0	1-Chloroanthraquinone	<chem>c12c(C(c3cccc3C1=O)=O)cccc2Cl</chem>	Sensitizer
257	117-11-3	1-Amino-5-chloroanthraquinone	<chem>c12c(C(c3c(cccc3C1=O)Cl)=O)cccc2N</chem>	Sensitizer
258	110-66-7	Amyl mercaptan	<chem>C(CCS)CC</chem>	Sensitizer
259	75567-37-2	Ingenol mebutate	<chem>C1=C([C@@H]([C@@]2([C@@]31[C@@@H](C[C@@H]1[C@@H]([C@@H](C=C([C@H]2O)CO)C3=O)[C@]1(C)C)C)O)OC(=O)/C(=C\C)C</chem>	Non-sensitizer
260	64-17-5	Ethanol	<chem>CCO</chem>	Sensitizer
261	62-53-3	Aniline	<chem>c1ccc(cc1)N</chem>	Sensitizer
262	106-25-2	Nerol	<chem>C(=C\C(O)\CC/C=C/C)C</chem>	Non-sensitizer
263	2682-20-4	Methylisothiazolinone	<chem>Cn1c(=O)ccs1</chem>	Sensitizer
264	106-23-0	Citronellal	<chem>C(CC/C=C/C)C(C)C</chem>	Non-sensitizer
265	110-27-0	Isopropyl myristate	<chem>C(CCCCCCCCCC)C(=O)OC(C)C</chem>	Non-sensitizer
266	488-10-8	Jasmone	<chem>CC\C=C/CC1=C(C)CCC1=O</chem>	Non-sensitizer
267	1490-04-6	Menthol	<chem>C1[C@@H]([C@@H]([C@@H]([C@@H](C1)O)C)C</chem>	Non-sensitizer
268	55-56-1	Chlorhexidine	<chem>c1(NC(NC(NCCCCNC(NC(Nc2ccc(Cl)cc2)=N)=N)=N)ccc(Cl)cc1</chem>	Sensitizer
269	4080-31-3	N-(3-Chloroallyl)hexaminium chloride	<chem>[N+]12(CN3CN(C1)CN(C2)C3)\C=C\Cl.[ClH-]</chem>	Non-sensitizer
270	68603-42-9	Coconut diethanolamide	n/a	Non-sensitizer
271	65277-42-1	Ketoconazole	<chem>CC(=O)N1CCN(CC1)c2ccc(cc2)OC[C@@H]3CO[C@@](O3)(Cn4ccnc4)c5ccc(cc5Cl)Cl</chem>	Sensitizer
272	59-87-0	Nitrofurazone	<chem>c1(cc(cc1)/C=N/NC(=O)N)[N+](=O)[O-]</chem>	Sensitizer
273	121-33-5	Vanillin	<chem>c1(cc(ccc1O)C=O)OC</chem>	Non-sensitizer
274	109-16-0	Triethylene glycol dimethacrylate	<chem>O(C(C)C)=O)CCOCCOCCO(C(C)C)=O</chem>	Sensitizer
275	26761-40-0	Diisodecyl phthalate	<chem>CC(C)CCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCC</chem>	Non-sensitizer
276	26027-38-3	Nonoxynols	<chem>c1(ccc(OCCO)cc1)CCCCCCCC</chem>	Non-sensitizer
277	110-97-4	Diisopropanolamine	<chem>C([C@@H](C)O)NC[C@@H](C)O</chem>	Non-sensitizer
278	811-97-2	1,1,1,2-Tetrafluoroethane	<chem>C(CF)(F)(F)F</chem>	Non-sensitizer
279	2835-95-2	5-Amino-o-cresol	<chem>c1(c(ccc(c1)N)C)O</chem>	Sensitizer
280	21087-64-9	Metribuzin	<chem>CC(C)C1C(=O)n(c(nn1)SC)N</chem>	Non-sensitizer

Number	CAS number	Chemical name	SMILES string	Binary sensitization status
281	564-25-0	Doxycycline	<chem>C[C@H]1c2cccc(c2C(=O)C3=C([C@]4([C@@H]([C@H]([C@H]13)O)[C@@H](C(=C(C4=O)C(=O)N)O)N(C)C)O)O</chem>	Sensitizer
282	105-55-5	N,N'-Diethylthiourea	<chem>C(NCC)(NCC)=S</chem>	Sensitizer
283	150-13-0	4-Aminobenzoic acid	<chem>c1cc(ccc1C(=O)O)N</chem>	Sensitizer
284	8001-54-5	Benzalkonium chloride compounds	<chem>c1(C[N+](C)(C)*)cccc1.[ClH-]</chem>	Sensitizer
285	100-51-6	Benzyl alcohol	<chem>OCC1CCCC1</chem>	Non-sensitizer
286	97-64-3	Ethyl lactate	<chem>CCOC(=O)C(C)O</chem>	Non-sensitizer
287	111-77-3	Diethylene glycol monomethyl ether	<chem>C(OCCO)COC</chem>	Non-sensitizer
288	28553-12-0	Diisononyl phthalate	<chem>CCCCCCC(C)COC(=O)c1cccc1C(=O)OCC(C)CCCCC</chem>	Non-sensitizer
289	92-87-5	Benzidine	<chem>c1(c2ccc(N)cc2)ccc(N)cc1</chem>	Sensitizer
290	7446-34-6	Selenium sulfide	<chem>S=[Se]</chem>	Sensitizer
291	102-76-1	Triacetin	<chem>C(COC(C)=O)(COC(C)=O)OC(C)=O</chem>	Non-sensitizer
292	55283-68-6	Ethalfuralin	<chem>c1(c(cc(C(F)(F)F)cc1[N+](=O)[O-])[N+](=O)[O-])N(CC(C)=C)CC</chem>	Sensitizer
293	110-19-0	Isobutyl acetate	<chem>C(COC(=O)C)(C)C</chem>	Non-sensitizer
294	6440-58-0	1,3-Dimethylol-5,5-dimethylhydantoin	<chem>CC1(C(=O)N(C(=O)N1CO)CO)C</chem>	Sensitizer
295	101-54-2	p-Aminodiphenylamine	<chem>c1(Nc2cccc2)ccc(N)cc1</chem>	Sensitizer
296	124-07-2	Octanoic acid	<chem>C(CCCCC)CC(O)=O</chem>	Non-sensitizer
297	137-30-4	Ziram	<chem>C(=S)(N(C)C)[S-].[S-]C(N(C)C)=S.[Zn+2]</chem>	Sensitizer
298	54-64-8	Thimerosal	<chem>c1(c(ccc1)C(=O)[O-])[S][Hg]CC.[Na+]</chem>	Sensitizer
299	104-61-0	Dihydro-5-pentyl-2(3H)-furanone	<chem>CCCCC1CCC(=O)O1</chem>	Non-sensitizer
300	79-57-2	Oxytetracycline	<chem>C[C@]1(c2cccc(c2C(=O)C3=C([C@]4([C@@H]([C@H]([C@H]13)O)[C@@H](C(=C(C4=O)C(=O)N)O)N(C)C)O)O)O</chem>	Sensitizer
301	868-77-9	2-Hydroxyethyl methacrylate	<chem>C(=O)(C(=C)C)OCCO</chem>	Sensitizer
302	92-48-8	Methyl coumarin	<chem>c12c(cc(=O)cc2)ccc(c1)C</chem>	Non-sensitizer
303	55-65-2	Guanethidine	<chem>N1(CCN(C(=N)N)CCN1)CCCCC1</chem>	Sensitizer
304	505-60-2	Bis(2-chloroethyl)sulfide	<chem>S(CCCl)CCCl</chem>	Sensitizer
305	95-48-7	o-Cresol	<chem>c1(c(ccc1)O)C</chem>	Sensitizer
306	63-25-2	Carbaryl	<chem>c12c(OC(NC)=O)cccc1cccc2</chem>	Sensitizer
307	81-14-1	Musk ketone	<chem>c1(c(c(c(C(=O)C)c1[N+](=O)[O-])C)C)[N+](=O)[O-]C(C)C</chem>	Non-sensitizer
308	21245-02-3	Padimate O	<chem>c1(C(=O)OCC(CCCC)CC)ccc(cc1)N(C)C</chem>	Sensitizer
309	95-95-4	2,4,5-Trichlorophenol	<chem>c1c(cc(c1Cl)Cl)Cl)O</chem>	Non-sensitizer
310	69430-24-6	Cyclomethicone	<chem>[Si](O*)(*)C(C)C</chem>	Non-sensitizer
311	126-73-8	Tributyl phopshate	<chem>CCCCOP(=O)(OCCCC)OCCCC</chem>	Non-sensitizer
312	80-08-0	Dapsone	<chem>S(c1ccc(N)cc1)(c1ccc(N)cc1)(=O)=O</chem>	Sensitizer
313	105-54-4	Ethyl n-butylate	<chem>C(=O)(CCC)OCC</chem>	Non-sensitizer
314	122-97-4	3-Phenylpropanol	<chem>c1(ccccc1)CCCO</chem>	Non-sensitizer
315	106-22-9	Citronellol	<chem>C(CC/C=C(/C)C)(CCO)C</chem>	Non-sensitizer
316	131-74-8	Ammonium picrate	<chem>c1(c(cc(c1)[N+](=O)[O-])[N+](=O)[O-])[O-][N+](=O)[O-].[NH4+]</chem>	Sensitizer
317	75-91-2	tert-Butyl hydroperoxide	<chem>C(OO)(C)C(C)C</chem>	Sensitizer
318	99-87-6	p-Cymene	<chem>c1(C(C)C)ccc(C)cc1</chem>	Non-sensitizer
319	111-90-0	Diethylene glycol monomethyl ether	<chem>C(OCC)OCCO</chem>	Non-sensitizer
320	684-93-5	N-nitroso-n-methylurea	<chem>CN(C(=O)N)N=O</chem>	Sensitizer
321	12002-03-8	Paris Green	<chem>CC(=O)[O-].CC(=O)[O-].[O-].[As]1O[As](O[As](O1)[O-])[O-].[O-].[As]1O[As](O[As](O1)[O-])[O-].[Cu+2].[Cu+2].[Cu+2].[Cu+2]</chem>	Sensitizer
322	542-92-7	1,3-Cyclopentadiene	<chem>C1C=CC=C1</chem>	Sensitizer
323	123-62-6	Propionic anhydride	<chem>O(C(C)=O)C(C(C)=O)</chem>	Sensitizer
324	85-68-7	Butyl benzyl phthalate	<chem>CCCCOC(=O)c1cccc1C(=O)OCC2CCCC2</chem>	Non-sensitizer
325	1222-05-5	Galaxolide	<chem>O1C[C@@H](c2c(cc3c(C([C@@H](C)C3(C)C)(C)C)c2)C1)C</chem>	Non-sensitizer
326	5471-51-2	Raspberry ketone	<chem>CC(=O)CCc1ccc(cc1)O</chem>	Non-sensitizer
327	105-60-2	Caprolactam	<chem>C1(CCCCCN1)=O</chem>	Sensitizer
328	108-78-1	Melamine	<chem>c1(nc(nc(n1)N)N)N</chem>	Non-sensitizer
329	35367-38-5	Diflubenzuron	<chem>c1(C(=O)NC(=O)Nc2ccc(cc2)Cl)c(cccc1F)F</chem>	Non-sensitizer

Number	CAS number	Chemical name	SMILES string	Binary sensitization status
330	79538-32-2	Tefluthrin	<chem>Cc1c(c(c(c1F)F)COC(=O)[C@H]2[C@H](C2(C)C)/C=C(C(F)(F)F)Cl)F</chem>	Non-sensitizer
331	25956-17-6	Allura red ac dye	<chem>c12c(cc(cc2)S(=O)(=O)[O-])ccc(c1/N=N/c1c(cc(c1)C)S(=O)(=O)[O-])OC.[Na+].[Na+]</chem>	Non-sensitizer
332	563-80-4	Methyl isopropyl ketone	<chem>C(C(C)=O)(C)C</chem>	Non-sensitizer
333	106-31-0	Butyric anhydride	<chem>C(=O)(OC(=O)CCC)CCC</chem>	Sensitizer
334	121-32-4	Ethyl vanillin	<chem>CCOc1cc(ccc1O)C=O</chem>	Non-sensitizer
335	143-08-8	1-Nonanol	<chem>CCCCCCCCCO</chem>	Non-sensitizer
336	13454-96-1	Platinum tetrachloride	<chem>[Pt](Cl)(Cl)(Cl)Cl</chem>	Sensitizer
337	107-46-0	Hexamethyldisiloxane	<chem>[Si](O[Si](C)(C)C)(C)(C)C</chem>	Non-sensitizer
338	111-13-7	2-Octanone	<chem>C(CC(=O)C)CCCC</chem>	Non-sensitizer
339	94-59-7	Safrole	<chem>c12c(ccc(c1)CC=C)OCO2</chem>	Non-sensitizer
340	2216-51-5	(L)-Menthol	<chem>C1[C@H]([C@@H]([C@H]([C@H](C1)O)C)C)C</chem>	Non-sensitizer
341	10025-65-7	Platinous chloride	<chem>[Pt](Cl)Cl</chem>	Sensitizer
342	39300-45-3	Dinocap	<chem>c1(c(cccc1)[N+](=O)[O-])OC(C=C)C=O.C(CCCC)C[C@@H](C)*.[N+](=O)[O-]</chem>	Sensitizer
343	6317-18-6	Methylene thiocyanate	<chem>C(SC#N)SC#N</chem>	Non-sensitizer
344	138-89-6	N,N-Dimethyl-p-nitrosoaniline	<chem>c1(ccc(N=O)cc1)N(C)C</chem>	Sensitizer
345	148-79-8	Thiabendazole	<chem>c1ccc2c(c1)[nH]c(n2)c3cscn3</chem>	Non-sensitizer
346	36653-82-4	1-Hexadecanol	<chem>CCCCCCCCCCCCCCCCO</chem>	Non-sensitizer
347	26571-11-9	Nonoxynol-9	<chem>c1(ccc(cc1)CCCCCCCC)OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO</chem>	Sensitizer
348	77-09-8	Phenolphthalein	<chem>C1(c2c(cccc2)C(O1)=O)(c1ccc(O)cc1)c1ccc(O)cc1</chem>	Sensitizer
349	101-81-5	1,1'-Methylenebibenzene	<chem>c1(Cc2ccccc2)ccccc1</chem>	Non-sensitizer
350	60-00-4	Ethylenediamine tetraacetic acid	<chem>N(CCN(CC(O)=O)CC(O)=O)(CC(O)=O)CC(O)=O</chem>	Sensitizer
351	21593-23-7	Cepharin	<chem>N12[C@@H]([C@@H](NC(CSc3ccncc3)=O)C2=O)SCC(=C1C(O)=O)COC(C)=O</chem>	Sensitizer
352	81-21-0	Dicyclopentadiene dioxide	<chem>C1[C@@H]2[C@@H]3[C@@H]([C@@H]([C@@H]1[C@@H]1[C@@H]2O1)C[C@@H]1[C@@H]3O1</chem>	Non-sensitizer
353	98-59-9	p-Toluenesulfonyl chloride	<chem>S(=O)(=O)(c1ccc(cc1)C)Cl</chem>	Sensitizer
354	96-08-2	1,2:8,9-Diepoxy-p-menthane	<chem>C12C(O1)(CCC(C2)C1C(O1)C)C</chem>	Non-sensitizer
355	104-93-8	1-Methoxy-4-methylbenzene	<chem>COc1ccc(C)cc1</chem>	Non-sensitizer
356	121-39-1	Ethyl-2,3-epoxy-3-phenylpropionate	<chem>C1(C(O1)C(=O)OCC)c1cccc1</chem>	Non-sensitizer
357	140-67-0	1-Methoxy-4-(2-propenyl)benzene	<chem>c1(ccc(OC)cc1)CC=C</chem>	Non-sensitizer
358	409-02-9	Methylheptenone	<chem>C(=C)CCC(=O)C(C)C</chem>	Non-sensitizer
359	103-64-0	beta-Bromostyrene	<chem>c1(ccccc1)/C=C/Br</chem>	Non-sensitizer
360	54-42-2	Idoxuridine	<chem>OC[C@H]1O[C@H](C[C@@H]1O)N2C=C(I)C(=O)NC2=O</chem>	Sensitizer
361	589-18-4	4-Methylbenzyl alcohol	<chem>Cc1ccc(CO)cc1</chem>	Non-sensitizer
362	8002-75-3	Palm Oil (From Fruit)	n/a	Non-sensitizer
363	12656-85-8	C.I. Pigment Red 104	n/a	Sensitizer
364	7440-06-4	Platinum	<chem>[Pt]</chem>	Sensitizer
365	9006-65-9	Dimethicone	n/a	Non-sensitizer
366	8006-64-2	Turpentine	n/a	Sensitizer
367	68647-73-4	Tea tree oil	n/a	Sensitizer
368	25265-71-8	Dipropylene glycol	n/a	Non-sensitizer
369	8000-27-9	Cedarwood oil	n/a	Non-sensitizer
370	8008-57-9	Oil of Orange	n/a	Non-sensitizer
371	8000-42-8	Oil of Caraway	n/a	Non-sensitizer
372	7440-02-0	Nickel, elemental	<chem>[Ni]</chem>	Sensitizer
373	8015-64-3	Angelica oils	n/a	Non-sensitizer
374	8016-23-7	Guaiac wood oil	n/a	Non-sensitizer
375	8006-84-6	Fennel oil	n/a	Sensitizer

Tab. S3: Raw numbers for global performance metrics

Model	Number of chemicals entered into model (n)	Number of predictions returned – base settings (n)					Number of predictions returned – optimized settings (n)				
		TP	TN	FP	FN	Total	TP	TN	FP	FN	Total
<b>Basketter et al. (2014)</b>											
PredSkin	123	91	10	10	12	123	54	1	7	1	63
Toxtree*	123	69	16	4	34	123	n/a	n/a	n/a	n/a	n/a
QSAR Toolbox**	123	53	5	6	5	69	53	5	6	5	69
REACHAcross™	131	75	13	7	28	123	34	8	1	10	53
Danish QSAR Database	131	41	13	3	28	85	33	9	3	24	69
CAESAR	123	67	8	11	20	106	47	5	1	10	63
TIMES-SS	123	38	17	1	57	113	61	11	0	20	92
Derek	123	85	17	3	17	122	85	17	3	13	118
<b>HSDB</b>											
PredSkin	361	206	37	94	24	361	113	1	26	0	140
Toxtree*	361	127	85	46	103	361	n/a	n/a	n/a	n/a	n/a
QSAR Toolbox**	361	103	34	39	17	193	103	34	39	17	193
REACHAcross™	375	169	78	52	57	356	75	37	18	10	140
Danish QSAR Database	375	98	81	20	43	242	75	72	14	28	189
CAESAR	361	138	34	89	51	312	44	14	42	5	105
TIMES-SS	361	98	107	19	104	328	59	41	19	18	137
Derek	361	154	85	44	72	355	154	78	44	50	326

TP: true positive; TN: true negative; FP: false positive; FN: false negative

\* Toxtree is a structural alert model and, therefore, does not have any optimization features.

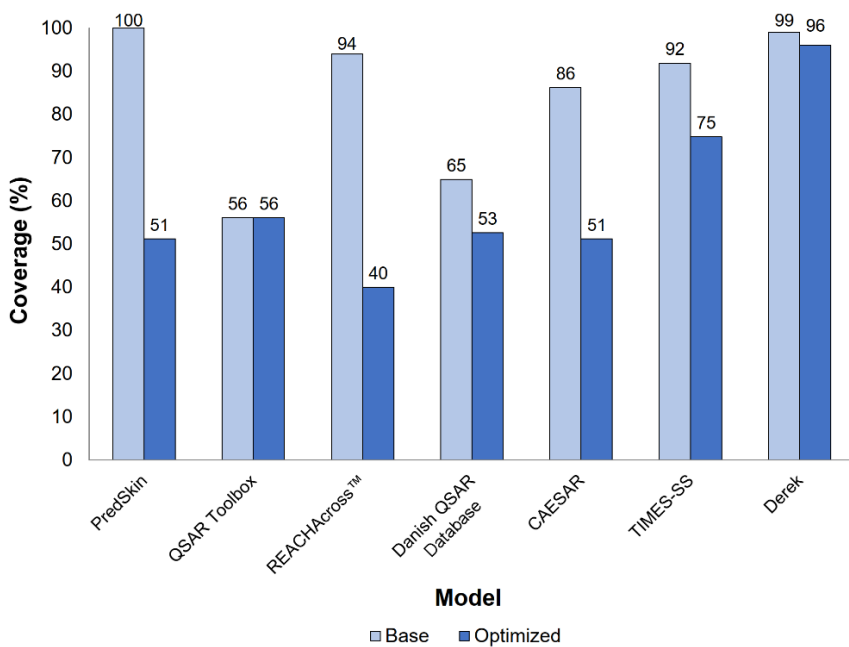
\*\*For QSAR Toolbox, both the base and optimized settings have the same numbers because the automated batch mode applies the same settings universally.

Tab. S4: Model sensitivity and specificity for high confidence results

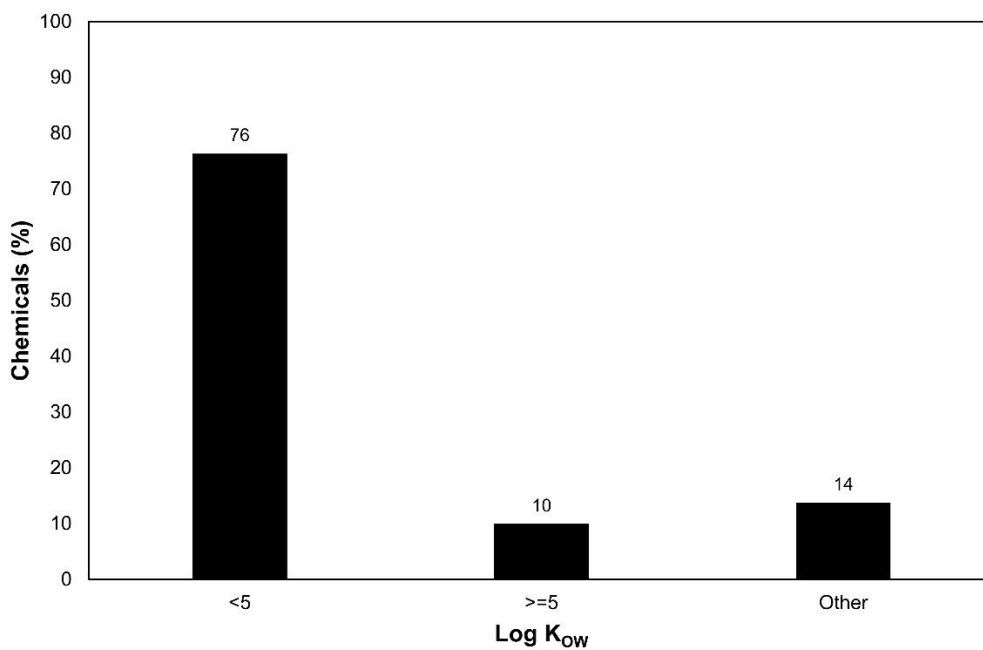
Model	Sensitivity (%)	Specificity (%)
<b>Basketter et al. (2014)</b>		
PredSkin	98	13
Toxtree	67	80
QSAR Toolbox	91	45
REACHAcross™	77	89
Danish QSAR Database	58	75
CAESAR	82	83
TIMES-SS	75	100
Derek	87	85
<b>HSDB</b>		
PredSkin	100	4
Toxtree	55	65
QSAR Toolbox	86	47
REACHAcross™	88	67
Danish QSAR Database	73	84
CAESAR	90	25
TIMES-SS	77	68
Derek	75	64

**Tab. S5: Model false predictions for high confidence results**

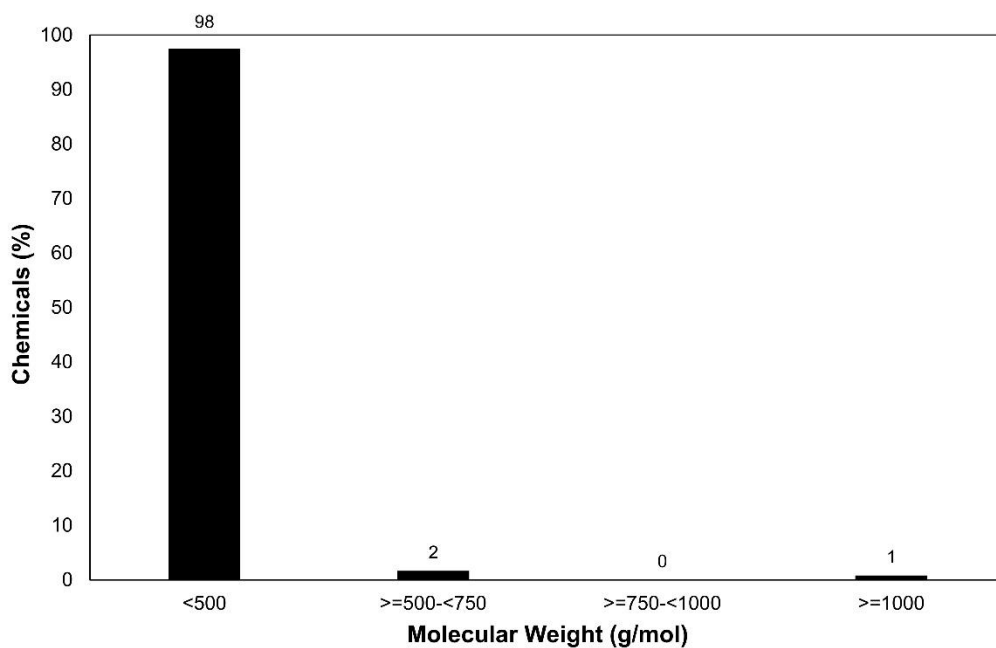
Model	False positive (%)	False negative (%)	False predictions (%)
<b>Basketter et al. (2014)</b>			
PredSkin	88	2	13
Toxtree	20	33	31
QSAR Toolbox	55	9	16
REACHAcross™	11	23	21
Danish QSAR Database	25	42	39
CAESAR	17	18	17
TIMES-SS	0	25	22
Derek	15	13	14
<b>HSDB</b>			
PredSkin	96	0	19
Toxtree	35	45	41
QSAR Toolbox	53	14	29
REACHAcross™	33	12	20
Danish QSAR Database	16	27	22
CAESAR	75	10	45
TIMES-SS	32	23	27
Derek	36	25	29



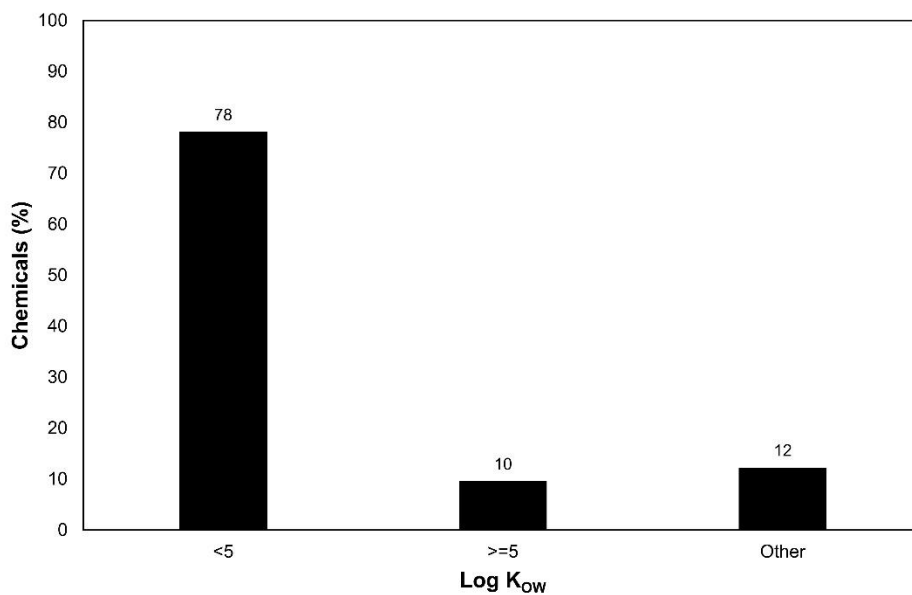
**Fig. S1: Model coverage for Basketter et al. (2014) data set using both base and optimized settings**



**Fig. S2: Partition coefficient distribution for Basketter et al. (2014) data set**  
 "Other" indicates that no experimental data were available, and a prediction could not be made due to a problem with the SMILES string.

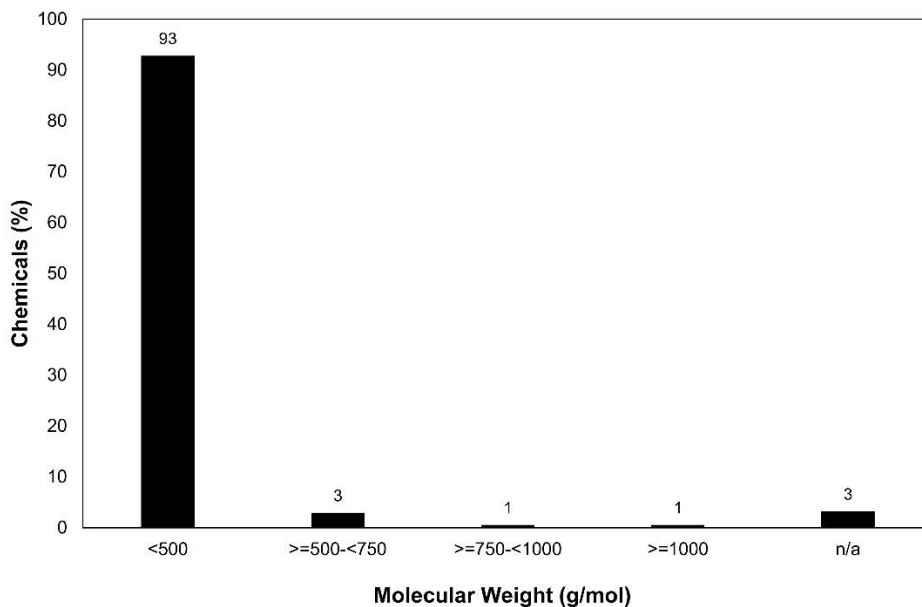


**Fig. S3: Molecular weight distribution for Basketter et al. (2014) data set**



**Fig. S4: Partition coefficient distribution for HSDB data set**

“Other” indicates that no experimental data were available, and a prediction could not be made due to a problem with the SMILES string.



**Fig. S5: Molecular weight distribution for HSDB data set**

“n/a” indicates that the chemical was a mixture, so no discrete molecular weight could be identified.