

Mapping Chemical Respiratory Sensitization: How Useful Are Our Current Computational Tools?

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Supplemental Information

#1	“Organic chemicals” [Mesh] OR “Inorganic chemicals” [Mesh] OR chemical*[tiab]
#2	"Occupational Exposure" [Mesh] OR "Inhalation Exposure" [Mesh] OR "Allergens/chemical synthesis" [Mesh] OR "Allergens/chemistry" [Mesh] OR "Allergens/toxicity" [Mesh] OR respiratory allergen*[tw] OR respiratory sensitizer*[tw] OR respiratory sensitiser*[tw] OR inhalational expos*[tw] OR inhalation expos*[tw] OR toxic inhalation*[tw] OR chemically induced[tw] OR chemical causation[tw] OR chemical cause*[tw] OR causing chemicals[tw] OR chemical determinant*[tw] OR occupational expos*[tw] OR chemical respirator*[tw] OR chemical allergen*[tw] OR sensitizing chemical*[tw] OR sensitising chemical*[tw]
#3	"Respiratory Hypersensitivity" [Mesh] OR "Alveolitis, Extrinsic Allergic" [Mesh] OR "Asthma/chemically induced" [Mesh:NoExp] OR "Asthma, Occupational/chemically induced" [Mesh] OR respiratory hypersensitivity[tw] OR occupational asthma[tw] OR hypersensitivity pneumonit*[tw] OR Extrinsic Allergic Alveolit*[tw] OR respiratory sensitization*[tw] OR respiratory sensitisation*[tw] OR occupational asthma*[tw] OR workplace asthma*[tw] OR respiratory allerg*[tw]
#4	#1 AND #2 AND #3
#5	animals [Mesh] NOT humans [Mesh]
#6	#4 NOT #5

Table S1: Scoping Search Strategy. *Supplemental Table 1 contains search terms included in our scoping search strategy.*

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
1	18503	3173-72-6	1,5-Naphthalene diisocyanate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
2	11443	584-84-9	2,4-Toluene diisocyanate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Lalko et al. 2012; Seed et al. 2015; HSDB
3	7040	91-08-7	2,6-Toluene diisocyanate	Sensitizer	Graham et al. 1997; Enoch et al. 2012; Lalko et al. 2012; HSDB
4	11082	551-16-6	6-Amino penicillanic acid	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
5	6249	69-53-4	Ampicillin	Sensitizer	Graham et al. 1997; Enoch et al. 2012
6	5904	61-33-6	Benzylpenicillin	Sensitizer	Graham et al. 1997; Enoch et al. 2012
7	78141	4424-06-0	Brilliant orange GR	Sensitizer	Graham et al. 1997
8	10255083	1260-17-9	Carminic acid	Sensitizer	Graham et al. 1997
9	27447	15686-71-2	Cephalexin	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
10	2713	55-56-1	Chlorhexidene	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015
11	3039	62-73-7	Dichlorvos	Sensitizer	Graham et al. 1997

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
12	7902	108-01-0	Dimethyl ethanolamine	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
13	7570	101-68-8	Diphenyl methane-4,4*- diisocyanate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Lalko et al. 2012; Seed et al. 2015; HSDB
14	65064	989-51-5	Epigallocatechin gallate	Sensitizer	Graham et al. 1997; Enoch et al. 2012; Seed et al. 2015
15	700	141-43-5	Ethanolamine	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
16	81530	7085-85-0	Ethyl cyanoacrylate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
17	3301	107-15-3	Ethylenediamine	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012 Seed et al. 2015
18	3346	55-38-9	Fenthion	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
19	13192	822-06-0	Hexamethylene diisocyanate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015; HSDB

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
20	169132	4098-71-9	Isophorone diisocyanate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015; HSDB
21	7923	108-31-6	Maleic anhydride	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015;
22	8711	137-05-3	Methyl-2-cyanoacrylate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
23	38853	555-30-6	Methyldopa	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
24	6811	85-44-9	Phthalic anhydride	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015; HSDB
25	43672	61477-96-1	Piperacillin	Sensitizer	Graham et al. 1997; Enoch et al. 2012
26	4837	110-85-0	Piperazine	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015
27	104836	16462-65-0	Plicatic acid	Sensitizer	Graham et al. 1997; Enoch et al. 2012; Seed et al. 2015
28	15910	1897-45-6	Tetrachloroisophthalonitrile	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Seed et al. 2015

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
29	8326	117-08-8	Tetrachlorophthalic anhydride	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015
30	5565	112-24-3	Triethylenetetramine	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
31	11089	552-30-7	Trimellitic anhydride	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015; HSDB
32	5280440	1401-69-0	Tylosin	Sensitizer	Graham et al. 1997; Enoch et al. 2012
33	67005	116-66-5	1,1,3,3,5-Pentamethyl-4,6-Dinitroindane	Non-sensitizer	Graham et al. 1997
34	n/a	470-67-7	1,4-Cineole	Non-sensitizer	Graham et al. 1997
35	8103	111-27-3	1-Hexanol	Non-sensitizer	Graham et al. 1997
36	94602	62346-96-7	2,4-Dimethyl benzyl acetate	Non-sensitizer	Graham et al. 1997
37	94569	54546-26-8	2-Butyl-4,4,6-trimethyl-1,3-dioxane	Non-sensitizer	Graham et al. 1997
38	62240	67874-72-0	2-tert-Amylcyclohexyl acetate	Non-sensitizer	Graham et al. 1997
39	108506	60763-42-0	3,6-Dimethyloctan-3-yl acetate	Non-sensitizer	Graham et al. 1997
40	61361	6066-49-5	3-Butyl phthalide	Non-sensitizer	Graham et al. 1997
41	61585	13171-00-1	4-Acetyl-6-tert-butyl-1,1-dimethylindane	Non-sensitizer	Graham et al. 1997
42	39801	50816-18-7	9-Decenyl acetate	Non-sensitizer	Graham et al. 1997
43	6930	88-29-9	Acetyl ethyltetramethyltetralin	Non-sensitizer	Graham et al. 1997

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
44	8878	142-19-8	Allyl heptylate	Non-sensitizer	Graham et al. 1997
45	7650	103-37-7	Benzyl butyrate	Non-sensitizer	Graham et al. 1997
46	7353	97-87-0	Butyl isobutyrate	Non-sensitizer	Graham et al. 1997
47	6616	79-92-5	Camphene	Non-sensitizer	Graham et al. 1997
48	5372353	65405-76-7	cis-3-Hexenyl anthranilate	Non-sensitizer	Graham et al. 1997
49	5362620	21662-09-9	cis-4-Decen-1-al	Non-sensitizer	Graham et al. 1997
50	40058	52671-32-6	Citronellyl nitrile	Non-sensitizer	Graham et al. 1997
51	20508	4442-79-9	Cyclohexylethyl alcohol	Non-sensitizer	Graham et al. 1997
52	11002	544-40-1	Dibutyl sulfide	Non-sensitizer	Graham et al. 1997
53	66768	95-41-0	Dihydro-isojasmone	Non-sensitizer	Graham et al. 1997
54	80865	6413-10-1	Ethyl acetoacetate ethylene glycol ketal	Non-sensitizer	Graham et al. 1997
55	7344	97-64-3	Ethyl lactate	Non-sensitizer	Graham et al. 1997
56	25238	10402-33-2	Eugenyl phenylacetate	Non-sensitizer	Graham et al. 1997
57	16821	2305-05-7	g-Dodecalactone	Non-sensitizer	Graham et al. 1997
58	5353011	94-48-4	Geranyl benzoate	Non-sensitizer	Graham et al. 1997
59	62592	5870-93-9	Heptyl butyrate	Non-sensitizer	Graham et al. 1997
60	8058	110-54-3	Hexane	Non-sensitizer	Graham et al. 1997
61	637523	16930-96-4	Hexyl tiglate	Non-sensitizer	Graham et al. 1997
62	7795	106-27-4	Isoamyl butyrate	Non-sensitizer	Graham et al. 1997
63	7336	97-45-0	l-Carvyl propionate	Non-sensitizer	Graham et al. 1997
64	89479	21280-29-5	Lactoscatone	Non-sensitizer	Graham et al. 1997
65	5323652	6622-76-0	Methyl tiglate	Non-sensitizer	Graham et al. 1997
66	20739	4621-04-9	p-Isopropylcyclohexanol	Non-sensitizer	Graham et al. 1997
67	62341	93-92-5	Phenylethyl acetate	Non-sensitizer	Graham et al. 1997
68	61035	112-19-6	Undecenyl acetate	Non-sensitizer	Graham et al. 1997
69	712	50-00-0	Formaldehyde	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015; HSDB*
70	5852	52-67-5	Penicillamine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
71	3767	54-85-3	Isoniazid	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
72	n/a	60-54-8	Tetracycline	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
73	176	64-19-7	Acetic acid	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
74	23663979	69-52-3	Ampicillin	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
75	23668834	69-57-8	Benzyl penicillin	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
76	3598	70-30-4	Hexachlorophene	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
77	5340	72-14-0	Sulfathiazole	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
78	6354	75-21-8	Ethylene oxide	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
79	6658	80-62-6	Methylmethacrylate	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015; HSDB*
80	85689	85-42-7	Hexahydrophthalic anhydride	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015; HSDB*
81	2723	88-04-0	Chloroxylenol	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012
82	6966	89-32-7	Pyromellitic dianhydride	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
83	3314	98-00-0	Furfuryl alcohol	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
84	7361	100-37-8	2-Diethylethanolamine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
85	7501	100-42-5	Styrene	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
86	4101	100-97-0	Hexamethylene tetramine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
87	7814	106-50-3	Paraphenylene diamine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
88	7972	109-02-4	N-methylmorpholine	Sensitizer	Jarvis et al. 2005
89	7993	109-55-7	3- dimethylaminopropylamine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015;
90	3485	111-30-8	Glutaraldehyde	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015; HSDB
91	8112	111-41-1	Aminoethylethanolamine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
92	8343	117-81-7	Diocetylphthalate	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012
93	73341	121-25-5	Amprolium hydrochloride	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
94	785	123-31-9	Hydroquinone	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
95	31269	123-77-3	Azodicarbonamide	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
96	196	124-04-9	Adipic acid	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
97	3641960	127-65-1	Chloramine-T	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Lalko et al. 2012; Seed et al. 2015

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
98	3092	148-01-6	2-methyl-3,5-dinitrobenzamide	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
99	9351	304-20-1	Hydralazine	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
100	67539	305-80-6	Pauli's Reagent (4-diazobenzenesulphonic acid)	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
101	9433	317-34-0	Aminophylline	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
102	10569	514-10-3	Abietic acid	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
103	5462328	561-27-3	Diacetyl morphine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
104	441328	957-68-6	7-aminocephalosporanic acid	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
105	637794	2746-19-2	Himic anhydride	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
106	16760159	2939-80-2	Captafol	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
107	77411	3779-63-3	1,3,5-tris-(6-isocyanatohexyl)-,1,3,5-triazinane-2,4,6-trione	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
108	19950	4035-89-6	Biuret of hexamethylene diisocyanate	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
109	442461	13466-78-9	3-carene	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012
110	76956083	28983-56-4	Methyl blue	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
111	3035399	31330-63-9	Tetrazene	Sensitizer	Jarvis et al. 2005; Seed et al. 2015

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
112	39859	36519-31-0	Salbutamol	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
113	170253	39878-87-0	Phenylglycine acid chloride	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
114	65324	49745-95-1	Dobutamine HCl	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012
115	2756	51481-61-9	Cimetidine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
116	62883	61336-70-7	Amoxicillin	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
117	124621	123354-92-7	Sodium isononanoyloxybenzene sulphonate	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
118	5464110	52-26-6	Morphine hydrochloride	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
119	8113	111-42-2	Diethanolamine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
120	8265	115-27-5	Chlorendic anhydride	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
121	10236	485-47-2	Ninhydrin	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
122	n/a	860-22-0	Indigotine	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
123	17142	2451-62-9	Triglycidyl isocyanurate	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
124	17520	2634-33-5	1,2-benzisothiazolin-3-one	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
125	83975	7696-12-0	Tetramethrin	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
126	53172	38661-72-2	1,3-Bis(isocyanatomethyl) cyclohexane	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
127	42008	56796-20-4	Cefmetazole	Sensitizer	Jarvis et al. 2005
128	23666879	59703-84-3	Piperacillin	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
129	94611	64265-57-2	polyfunctional aziridine	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
130	4212	65271-80-9	Mitoxanthrone	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
131	47964	66592-87-8	Cefadroxil	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
132	5481173	72558-82-8	Ceftazidime	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
133	91731	79622-59-6	Fluazinam	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
134	5362114	82547-81-7	Cefteram pivoxil	Sensitizer	Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015
135	n/a	125700-67-6	2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate	Sensitizer	Jarvis et al. 2005; Seed et al. 2015
136	93377	68123-13-7	Basic blue 99	Sensitizer	Lalko et al. 2012
137	102090420	17095-24-8	Black GR Reactive Dye	Sensitizer	Lalko et al. 2012
138	7954	108-77-0	Cyanuric chloride	Sensitizer	Lalko et al. 2012
139	82984	12225-83-1	Orange 3R reactive dye	Sensitizer	Lalko et al. 2012
140	n/a	10343-58-5	Reactive yellow	Sensitizer	Lalko et al. 2012
141	77336	3740-18-9	2,4-dichloro-5-chlorsulfonyl-benzoic acid	Sensitizer	Enoch et al. 2012; Seed et al. 2015
142	2723869	16691-43-3	3-amino-5-mercapto-1,2,4-triazole	Sensitizer	Enoch et al. 2012; Seed et al. 2015

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
143	4075	89-57-6	5-aminosalicylic acid	Sensitizer	Enoch et al. 2012; Seed et al. 2015
144	6400459	37539-03-0	7-amino-3-thiomethyl-3-cephalosporanic acid	Sensitizer	Seed et al. 2015
145	2286	1675-54-3	Diglycidyl ether of bisphenol A	Sensitizer	Enoch et al. 2012; Seed et al. 2015
146	12736	693-23-2	Dodecanedioic acid	Sensitizer	Enoch et al. 2012; Seed et al. 2015
147	12560	114-07-8	Erythromycin	Sensitizer	Seed et al. 2015
148	90504	24447-78-7	Ethoxylated bisphenol A diacrylate	Sensitizer	Seed et al. 2015
149	3314	97-53-0	Eugenol	Sensitizer	Enoch et al. 2012; Seed et al. 2015
150	188203	77430-27-4	Glycyl compound	Sensitizer	Enoch et al. 2012; Seed et al. 2015
151	8753	139-07-1	Lauryl dimethyl benzyl ammonium chloride	Sensitizer	Seed et al. 2015
152	6438396	64761-66-6	MM22383	Sensitizer	Enoch et al. 2012; Seed et al. 2015
153	4807	643-79-8	Ortho-phthalaldehyde (1,2-Phthalic dicarboxaldehyde)	Sensitizer	Seed et al. 2015
154	6042	59-43-8	Thiamine	Sensitizer	Enoch et al. 2012; Seed et al. 2015
155	27200	15318-45-3	Thiamphenicol	Sensitizer	Enoch et al. 2012; Seed et al. 2015
156	7618	102-71-6	Triethanolamine	Sensitizer	Seed et al. 2015
157	27423	15625-89-5	Trimethylolpropane triacrylate	Sensitizer	Enoch et al. 2012; Seed et al. 2015
158	60196281	74610-55-2	Tylosin tartrate	Sensitizer	Seed et al. 2015
159	75500	2422-91-5	Triphenylmethane triisocyanate	Sensitizer	Seed et al. 2015
160	n/a	26471-62-5	Toluene diisocyanate	Sensitizer	HSDB
161	7672	103-71-9	Phenyl isocyanate	Sensitizer	HSDB

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
162	16760159	2425-06-1	Captafol	Sensitizer	Enoch et al. 2012; HSDB
163	11167	556-61-6	Methyl isothiocyanate	Sensitizer	HSDB
164	25517	12125-02-9	Ammonium chloride	Sensitizer	HSDB
165	7607	102-36-3	3,4-Dichlorophenyl isocyanate	Sensitizer	HSDB
166	7693	104-12-1	4-Chlorophenyl isocyanate	Sensitizer	HSDB
167	8111	111-40-0	Diethylenetriamine	Sensitizer	HSDB
168	6581	79-10-7	Acrylic acid	Non-sensitizer	HSDB
169	18502	3173-53-3	Cyclohexylisocyanate	Sensitizer	Graham et al. 1997; Jarvis et al. 2005; Enoch et al. 2012; Seed et al. 2015; HSDB
170	6588	79-27-6	1,1,2,2-Tetrabromoethane	Non-sensitizer	Enoch et al. 2012
171	7115	92-94-4	1,1':4',1'-Terphenyl	Non-sensitizer	Enoch et al. 2012
172	7247	95-63-6	1,2,4-Trimethylbenzene	Non-sensitizer	Enoch et al. 2012
173	7839	106-93-4	1,2-Dibromoethane	Non-sensitizer	Enoch et al. 2012
174	10707	528-29-0	1,2-Dinitrobenzene	Non-sensitizer	Enoch et al. 2012
175	4685	106-46-7	1,4-Dichlorobenzene	Non-sensitizer	Enoch et al. 2012
176	7474	100-00-5	1-Chloro-4-nitrobenzene	Non-sensitizer	Enoch et al. 2012
177	13387	872-50-4	1-Methyl-2-pyrrolidone	Non-sensitizer	Enoch et al. 2012
178	8134	111-77-3	2-(2-Methoxyethoxy)ethanol	Non-sensitizer	Enoch et al. 2012
179	1486	94-75-7	2,4-Dichlorophenoxyacetic acid	Non-sensitizer	Enoch et al. 2012
180	7958	108-83-8	2,6-Dimethylheptan-4-one	Non-sensitizer	Enoch et al. 2012
181	31404	128-37-0	2,6-Di-tert-butyl-p-cresol	Non-sensitizer	Enoch et al. 2012
182	10757	532-27-4	2-Chloroacetophenone	Non-sensitizer	Enoch et al. 2012
183	62783	24468-13-1	2-Ethylhexyl chloroformate	Non-sensitizer	Enoch et al. 2012
184	61249	999-61-1	2-Hydroxypropyl acrylate	Non-sensitizer	Enoch et al. 2012
185	398	79-46-9	2-Nitropropane	Non-sensitizer	Enoch et al. 2012
186	10439	504-29-0	2-Pyridylamine	Non-sensitizer	Enoch et al. 2012
187	6984	89-72-5	2-sec-Butylphenol	Non-sensitizer	Enoch et al. 2012
188	6544	78-59-1	3,5,5-Trimethylcyclohex-2-enone	Non-sensitizer	Enoch et al. 2012
189	7308	96-69-5	6,6'-Di-tert-butyl-4,4'-thiodi-m-cresol	Non-sensitizer	Enoch et al. 2012
190	180	67-64-1	Acetone	Non-sensitizer	Enoch et al. 2012
191	7855	107-13-1	Acrylonitrile	Non-sensitizer	Enoch et al. 2012

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
192	33613	26787-78-0	Amoxicillin	Sensitizer	Enoch et al. 2012
193	8732	137-88-2	Amprolium hydrochloride	Sensitizer	Enoch et al. 2012
194	2347	85-68-7	Benzyl butyl phthalate	Non-sensitizer	Enoch et al. 2012
195	159055	76-22-2	Bornan-2-one	Non-sensitizer	Enoch et al. 2012
196	9411	314-40-9	Bromacil (ISO)	Non-sensitizer	Enoch et al. 2012
197	263	71-36-3	Butan-1-ol	Non-sensitizer	Enoch et al. 2012
198	18594026	133-06-2	Captan (ISO)	Non-sensitizer	Enoch et al. 2012
199	47965	50370-12-2	Cefadroxil	Sensitizer	Enoch et al. 2012
200	33	107-20-0	Chloroacetaldehyde	Non-sensitizer	Enoch et al. 2012
201	6372	75-45-6	Chlorodifluoromethane	Non-sensitizer	Enoch et al. 2012
202	2730	2921-88-2	Chloropyrifos (ISO)	Non-sensitizer	Enoch et al. 2012
203	643833	156-59-2	cis 1,2-dichloroethylene	Non-sensitizer	Enoch et al. 2012
204	6429	76-14-2	Cryofluorane(INN)	Non-sensitizer	Enoch et al. 2012
205	7966	108-93-0	Cyclohexanol	Non-sensitizer	Enoch et al. 2012
206	8560	131-17-9	Diallyl phthalate	Non-sensitizer	Enoch et al. 2012
207	3026	84-74-2	Dibutyl phthalate	Non-sensitizer	Enoch et al. 2012
208	6777	84-61-7	Dicyclohexyl phthalate	Non-sensitizer	Enoch et al. 2012
209	6781	84-66-2	Diethyl phthalate	Non-sensitizer	Enoch et al. 2012
210	6163	64-67-5	Diethyl sulphate	Non-sensitizer	Enoch et al. 2012
211	6782	84-69-5	Diisobutyl phthalate	Non-sensitizer	Enoch et al. 2012
212	33599	26761-40-0	Diisodecyl phthalate	Non-sensitizer	Enoch et al. 2012
213	3018042	28553-12-0	Diisononyl phthalate	Non-sensitizer	Enoch et al. 2012
214	33934	27554-26-3	Diisooctyl phthalate	Non-sensitizer	Enoch et al. 2012
215	8554	131-11-3	Dimethyl phthalate	Non-sensitizer	Enoch et al. 2012
216	6787	84-76-4	Dinonyl phthalate	Non-sensitizer	Enoch et al. 2012
217	7583	101-84-8	Diphenyl ether	Non-sensitizer	Enoch et al. 2012
218	11487	122-39-4	Diphenylamine	Non-sensitizer	Enoch et al. 2012

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
219	7570	26447-40-5	Diphenylmethane di-isocyanate	Sensitizer	Enoch et al. 2012
220	3224	115-29-7	Endosulfan	Non-sensitizer	Enoch et al. 2012
221	702	64-17-5	Ethanol	Non-sensitizer	Enoch et al. 2012
222	10928	541-41-3	Ethyl chloroformate	Non-sensitizer	Enoch et al. 2012
223	8025	109-94-4	Ethyl formate	Non-sensitizer	Enoch et al. 2012
224	3562	151-67-7	Halothane	Non-sensitizer	Enoch et al. 2012
225	8051	110-43-0	Heptan-2-one	Non-sensitizer	Enoch et al. 2012
226	11583	591-78-6	Hexan-2-one	Non-sensitizer	Enoch et al. 2012
227	3637	86-54-4	Hydralazine	Sensitizer	Enoch et al. 2012
228	6556	78-78-4	Isopentane	Non-sensitizer	Enoch et al. 2012
229	4004	121-75-5	Malathion	Non-sensitizer	Enoch et al. 2012
230	15413	1634-04-4	Methyl-tert-butyl ether	Non-sensitizer	Enoch et al. 2012
231	198243	26590-20-5	Methyltetrahydrophthalic anhydride	Sensitizer	Enoch et al. 2012
232	11723	598-56-1	N,N-Dimethylethylamine	Non-sensitizer	Enoch et al. 2012
233	10041	463-82-1	Neopentane	Non-sensitizer	Enoch et al. 2012
234	89594	54-11-5	Nicotine	Non-sensitizer	Enoch et al. 2012
235	7515	100-61-8	N-Methylaniline	Non-sensitizer	Enoch et al. 2012
236	971	144-62-7	Oxalic acid	Non-sensitizer	Enoch et al. 2012
237	4790	298-02-2	Phorate	Non-sensitizer	Enoch et al. 2012
238	15965	1918-02-1	Picloram (ISO)	Non-sensitizer	Enoch et al. 2012
239	6954	88-89-1	Picric acid	Non-sensitizer	Enoch et al. 2012
240	8893	142-64-3	Piperazine dihydrochloride	Non-sensitizer	Enoch et al. 2012
241	4944	114-26-1	Propoxur	Non-sensitizer	Enoch et al. 2012
242	4946	525-66-6	Propranolol	Non-sensitizer	Enoch et al. 2012
243	7397	98-59-9	p-Toluenesulphonyl chloride	Non-sensitizer	Enoch et al. 2012
244	289	120-80-9	Pyrocatechol	Non-sensitizer	Enoch et al. 2012
245	6758	83-79-4	Rotenone (ISO)	Non-sensitizer	Enoch et al. 2012
246	2083	18559-94-9	Salbutamol	Sensitizer	Enoch et al. 2012
247	23690431	136-78-7	Sodium 2-(2,4-dichlorophenoxy)ethyl sulphate	Non-sensitizer	Enoch et al. 2012

Number	CID	CASRN	Chemical Name	Sensitization Status	Reference(s)
248	5988	57-50-1	Sucrose	Non-sensitizer	Enoch et al. 2012
249	3032425	2422-88-0	1,1,3-Tributylthiourea (TBTU)	Sensitizer	Enoch et al. 2012
250	31373	127-18-4	Tetrachloroethylene	Non-sensitizer	Enoch et al. 2012
251	1140	108-88-3	Toluene	Non-sensitizer	Enoch et al. 2012
252	31357	126-73-8	Tributyl phosphate	Non-sensitizer	Enoch et al. 2012
253	6423	76-06-2	Trichloronitromethane	Non-sensitizer	Enoch et al. 2012
254	8376	118-96-7	Trinitrotoluene	Non-sensitizer	Enoch et al. 2012
255	6527	78-30-8	Tri-o-tolyl phosphate	Non-sensitizer	Enoch et al. 2012
256	8289	115-86-6	Triphenyl phosphate	Non-sensitizer	Enoch et al. 2012
257	186099	25656-78-4	Triphenylmethane triisocyanate	Sensitizer	Enoch et al. 2012

*The chemical sensitization status of this chemical was a non-sensitizer according to HSDB; however, the sensitization status did not agree with the status in the other references. A conservative approach was taken to be protective of human health, and the chemical was labeled as a sensitizer.

Table S2: Data Sets. *Supplemental Table 2 presents the complete discrete chemical data set. Duplicates have been removed, and chemicals without a usable CASRN or SMILES string were removed. Some chemicals curated from HSDB were classified as non-sensitizers based on available data; however, this sensitization status did not agree with the other references for that chemical (as indicated by an asterisk next to “HSDB” in the References column). Therefore, these chemicals were classified as sensitizers based on a weight-of-evidence approach and to be protective of human health.*

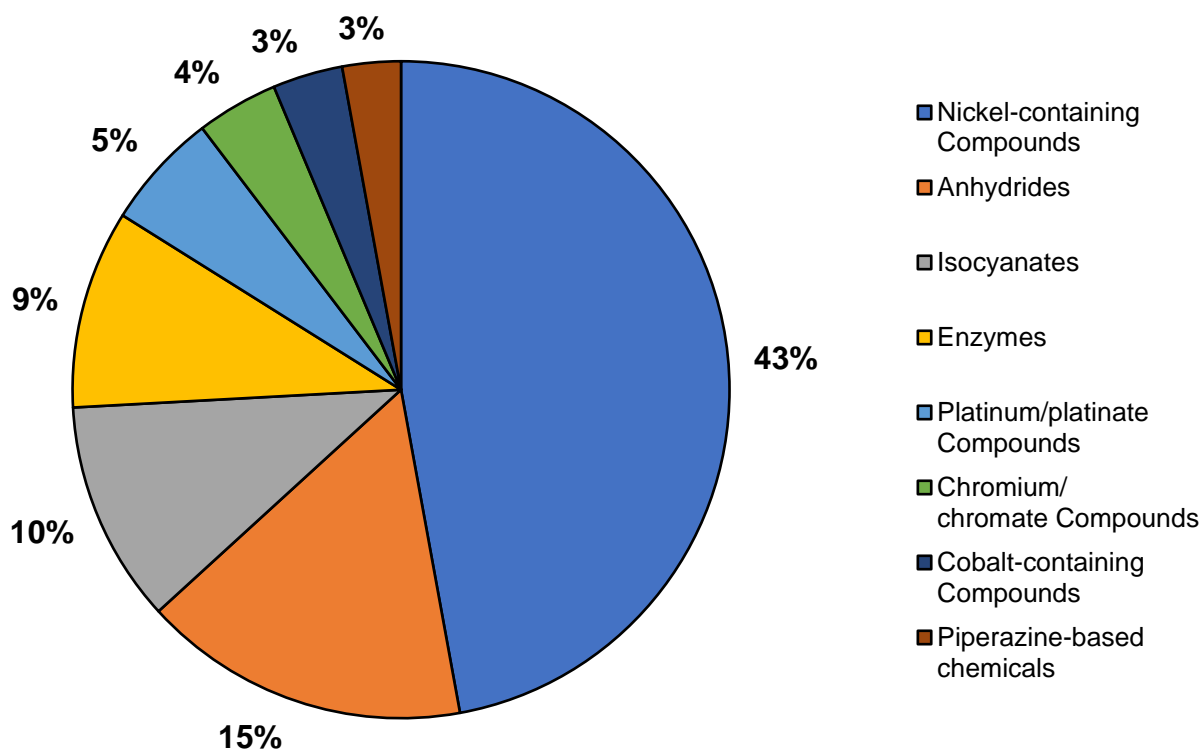


Figure S1: Harmonized CLP Classification Respiratory Sensitization Chemical Category Distribution. *Supplemental Figure 1 presents the harmonized CLP classifications for respiratory sensitization (n=191) by chemical class. Most chemicals with harmonized classifications were metals (55%) in addition to other well-accepted respiratory sensitizers (anhydrides and isocyanates).*

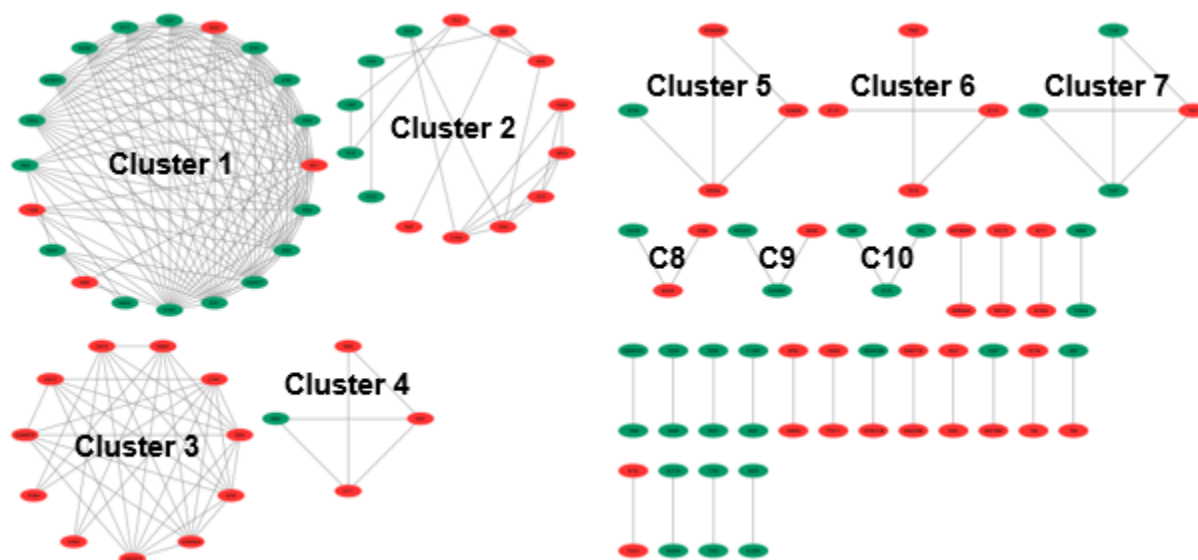


Figure S2: Chemical Similarity Map for the Discrete Chemical Data Set with all Clusters Identified. Supplemental Figure 2 displays the chemical similarity map (similarity cutoff=80%) for all chemicals in the data set that had at least one neighbor ($n=110$) and identifies each cluster with a number. Cluster 8, Cluster 9, and Cluster 10 were abbreviated to C8, C9, and C10, respectively, to adhere to size constraints of the figure. Each chemical in each cluster is identified by CASRN, CID, Chemical name, and sensitization status with the corresponding number of neighbors (using a similarity cutoff of 80%) in Table S2.

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
1	1	84-66-2	6781	Diethyl phthalate	Non-sensitizer	17
	2	6066-49-5	61361	3-Butyl phthalide	Non-sensitizer	17
	3	131-11-3	8554	Dimethyl phthalate	Non-sensitizer	16
	4	131-17-9	8560	Diallyl phthalate	Non-sensitizer	16
	5	94-48-4	5353011	Geranyl benzoate	Non-sensitizer	16
	6	85-44-9	6811	Phthalic anhydride	Sensitizer	16
	7	84-76-4	6787	Dinonyl phthalate	Non-sensitizer	15
	8	84-69-5	6782	Diisobutyl phthalate	Non-sensitizer	15
	9	84-74-2	3026	Dibutyl phthalate	Non-sensitizer	15
	10	117-81-7	8343	Diocetylphthalate	Sensitizer	14
	11	84-61-7	6777	Dicyclohexyl phthalate	Non-sensitizer	14
	12	85-68-7	2347	Benzyl butyl phthalate	Non-sensitizer	14
	13	27554-26-3	33934	Diisooctyl phthalate	Non-sensitizer	12
	14	28553-12-0	3018042	Diisononyl phthalate	Non-sensitizer	12
	15	26761-40-0	33599	Diisodecyl phthalate	Non-sensitizer	12
	16	103-37-7	7650	Benzyl butyrate	Non-sensitizer	9
	17	552-30-7	11089	Trimellitic anhydride	Sensitizer	6
	18	93-92-5	62341	Phenylethyl acetate	Non-sensitizer	5
	19	89-32-7	6966	Pyromellitic dianhydride	Sensitizer	3
	20	62346-96-7	94602	2,4-Dimethyl benzyl acetate	Non-sensitizer	2
2	1	584-84-9	11443	2,4-Toluene diisocyanate	Sensitizer	5
	2	91-08-7	7040	2,6-Toluene diisocyanate	Sensitizer	5
	3	3173-72-6	18503	1,5-Naphthalene diisocyanate	Sensitizer	4
	4	26447-40-5	7570	Diphenylmethane di-isocyanate	Sensitizer	4
	5	2422-91-5	75500	Triphenylmethane triisocyanate	Sensitizer	3
	6	106-50-3	7814	Paraphenylene diamine	Sensitizer	3
	7	103-71-9	7672	Phenyl isocyanate	Sensitizer	3
	8	104-12-1	7693	4-Chlorophenyl isocyanate	Sensitizer	3
	9	118-96-7	8376	Trinitrotoluene	Non-sensitizer	2
	10	122-39-4	11487	Diphenylamine	Non-sensitizer	2
	11	100-61-8	7515	N-Methylaniline	Non-sensitizer	2
	12	100-00-5	7474	1-Chloro-4-nitrobenzene	Non-sensitizer	2
	13	102-36-3	7607	3,4-Dichlorophenyl isocyanate	Sensitizer	1
	14	528-29-0	10707	1,2-Dinitrobenzene	Non-sensitizer	1
3	1	69-53-4	6249	Ampicillin	Sensitizer	8
	2	61-33-6	5904	Benzylpenicillin	Sensitizer	8
	3	15686-71-2	27447	Cephalexin	Sensitizer	8
	4	69-52-3	23663979	Ampicillin	Sensitizer	8

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
	5	69-57-8	23668834	Benzyl penicillin	Sensitizer	8
	6	61336-70-7	62883	Amoxicillin	Sensitizer	7
	7	26787-78-0	33613	Amoxicillin	Sensitizer	7
	8	61477-96-1	43672	Piperacillin	Sensitizer	6
	9	59703-84-3	23666879	Piperacillin	Sensitizer	6
	10	50370-12-2	47965	Cefadroxil	Sensitizer	3
	11	66592-87-8	47964	Cefadroxil	Sensitizer	3
4	1	110-85-0	4837	Piperazine	Sensitizer	3
	2	111-40-0	8111	Diethylenetriamine	Sensitizer	3
	3	112-24-3	5565	Triethylenetetramine	Sensitizer	2
	4	142-64-3	8893	Piperazine dihydrochloride	Non-sensitizer	2
5	1	989-51-5	65064	Epigallocatechin gallate	Sensitizer	3
	2	1260-17-9	10255083	Carminic acid	Sensitizer	2
	3	16462-65-0	104836	Plicatic acid	Sensitizer	2
	4	83-79-4	6758	Rotenone (ISO)	Non-sensitizer	1
6	1	111-42-2	8113	Diethanolamine	Sensitizer	2
	2	102-71-6	7618	Triethanolamine	Sensitizer	2
	3	111-41-1	8112	Aminoethylethanolamine	Sensitizer	1
	4	108-01-0	7902	Dimethyl ethanolamine	Sensitizer	1
7	1	95-63-6	7247	1,2,4-Trimethylbenzene	Non-sensitizer	3
	2	100-42-5	7501	Styrene	Sensitizer	3
	3	108-88-3	1140	Toluene	Non-sensitizer	2
	4	92-94-4	7115	1,1':4',1'-Terphenyl	Non-sensitizer	2
8	1	24447-78-7	90504	Ethoxylated bisphenol A diacrylate	Sensitizer	2
	2	10402-33-2	25238	Eugenyl phenylacetate	Non-sensitizer	1
	3	1675-54-3	2286	Diglycidyl ether of bisphenol A	Sensitizer	1
9	1	6622-76-0	5323652	Methyl tiglate	Non-sensitizer	2
	2	80-62-6	6658	Methylmethacrylate	Sensitizer	1
	3	16930-96-4	637523	Hexyl tiglate	Non-sensitizer	1
10	1	111-27-3	8103	1-Hexanol	Non-sensitizer	2
	2	108-93-0	7966	Cyclohexanol	Non-sensitizer	1
	3	71-36-3	263	Butan-1-ol	Non-sensitizer	1
No cluster identified;	1	128-37-0	31404	2,6-Di-tert-butyl-p-cresol	Non-sensitizer	1
	2	89-72-5	6984	2-sec-Butylphenol	Non-sensitizer	1

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
chemicals with only one neighbor in chemical similarity map	3	94-75-7	1486	2,4-Dichlorophenoxyacetic acid	Non-sensitizer	1
	4	136-78-7	23690431	Sodium 2-(2,4-dichlorophenoxy)ethyl sulphate	Non-sensitizer	1
	5	4442-79-9	20508	Cyclohexylethyl alcohol	Non-sensitizer	1
	6	4621-04-9	20739	p-Isopropylcyclohexanol	Non-sensitizer	1
	7	97-87-0	7353	Butyl isobutyrate	Non-sensitizer	1
	8	106-27-4	7795	Isoamyl butyrate	Non-sensitizer	1
	9	79-27-6	6588	1,1,2,2-Tetrabromoethane	Non-sensitizer	1
	10	13171-00-1	61585	4-Acetyl-6-tert-butyl-1,1-dimethylindane	Non-sensitizer	1
	11	106-93-4	7839	1,2-Dibromoethane	Non-sensitizer	1
	12	88-29-9	6930	Acetyl ethyltetramethyltetralin	Non-sensitizer	1
	13	1401-69-0	5280440	Tylosin	Sensitizer	1
	14	74610-55-2	60196281	Tylosin tartrate	Sensitizer	1
	15	36519-31-0	39859	Salbutamol	Sensitizer	1
	16	4098-71-9	169132	Isophorone diisocyanate	Sensitizer	1
	17	18559-94-9	2083	Salbutamol	Sensitizer	1
	18	38661-72-2	53172	1,3-Bis(isocyanatomethyl)cyclohexane	Sensitizer	1
	19	3779-63-3	77411	1,3,5-tris-(6-isocyanato-hexyl)-,1,3,5-triazinane-2,4,6-trione	Sensitizer	1
	20	7085-85-0	81530	Ethyl cyanoacrylate	Sensitizer	1
	21	4035-89-6	19950	Biuret of hexamethylene diisocyanate	Sensitizer	1
	22	137-05-3	8711	Methyl-2-cyanoacrylate	Sensitizer	1
	23	2425-06-1	16760159	Captafol	Sensitizer	1
	24	133-06-2	18594026	Captan (ISO)	Non-sensitizer	1
	25	561-27-3	5462328	Diacetyl morphine	Sensitizer	1
	26	52-26-6	5464110	Morphine hydrochloride	Sensitizer	1
	27	304-20-1	9351	Hydralazine	Sensitizer	1
	28	86-54-4	3637	Hydralazine	Sensitizer	1
	29	127-65-1	3641960	Chloramine-T	Sensitizer	1
	30	98-59-9	7397	p-Toluenesulphonyl chloride	Non-sensitizer	1
	31	124-04-9	196	Adipic acid	Sensitizer	1
	32	693-23-2	12736	Dodecanedioic acid	Sensitizer	1
	33	123-31-9	785	Hydroquinone	Sensitizer	1
	34	120-80-9	289	Pyrocatechol	Non-sensitizer	1
	35	121-25-5	73341	Amprolium hydrochloride	Sensitizer	1
	36	137-88-2	8732	Amprolium hydrochloride	Sensitizer	1
	37	78-30-8	6527	Tri-o-tolyl phosphate	Non-sensitizer	1

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
	38	115-86-6	8289	Triphenyl phosphate	Non-sensitizer	1
	39	110-43-0	8051	Heptan-2-one	Non-sensitizer	1
	40	591-78-6	11583	Hexan-2-one	Non-sensitizer	1
No Neighbors (Not pictured in Figure S2)	1	551-16-6	11082	6-Amino penicillanic acid	Sensitizer	0
	2	4424-06-0	78141	Brilliant orange GR	Sensitizer	0
	3	55-56-1	2713	Chlorhexidene	Sensitizer	0
	4	62-73-7	3039	Dichlorvos	Sensitizer	0
	5	101-68-8	7570	Diphenyl methane-4,4*-diisocyanate	Sensitizer	0
	6	141-43-5	700	Ethanolamine	Sensitizer	0
	7	107-15-3	3301	Ethylenediamine	Sensitizer	0
	8	55-38-9	3346	Fenthion	Sensitizer	0
	9	822-06-0	13192	Hexamethylene diisocyanate	Sensitizer	0
	10	108-31-6	7923	Maleic anhydride	Sensitizer	0
	11	555-30-6	38853	Methyldopa	Sensitizer	0
	12	1897-45-6	15910	Tetrachloroisophthalonitrile	Sensitizer	0
	13	117-08-8	8326	Tetrachlorophthalic anhydride	Sensitizer	0
	14	116-66-5	67005	1,1,3,3,5-Pentamethyl-4,6-Dinitroindane	Non-sensitizer	0
	15	470-67-7		1,4-Cineole	Non-sensitizer	0
	16	54546-26-8	94569	2-Butyl-4,4,6-trimethyl-1,3-dioxane	Non-sensitizer	0
	17	67874-72-0	62240	2-tert-Amylcyclohexyl acetate	Non-sensitizer	0
	18	60763-42-0	108506	3,6-Dimethyloctan-3-yl acetate	Non-sensitizer	0
	19	50816-18-7	39801	9-Decenyl acetate	Non-sensitizer	0
	20	142-19-8	8878	Allyl heptylate	Non-sensitizer	0
	21	79-92-5	6616	Camphene	Non-sensitizer	0
	22	65405-76-7	5372353	cis-3-Hexenyl anthranilate	Non-sensitizer	0
	23	21662-09-9	5362620	cis-4-Decen-1-al	Non-sensitizer	0
	24	52671-32-6	40058	Citronellyl nitrile	Non-sensitizer	0
	25	544-40-1	11002	Dibutyl sulfide	Non-sensitizer	0
	26	95-41-0	66768	Dihydro-isojasmone	Non-sensitizer	0
	27	6413-10-1	80865	Ethyl acetoacetate ethylene glycol ketal	Non-sensitizer	0
	28	97-64-3	7344	Ethyl lactate	Non-sensitizer	0
	29	2305-05-7	16821	g-Dodecalactone	Non-sensitizer	0
	30	5870-93-9	62592	Heptyl butyrate	Non-sensitizer	0
	31	110-54-3	8058	Hexane	Non-sensitizer	0
	32	97-45-0	7336	l-Carvyl propionate	Non-sensitizer	0

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
	33	21280-29-5	89479	Lactoscatone	Non-sensitizer	0
	34	112-19-6	61035	Undecenyl acetate	Non-sensitizer	0
	35	50-00-0	712	Formaldehyde	Sensitizer	0
	36	52-67-5	5852	Penicillamine	Sensitizer	0
	37	54-85-3	3767	Isoniazid	Sensitizer	0
	38	60-54-8		Tetracycline	Sensitizer	0
	39	64-19-7	176	Acetic acid	Sensitizer	0
	40	70-30-4	3598	Hexachlorophene	Sensitizer	0
	41	72-14-0	5340	Sulfathiazole	Sensitizer	0
	42	75-21-8	6354	Ethylene oxide	Sensitizer	0
	43	85-42-7	85689	Hexahydrophthalic anhydride	Sensitizer	0
	44	88-04-0	2723	Chloroxylenol	Sensitizer	0
	45	98-00-0	3314	Furfuryl alcohol	Sensitizer	0
	46	100-37-8	7361	2-Diethylethanolamine	Sensitizer	0
	47	100-97-0	4101	Hexamethylene tetramine	Sensitizer	0
	48	109-02-4	7972	N-methylmorpholine	Sensitizer	0
	49	109-55-7	7993	3-dimethylaminopropylamine	Sensitizer	0
	50	111-30-8	3485	Glutaraldehyde	Sensitizer	0
	51	123-77-3	31269	Azodicarbonamide	Sensitizer	0
	52	148-01-6	3092	2-methyl-3,5-dinitrobenzamide	Sensitizer	0
	53	305-80-6	67539	Pauli's Reagent (4-diazobenzenesulphonic acid)	Sensitizer	0
	54	317-34-0	9433	Aminophylline	Sensitizer	0
	55	514-10-3	10569	Abietic acid	Sensitizer	0
	56	957-68-6	441328	7-aminocephalosporanic acid	Sensitizer	0
	57	2746-19-2	637794	Himic anhydride	Sensitizer	0
	58	2939-80-2	16760159	Captafol	Sensitizer	0
	59	13466-78-9	442461	3-carene	Sensitizer	0
	60	28983-56-4	76956083	Methyl blue	Sensitizer	0
	61	31330-63-9	3035399	Tetrazene	Sensitizer	0
	62	39878-87-0	170253	Phenylglycine acid chloride	Sensitizer	0
	63	49745-95-1	65324	Dobutamine HCl	Sensitizer	0
	64	51481-61-9	2756	Cimetidine	Sensitizer	0
	65	123354-92-7	124621	Sodium iso-nonanoyloxybenzene sulphonate	Sensitizer	0
	66	115-27-5	8265	Chlorendic anhydride	Sensitizer	0
	67	485-47-2	10236	Ninhydrin	Sensitizer	0
	68	860-22-0		Indigotine	Sensitizer	0

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
	69	2451-62-9	17142	Triglycidyl isocyanurate	Sensitizer	0
	70	2634-33-5	17520	1,2-benzisothiazolin-3-one	Sensitizer	0
	71	7696-12-0	83975	Tetramethrin	Sensitizer	0
	72	56796-20-4	42008	Cefmetazole	Sensitizer	0
	73	64265-57-2	94611	polyfunctional aziridine	Sensitizer	0
	74	65271-80-9	4212	Mitoxanthrone	Sensitizer	0
	75	72558-82-8	5481173	Ceftazidime	Sensitizer	0
	76	79622-59-6	91731	Fluazinam	Sensitizer	0
	77	82547-81-7	5362114	Cefteram pivoxil	Sensitizer	0
	78	125700-67-6		2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate	Sensitizer	0
	79	68123-13-7	93377	Basic blue 99	Sensitizer	0
	80	17095-24-8	1.02E+08	Black GR Reactive Dye	Sensitizer	0
	81	108-77-0	7954	Cyanuric chloride	Sensitizer	0
	82	12225-83-1	82984	Orange 3R reactive dye	Sensitizer	0
	83	10343-58-5		Reactive yellow	Sensitizer	0
	84	3740-18-9	77336	2,4-dichloro-5-chlorosulfonylbenzoic acid	Sensitizer	0
	85	16691-43-3	2723869	3-amino-5-mercapto-1,2,4-triazole	Sensitizer	0
	86	89-57-6	4075	5-aminosalicylic acid	Sensitizer	0
	87	37539-03-0	6400459	7-amino-3-thiomethyl-3-cephalosporanic acid	Sensitizer	0
	88	114-07-8	12560	Erythromycin	Sensitizer	0
	89	97-53-0	3314	Eugenol	Sensitizer	0
	90	77430-27-4	188203	Glycyl compound	Sensitizer	0
	91	139-07-1	8753	Lauryl dimethyl benzyl ammonium chloride	Sensitizer	0
	92	64761-66-6	6438396	MM22383	Sensitizer	0
	93	643-79-8	4807	Ortho-phthalaldehyde(1,2-Phthalic dicarboxaldehyde)	Sensitizer	0
	94	59-43-8	6042	Thiamine	Sensitizer	0
	95	15318-45-3	27200	Thiamphenicol	Sensitizer	0

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
	96	15625-89-5	27423	Trimethylolpropane triacrylate	Sensitizer	0
	97	26471-62-5		Toluene diisocyanate	Sensitizer	0
	98	556-61-6	11167	Methyl isothiocyanate	Sensitizer	0
	99	12125-02-9	25517	Ammonium chloride	Sensitizer	0
	100	79-10-7	6581	Acrylic acid	Non-sensitizer	0
	101	3173-53-3	18502	Cyclohexylisocyanate	Sensitizer	0
	102	106-46-7	4685	1,4-Dichlorobenzene	Non-sensitizer	0
	103	872-50-4	13387	1-Methyl-2-pyrrolidone	Non-sensitizer	0
	104	111-77-3	8134	2-(2-Methoxyethoxy)ethanol	Non-sensitizer	0
	105	108-83-8	7958	2,6-Dimethylheptan-4-one	Non-sensitizer	0
	106	532-27-4	10757	2-Chloroacetophenone	Non-sensitizer	0
	107	24468-13-1	62783	2-Ethylhexyl chloroformate	Non-sensitizer	0
	108	999-61-1	61249	2-Hydroxypropyl acrylate	Non-sensitizer	0
	109	79-46-9	398	2-Nitropropane	Non-sensitizer	0
	110	504-29-0	10439	2-Pyridylamine	Non-sensitizer	0
	111	78-59-1	6544	3,5,5-Trimethylcyclohex-2-enone	Non-sensitizer	0
	112	96-69-5	7308	6,6'-Di-tert-butyl-4,4'-thiodi-m-cresol	Non-sensitizer	0
	113	67-64-1	180	Acetone	Non-sensitizer	0
	114	107-13-1	7855	Acrylonitrile	Non-sensitizer	0
	115	76-22-2	159055	Bornan-2-one	Non-sensitizer	0
	116	314-40-9	9411	Bromacil (ISO)	Non-sensitizer	0
	117	107-20-0	33	Chloroacetaldehyde	Non-sensitizer	0
	118	75-45-6	6372	Chlorodifluoromethane	Non-sensitizer	0
	119	2921-88-2	2730	Chloropyrifos (ISO)	Non-sensitizer	0
	120	156-59-2	643833	cis 1,2-dichloroethylene	Non-sensitizer	0
	121	76-14-2	6429	Cryofluorane(INN)	Non-sensitizer	0
	122	64-67-5	6163	Diethyl sulphate	Non-sensitizer	0
	123	101-84-8	7583	Diphenyl ether	Non-sensitizer	0
	124	115-29-7	3224	Endosulfan	Non-sensitizer	0
	125	64-17-5	702	Ethanol	Non-sensitizer	0
	126	541-41-3	10928	Ethyl chloroformate	Non-sensitizer	0
	127	109-94-4	8025	Ethyl formate	Non-sensitizer	0
	128	151-67-7	3562	Halothane	Non-sensitizer	0
	129	78-78-4	6556	Isopentane	Non-sensitizer	0
	130	121-75-5	4004	Malathion	Non-sensitizer	0
	131	1634-04-4	15413	Methyl-tert-butyl ether	Non-sensitizer	0
	132	26590-20-5	198243	Methyltetrahydrophthalic anhydride	Sensitizer	0
	133	598-56-1	11723	N,N-Dimethylethylamine	Non-sensitizer	0

Cluster	Number Within Cluster	CASRN	CID	Chemical Name	Respiratory Sensitization Status	Number of Neighbors
	134	463-82-1	10041	Neopentane	Non-sensitizer	0
	135	54-11-5	89594	Nicotine	Non-sensitizer	0
	136	144-62-7	971	Oxalic acid	Non-sensitizer	0
	137	298-02-2	4790	Phorate	Non-sensitizer	0
	138	1918-02-1	15965	Picloram (ISO)	Non-sensitizer	0
	139	88-89-1	6954	Picric acid	Non-sensitizer	0
	140	114-26-1	4944	Propoxur	Non-sensitizer	0
	141	525-66-6	4946	Propranolol	Non-sensitizer	0
	142	57-50-1	5988	Sucrose	Non-sensitizer	0
	143	2422-88-0	3032425	1,1,3-Tributylthiourea (TBTU)	Sensitizer	0
	144	127-18-4	31373	Tetrachloroethylene	Non-sensitizer	0
	145	126-73-8	31357	Tributyl phosphate	Non-sensitizer	0
	146	76-06-2	6423	Trichloronitromethane	Non-sensitizer	0
	147	25656-78-4	186099	Triphenylmethane triisocyanate	Sensitizer	0

Table S3: Chemical Identifiers by Clusters in the Chemical Similarity Map. *Supplemental Table 3 identifies the chemicals by cluster as displayed in the chemical similarity map in Figure S2. The similarity cutoff for the chemical similarity map in Figure S2 is 80%. There are 257 discrete chemicals in the overall data set, and, of these, 147 chemicals had no neighbor at an 80% similarity cutoff. As these chemicals have no neighbors, the singleton chemicals are not displayed in the chemical similarity map in Figure S2. In addition, several of the chemicals only had one neighbor (n=40). While they are displayed on the chemical similarity map, the individual pairs are not identified as individual clusters on the chemical similarity map or in the table; they are simply listed as a cluster of all chemicals with only one neighbor.*

Performance Metric	Toxtree		COEH (Conservative)		COEH (Not Conservative)	
	n	%	n	%	n	%
Sensitivity	104	74	106	78	94	69
Specificity	79	68	30	66	42	84
False Positive	37	32	39	34	19	16
False Negative	37	26	30	22	42	31
Coverage	257	100	252	98	252	98

Table S4: Performance Metrics. *The total data set is 257 chemicals. Coverage is defined as the number of chemicals that returned a prediction after inputting all 257 chemicals. COEH assigns 3 different predictions to chemicals: Hazardous; Borderline, may be hazardous; and Low index, may still be hazardous. Chemicals designated as “Hazardous” were always considered to be respiratory sensitizers, and chemicals designated as “Low index; may still be hazardous” were designated as non-respiratory sensitizers. For the COEH (Conservative) approach, we considered chemicals designated “Borderline, may be hazardous” as respiratory sensitizers. For the COEH (Not Conservative) approach, chemicals designated as “Borderline, may be hazardous” as non-respiratory sensitizers.*

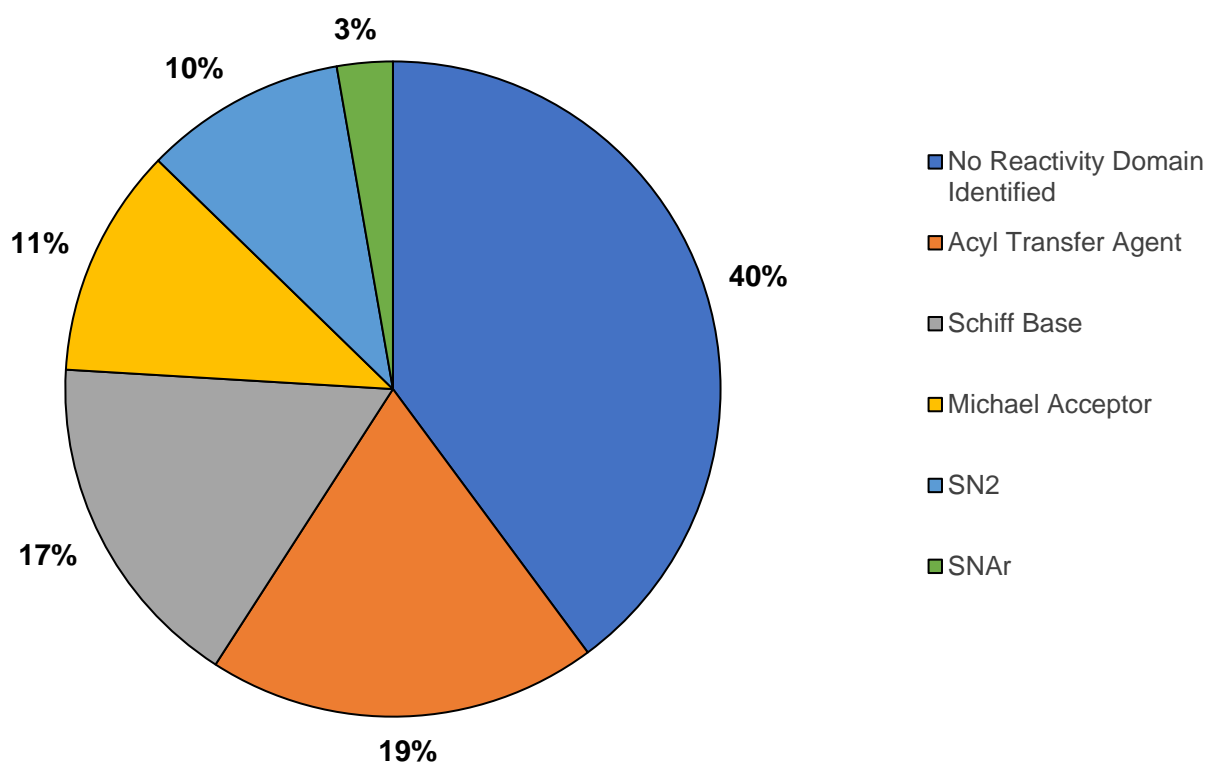


Figure S3: Skin Sensitization Reactivity Alert Distribution. *Skin sensitization reactivity domain alerts were assigned using Toxtree for all chemicals in the data set. Some chemicals had more than one alert, and this figure accounts for all alerts from each chemical.*