Table S1. Chemicals used to construct models for predicting chemical reactivity to cysteine in this study.

	CAS	Chemical Name	SMILES	experimental result		dataset	prediction result		
				Cys % depletion	target class		RF-based	GCN-based	Consensus
1	100-06-1	4-Acetylanisole	CC(=O)C1=CC=C(C=C1)OC	4.72	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
2	100-11-8	4-Nitrobenzyl bromide	C1=CC(=CC=C1CBr)[N+](=O)[O-]	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
3	100-39-0	Benzyl bromide	C1=CC=C(C=C1)CBr	100	Moderate-High	training	Minimal-Low	Moderate-High	Inconclusive
4	101-68-8	Diphenylmethane diisocyanate	C1=CC(=CC=C1CC2=CC=C(C=C2)N=C=O)N=C=O	89.2	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
5	101-77-9	Methylenedianiline	C1=CC(=CC=C1CC2=CC=C(C=C2)N)N	1.38	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
6	101-83-7	Dicyclohexylamine	C1CCC(CC1)NC2CCCCC2	3.81	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
7	102-71-6	Triethanolamine	C(CO)N(CCO)CCO	0.63	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
8	103-11-7	2-Ethylhexyl acrylate	CCCCC(CC)COC(=O)C=C	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
9	103-41-3	Benzyl cinnamate	C1=CC=C(C=C1)COC(=O)/C=C/C2=CC=CC=C2	4.3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
10	104-27-8	1-(4-Methoxyphenyl)pent-1-en-3-one	CCC(=O)/C=C/C1=CC=C(C=C1)OC	29.91	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
11	104-76-7	2-Ethylhexan-1-ol	CCCCC(CC)CO	1.27	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
12	105-95-3	Ethylene brassylate	C1CCCCCC(=O)OCCOC(=O)CCCCC1	0.03	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
13	106-47-8	4-Chloroaniline	C1=CC(=CC=C1N)Cl	1.8	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
14	106-51-4	1,4-Benzoquinone	C1=CC(=O)C=CC1=O	99.73	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
15	107-21-1	Ethylene glycol	C(CO)O	0.65	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
16	107-88-0	1,3-Butanediol	CC(CCO)O	0.16	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
17	107-98-2	1-Methoxy-2-propanol	CC(COC)O	3.21	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
18	108-01-0	Deanol	CN(C)CCO	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
19	108-65-6	1-Methoxy-2-propyl acetate	CC(COC)OC(=O)C	-0.04	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
20	108-77-0	Cyanuric chloride	C1(=NC(=NC(=N1)Cl)Cl)Cl	79.8	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
21	109-55-7	3-Dimethylamino propylamine	CN(C)CCCN	10.18	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
22	109-65-9	1-Bromobutane	CCCCBr	13.77	Minimal-Low	training	Minimal-Low	Moderate-High	Inconclusive
23	110-15-6	Succinic acid	C(CC(=O)O)C(=O)O	59.6	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
24	110-27-0	Isopropyl myristate	CCCCCCCCCCCCCC(=O)OC(C)C	5.9	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
25	110-54-3	Hexane	CCCCCC	0.33	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
26	110-63-4	1,4-Butanediol	C(CCO)CO	0.02	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
27	110-85-0	Piperazine	C1CNCCN1	3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
28	110-91-8	Morpholine	C1COCCN1	3.85	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
29	110-98-5	1,1-Oxydi-2-propanol	CC(COCC(C)O)O	0.63	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
30	111-12-6	Methyl heptine carbonate	CCCCCC#CC(=O)OC	99.2	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
31	111-42-2	Diethanolamine	C(CO)NCCO	6.67	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
32	111-46-6	Diethylene glycol	C(COCCO)O	0.64	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
33	1118-71-4	Dipivaloylmethane	CC(C)(C)C(=O)CC(=O)C(C)(C)C	1.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
34	112-07-2	2-Butoxyethyl acetate	CCCCOCCOC(=O)C	13.1	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
35	112-15-2	Carbitol acetate	CCOCCOCCOC(=O)C	0.61	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
36	112-38-9	Undecylenic acid	C=CCCCCCCCCC(=O)O	11.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
37	1154-59-2	Tetrachlorosalicylanilide	C1=CC(=C(C=C1NC(=O)C2=C(C(=CC(=C2)Cl)Cl)O)Cl)Cl	36.8	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
38	118-58-1	Benzyl salicylate	C1=CC=C(C=C1)COC(=O)C2=CC=CC=C2O	6.325	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
39	118-61-6	Ethyl salicylate	CCOC(=O)C1=CC=CC=C1O	0.65	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
40	119-10-8	4-Methyl-2-nitroanisole	CC1=CC(=C(C=C1)OC)[N+](=O)[O-]	3.3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
41	119-36-8	Methyl salicylate	COC(=O)C1=CC=CC=C1O	0.34	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
42	119-84-6	3,4-Dihydrocoumarin	C1CC(=O)OC2=CC=CC=C21	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
43	121-57-3	Sulfanilic acid	C1=CC(=CC=C1N)S(=O)(=O)O	5.3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
44	122-57-6	Benzylideneacetone	CC(=O)/C=C/C1=CC=CC=C1	94.68	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
45	122-99-6	2-Phenoxyethanol	C1=CC=C(C=C1)OCCO	11.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
46	123-86-4	Butyl acetate	CCCCOC(=O)C	0.39	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
47	124-04-9	Adipic acid	C(CCC(=O)O)CC(=O)O	2.67	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
48	124-12-9	Octanenitrile	CCCCCCCC#N	0	Minimal-Low	training	Minimal-Low	Moderate-High	Inconclusive
49	124-17-4	2-(2-Butoxyethoxy)ethyl acetate	CCCCOCCOCCOC(=O)C	0.49	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
50	134-62-3	Diethyl toluamide	CCN(CC)C(=O)C1=CC=CC(=C1)C	6.7	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
51	137-26-8	Thiram	CN(C)C(=S)SSC(=S)N(C)C	99.5	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
52	138-89-6	N,N-Dimethyl-4-nitrosoaniline	CN(C)C1=CC=C(C=C1)N=O	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
53	141-02-6	Bis(2-ethylhexyl) fumarate	CCCCC(CC)COC(=O)/C=C/C(=O)OCC(CC)CCCC	7.65	Minimal-Low	training	Minimal-Low	Moderate-High	Inconclusive

Table S1. (Continued).

	CAS	Chemical Name	SMILES	experimental result		dataset	prediction result		
				Cys % depletion	target class		RF-based	GCN-based	Consensus
54	141-05-9	Diethyl maleate	CCOC(=O)/C=CC(=O)OCC	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
55	141-32-2	Butyl acrylate	CCCCOC(=O)C=C	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
56	141-43-5	Ethanolamine	C(CO)N	8	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
57	149021-58-9	Acrylic acid 2-propylheptyl ester	CCCCCC(CCC)COC(=O)C=C	96.8	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
58	150-13-0	4-Aminobenzoic acid	C1=CC(=CC=C1C(=O)O)N	10.7	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
59	15646-46-5	Oxazolone	CCOC=C1C(=O)OC(=N1)C2=CC=CC=C2	75.5	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
60	16867-03-1	2-Amino-3-hydroxypyridine	C1=CC(=C(N=C1)N)O	55.43	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
61	17369-59-4	3-Propylidenephthalide	CC/C=C1/C2=CC=CC=C2C(=O)O1	14.3	Minimal-Low	training	Minimal-Low	Moderate-High	Inconclusive
62	1885-38-7	Cinnamyl nitrile	C1=CC=C(C=C1)/C=C/C#N	4.04	Minimal-Low	training	Minimal-Low	Moderate-High	Inconclusive
63	1897-45-6	Chlorothalonil	C(#N)C1=C(C(=C(C(=C1Cl)Cl)Cl)C#N)Cl	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
64	20048-27-5	Bandrowski's base	C1=CC(=CC=C1N)N=C2C=C(C(=NC3=CC=C(C=C3)N)C=C2N)N	87.5	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
65	2050-14-8	2,2'-Dihydroxyazobenzene	C1=CC=C(C(=C1)N=NC2=CC=CC=C2O)O	7.19	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
66	2345-34-8	4-Acetoxybenzoic acid	CC(=O)OC1=CC=C(C=C1)C(=O)O	90.6	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
67	23593-75-1	Clotrimazole	C1=CC=C(C=C1)C(C2=CC=CC=C2)(C3=CC=CC=C3Cl)N4C=CN=C4	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
68	23911-56-0	1-(3-Methylbenzofuran-2-yl)ethanone	CC1=C(OC2=CC=CC=C12)C(=O)C	0.3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
69	2426-08-6	Butyl glycidyl ether	CCCCOCC1CO1	67.3	Moderate-High	training	Minimal-Low	Moderate-High	Inconclusive
70	2442-10-6	1-Octen-3-yl acetate	CCCCCC(C=C)OC(=O)C	4.05	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
71	30007-47-7	5-Bromo-5-nitro-1,3-dioxane	C1C(COCO1)([N+](=O)[O-])Br	99.7	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
72	30618-84-9	Glyceryl monothioglycolate	C(C(COC(=O)CS)O)O	0.6	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
73	3395-91-3	Methyl 3-bromopropionate	COC(=O)CCBr	97.3	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
74	369-36-8	2-Fluoro-5-nitroaniline	C1=CC(=C(C=C1[N+](=O)[O-])N)F	11.1	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
75	4098-71-9	Isophorone diisocyanate	CC1(CC(CC(C1)(C)CN=C=O)N=C=O)C	99.76	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
76	485-47-2	Ninhydrin	C1=CC=C2C(=C1)C(=O)C(C2=O)(O)O	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
77	492-94-4	Furil	C1=COC(=C1)C(=O)C(=O)C2=CC=CO2	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
78	50-00-0	Formaldehyde	C=O	60.41	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
79	50-21-5	Lactic acid	CC(C(=O)O)O	3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
80	5231-87-8	Diethyl squarate	CCOC1=C(C(=O)C1=O)OCC	2.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
81	52-51-7	Bronopol	C(C(CO)([N+](=O)[O-])Br)O	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
82	540-51-2	2-Bromoethanol	C(CBr)O	13	Minimal-Low	training	Moderate-High	Minimal-Low	Inconclusive
83	540-97-6	Dodecamethylcyclohexasiloxane	C[Si]1(O[Si](O[Si](O[Si](O[Si](O[Si](O1)(C)C)(C)C)(C)C)(C)C)(C)C)C	-0.03	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
84	541-02-6	Decamethylcyclopentasiloxane	C[Si]1(O[Si](O[Si](O[Si](O[Si](O1)(C)C)(C)C)(C)C)(C)C)C	0.03	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
85	5466-77-3	Octinoxate	CCCCC(CC)COC(=O)/C=C/C1=CC=C(C=C1)OC	0.3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
86	55406-53-6	Iodopropynyl butylcarbamate	CCCCNC(=O)OCC#CI	99.7	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
87	55-56-1	Chlorhexidine	C1=CC(=CC=C1N/C(=N/C(=NCCCCCCN=C(/N=C(/NC2=CC=C(C=C2)Cl)N)N)N)/N)Cl	0.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
88	556-67-2	Octamethylcyclotetrasiloxane	C[Si]1(O[Si](O[Si](O[Si](O1)(C)C)(C)C)(C)C)C	-0.01	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
89	563-70-2	Bromonitromethane	C([N+](=O)[O-])Br	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
90	56-81-5	Glycerol	C(C(CO)O)O	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
91	57-55-6	Propylene glycol	CC(CO)O	0.35	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
92	579-07-7	1-Phenyl-1,2-propanedione	CC(=O)C(=O)C1=CC=CC=C1	47.1	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
93	57-97-6	7,12-Dimethylbenz[a]anthracene	CC1=C2C=CC3=CC=CC=C3C2=C(C4=CC=CC=C14)C	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
94	582-17-2	2,7-Dihydroxynaphthalene	C1=CC(=CC2=C1C=CC(=C2)O)O	6.5	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
95	584-84-9	2,4-Diisocyanato-1-methylbenzene	CC1=C(C=C(C=C1)N=C=O)N=C=O	63.4	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
96	59-01-8	Kanamycin	C1[C@H]([C@@H]([C@H]([C@@H]([C@H]1N)O[C@@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CN)O)O)O)O)O[C@@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)N)O)N	5.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
97	5965-66-2	beta-Lactose	C([C@@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)O[C@@H]2[C@H](O[C@H]([C@@H]([C@H]2O)O)O)CO)O)O)O)O	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
98	600-22-6	Methyl pyruvate	CC(=O)C(=O)OC	0	Minimal-Low	training	Minimal-Low	Moderate-High	Inconclusive
99	613-29-6	N,N-Dibutylaniline	CCCCN(CCCC)C1=CC=CC=C1	1.6	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
100	61-33-6	Penicillin G	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)CC3=CC=CC=C3)C(=O)O)C	14.3	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
101	61789-40-0	Cocamidopropyl betaine	CCCCCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]	3.88	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
102	623-91-6	Diethyl fumarate	CCOC(=O)/C=C/C(=O)OCC	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
103	624-48-6	Dimethyl maleate	COC(=O)/C=CC(=O)OC	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
104	6259-76-3	Hexyl salicylate	CCCCCCOC(=O)C1=CC=CC=C1O	3.9	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low

Table S1. (Continued).

	CAS	Chemical Name	SMILES	experimental result		dataset	prediction result		
				Cys % depletion	target class		RF-based	GCN-based	Consensus
105	638-45-9	1-Iodohexane	CCCCCCI	32.2	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
106	6440-58-0	Dimethyloldimethyl hydantoin	CC1(C(=O)N(C(=O)N1CO)CO)C	60	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
107	65-85-0	Benzoic acid	C1=CC=C(C=C1)C(=O)O	16.2	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
108	66-27-3	Methyl methanesulfonate	COS(=O)(=O)C	93	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
109	67-63-0	Isopropanol	CC(C)O	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
110	68039-69-0	1-Cyclohexylethyl 2-butenoate	CC=CC(=O)OC(C)C1CCCCC1	8.4	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
111	6846-50-0	Kodaflex txib	CC(C)C(C(C)(C)COC(=O)C(C)C)OC(=O)C(C)C	1	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
112	69-72-7	Salicylic acid	C1=CC=C(C(=C1)C(=O)O)O	8.71	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
113	70356-09-1	Avobenzone	CC(C)(C)C1=CC=C(C=C1)C(=O)CC(=O)C2=CC=C(C=C2)OC	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
114	71-36-3	1-Butanol	CCCCO	0.7	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
115	78439-06-2	Ceftazidimum	CC(C)(C(=O)O)ON=C(C1=CSC(=N1)N)C(=O)NC2C3N(C2=O)C(=C(CS3)C[N+]4=CC=CC=C4)C(=O)[O-]	89.67	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
116	80-62-6	Methylmethacrylate	CC(=C)C(=O)OC	55.25	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
117	811412-48-3	3-Decen-5-one, 4-methyl-, (3E)-	CCCCCC(=O)/C(=C/CC)/C	7.6	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
118	81925-81-7	5-Methyl-2-hepten-4-one	CCC(C)C(=O)/C=C/C	99.9	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
119	822-06-0	Hexamethylene diisocyanate	C(CCCN=C=O)CCN=C=O	97.6	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
120	85-68-7	Benzyl butyl phthalate	CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2	3.6	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
121	868839-23-0	Propylheptyl caprylate	CCCCCCCC(=O)OCC(CCC)CCCCC	6.79	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
122	874-23-7	2-Acetylcyclohexanone	CC(=O)C1CCCCC1=O	18.23	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
123	87-69-4	L-Tartaric acid	[C@@H]([C@H](C(=O)O)O)(C(=O)O)O	6.6	Minimal-Low	training	Moderate-High	Minimal-Low	Inconclusive
124	87-86-5	Pentachlorophenol	C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)O	0	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
125	886-38-4	Diphenylcyclopropenone	C1=CC=C(C=C1)C2=C(C2=O)C3=CC=CC=C3	98.83	Moderate-High	training	Moderate-High	Minimal-Low	Inconclusive
126	923-26-2	2-Hydroxypropyl methacrylate	CC(COC(=O)C(=C)C)O	58.39	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
127	92-48-8	6-Methylcoumarin	CC1=CC2=C(C=C1)OC(=O)C=C2	1.41	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
128	94-02-0	Ethyl benzoylacetate	CCOC(=O)CC(=O)C1=CC=CC=C1	11.2	Minimal-Low	training	Minimal-Low	Minimal-Low	Minimal-Low
129	94-36-0	Benzoyl peroxide	C1=CC=C(C=C1)C(=O)OOC(=O)C2=CC=CC=C2	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
130	96-27-5	Thioglycerol	C(C(CS)O)O	27.3	Moderate-High	training	Minimal-Low	Moderate-High	Inconclusive
131	96-33-3	Methyl acrylate	COC(=O)C=C	100	Moderate-High	training	Moderate-High	Moderate-High	Moderate-High
132	100-43-6	4-Vinylpyridine	C=CC1=CC=NC=C1	92.1	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
133	101-85-9	Amylcinnamyl alcohol	CCCCCC(=CC1=CC=CC=C1)CO	23	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
134	103694-68-4	Majantol	CC1=CC(=CC=C1)CC(C)(C)CO	0.14	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
135	104-46-1	Anethole	C/C=C/C1=CC=C(C=C1)OC	0	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
136	105-76-0	Dibutyl maleate	CCCCOC(=O)/C=CC(=O)OCCCC	100	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
137	107-15-3	Ethylene diamine	C(CN)N	18.6	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
138	108-90-7	Chlorobenzene	C1=CC=C(C=C1)Cl	1.33	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
139	108-91-8	Cyclohexylamine	C1CCC(CC1)N	1.05	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
140	109-89-7	Diethylamine	CCNCC	4.1	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
141	110-16-7	Maleic acid	C(=CC(=O)O)C(=O)O	44.2	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
142	111-25-1	1-Bromohexane	CCCCCCBr	14.1	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
143	111-80-8	Methyl 2-nonynoate	CCCCCCC#CC(=O)OC	100	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
144	112-24-3	Triethylenetetramine	C(CNCCNCCN)N	0	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
145	13706-86-0	5-Methyl-2,3-hexanedione	CC(C)CC(=O)C(=O)C	25.79	Moderate-High	validation	Minimal-Low	Moderate-High	Inconclusive
146	144-62-7	Oxalic acid	C(=O)(C(=O)O)O	0.9	Minimal-Low	validation	Moderate-High	Moderate-High	Moderate-High
147	149-30-4	2-Mercaptobenzothiazole	C1=CC=C2C(=C1)NC(=S)S2	99.88	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
148	1565-94-2	Silux	CC(=C)C(=O)OCC(COC1=CC=C(C=C1)C(C)(C)C2=CC=C(C=C2)OCC(COC(=O)C(=C)C)O)O	35.6	Moderate-High	validation	Minimal-Low	Moderate-High	Inconclusive
149	24851-98-7	Methyl dihydrojasmonate	CCCCCC1C(CCC1=O)CC(=O)OC	22.5	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
150	2634-33-5	1,2-Benzisothiazolin-3-one	C1=CC=C2C(=C1)C(=O)NS2	97.65	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
151	2682-20-4	Methylisothiazolinone	CN1C(=O)C=CS1	97.9	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
152	3055-86-5	3-Phenoxypropanenitrile	C1=CC=C(C=C1)OCCC#N	0	Minimal-Low	validation	Minimal-Low	Moderate-High	Inconclusive
153	3326-32-7	Fluorescein-5-isothiocyanate	C1=CC2=C(C=C1N=C=S)C(=O)OC23C4=C(C=C(C=C4)O)OC5=C3C=CC(=C5)O	100	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
154	35691-65-7	Methyldibromo glutaronitrile	C(CC(CBr)(C#N)Br)C#N	100	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
155	36727-29-4	3,5,5-Trimethylhexanoyl chloride	CC(CC(=O)Cl)CC(C)(C)C	29.3	Moderate-High	validation	Moderate-High	Minimal-Low	Inconclusive
156	478695-70-4	Propanedioic acid, 1-(3,3-dimethylcyclohexyl)ethyl ethyl ester	CCOC(=O)CC(=O)OC(C)C1CCCC(C1)(C)C	1.17	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low

Table S1. (Continued).

	CAS	Chemical Name	SMILES	experimental result		dataset	prediction result		
				Cys % depletion	target class		RF-based	GCN-based	Consensus
157	513-85-9	2,3-Butanediol	CC(C(C)O)O	0.21	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
158	56539-66-3	3-Methoxy-3-methylbutan-1-ol	CC(C)(CCO)OC	0.45	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
159	584-03-2	1,2-Butanediol	CCC(CO)O	0.27	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
160	59-30-3	Folic acid	C1=CC(=CC=C1C(=O)N[C@@H](CCC(=O)O)C(=O)O)NCC2=CN=C3C(=N2)C(=O)NC(=N3)N	0	Minimal-Low	validation	Moderate-High	Minimal-Low	Inconclusive
161	62-53-3	Aniline	C1=CC=C(C=C1)N	0	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
162	63500-71-0	2-Isobutyl-4-methyltetrahydropyran-4-ol	CC(C)CC1CC(CCO1)(C)O	1.34	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
163	637-07-0	Clofibrate	CCOC(=O)C(C)(C)OC1=CC=C(C=C1)Cl	2.26	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
164	63-74-1	Sulfanilamide	C1=CC(=CC=C1N)S(=O)(=O)N	3.8	Minimal-Low	validation	Minimal-Low	Moderate-High	Inconclusive
165	67-68-5	DMSO	CS(=O)C	0.4	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
166	68-12-2	N,N-Dimethylformamide	CN(C)C=O	1.2	Minimal-Low	validation	Minimal-Low	Moderate-High	Inconclusive
167	84-66-2	Diethyl phthalate	CCOC(=O)C1=CC=CC=C1C(=O)OCC	0.76	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
168	94-09-7	Benzocaine	CCOC(=O)C1=CC=C(C=C1)N	29.2	Moderate-High	validation	Minimal-Low	Minimal-Low	Minimal-Low
169	97-90-5	Ethyleneglycol dimethacrylate	CC(=C)C(=O)OCCOC(=O)C(=C)C	93.47	Moderate-High	validation	Moderate-High	Moderate-High	Moderate-High
170	99-76-3	Methylparaben	COC(=O)C1=CC=C(C=C1)O	11	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
171	99-96-7	4-Hydroxybenzoic acid	C1=CC(=CC=C1C(=O)O)O	3	Minimal-Low	validation	Minimal-Low	Minimal-Low	Minimal-Low
172	105-75-9	Dibutyl fumarate	CCCCOC(=O)/C=C/C(=O)OCCCC	100	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
173	107-22-2	Glyoxal	C(=O)C=O	56.5	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
174	107-41-5	Hexylene glycol	CC(CC(C)(C)O)O	0.37	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
175	108-95-2	Phenol	C1=CC=C(C=C1)O	15.4	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
176	110-17-8	Fumaric acid	C(=C/C(=O)O)\C(=O)O	38.6	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
177	1101843-02-0	Methyl jasmonate	CC/C=CCC1C(CCC1=O)CC(=O)OC	18.6	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
178	110-86-1	Pyridine	C1=CC=NC=C1	1.5	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
179	111-40-0	Diethylenetriamine	C(CNCCN)N	5.7	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
180	112-05-0	Nonanoic acid	CCCCCCCCC(=O)O	0	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
181	120-51-4	Benzyl benzoate	C1=CC=C(C=C1)COC(=O)C2=CC=CC=C2	0.88	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
182	124-07-2	Octanoic acid	CCCCCCCC(=O)O	0	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
183	125-12-2	Bornyl acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	0.4	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
184	131-57-7	Oxybenzone	COC1=CC(=C(C=C1)C(=O)C2=CC=CC=C2)O	4.6	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
185	140-88-5	Ethyl acrylate	CCOC(=O)C=C	100	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
186	142-16-5	Bis(2-ethylhexyl) maleate	CCCCC(CC)COC(=O)/C=CC(=O)OCC(CC)CCCC	5.45	Minimal-Low	test	Minimal-Low	Moderate-High	Inconclusive
187	145551-14-0	Phenethyl dimethyl caffeate	COC1=C(C=C(C=C1)/C=C/C(=O)OCCC2=CC=CC=C2)OC	5.5	Minimal-Low	test	Minimal-Low	Moderate-High	Inconclusive
188	1675-54-3	Bisphenol A-diglycidyl ether	CC(C)(C1=CC=C(C=C1)OCC2CO2)C3=CC=C(C=C3)OCC4CO4	42.5	Moderate-High	test	Minimal-Low	Moderate-High	Inconclusive
189	1680-31-5	Dicaprylyl carbonate	CCCCCCCCOC(=O)OCCCCCCCC	4.76	Minimal-Low	test	Moderate-High	Minimal-Low	Inconclusive
190	2508-19-2	Picrylsulfonic acid	C1=C(C=C(C(=C1[N+](=O)[O-])S(=O)(=O)O)[N+](=O)[O-])[N+](=O)[O-]	99.7	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
191	25265-77-4	Texanol	CC(C)C(C(C)(C)COC(=O)C(C)C)O	1.91	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
192	26172-55-4	Methylchloroisothiazolinone	CN1C(=O)C=C(S1)Cl	96.3	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
193	39236-46-9	Imidazolidinyl urea	C(NC(=O)NC1C(=O)NC(=O)N1CO)NC(=O)NC2C(=O)NC(=O)N2CO	59	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
194	431-03-8	2,3-Butanedione	CC(=O)C(=O)C	92.83	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
195	50-23-7	Hydrocortisone	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	39.1	Moderate-High	test	Minimal-Low	Minimal-Low	Minimal-Low
196	544-77-4	1-Iodohexadecane	CCCCCCCCCCCCCCCCI	85.5	Moderate-High	test	Minimal-Low	Moderate-High	Inconclusive
197	6197-30-4	Octocrylene	CCCCC(CC)COC(=O)C(=C(C1=CC=CC=C1)C2=CC=CC=C2)C#N	1.9	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
198	624-49-7	Dimethyl fumarate	COC(=O)/C=C/C(=O)OC	100	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
199	64-19-7	Acetic acid	CC(=O)O	4.33	Minimal-Low	test	Minimal-Low	Moderate-High	Inconclusive
200	64-67-5	Diethyl sulfate	CCOS(=O)(=O)OCC	26	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
201	69300-15-8	2-Methyldecanenitrile	CCCCCCCCC(C)C#N	3	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
202	69-65-8	Mannitol	C([C@H]([C@H]([C@@H]([C@@H](CO)O)O)O)O)O	12.67	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
203	7493-74-5	Allyl phenoxyacetate	C=CCOC(=O)COC1=CC=CC=C1	0.61	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
204	81-07-2	Saccharin	C1=CC=C2C(=C1)C(=O)NS2(=O)=O	2.4	Minimal-Low	test	Moderate-High	Moderate-High	Moderate-High
205	818-61-1	2-Hydroxyethyl acrylate	C=CC(=O)OCCO	92.64	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
206	84-74-2	Dibutyl Phthalate	CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC	0	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
207	90-15-3	1-Naphthol	C1=CC=C2C(=C1)C=CC=C2O	68.2	Moderate-High	test	Minimal-Low	Minimal-Low	Minimal-Low
208	91-08-7	2,6-Diisocyanatotoluene	CC1=C(C=CC=C1N=C=O)N=C=O	86.3	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High
209	91-64-5	Coumarin	C1=CC=C2C(=C1)C=CC(=O)O2	7	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
210	94-13-3	Propylparaben	CCCOC(=O)C1=CC=C(C=C1)O	8.2	Minimal-Low	test	Minimal-Low	Minimal-Low	Minimal-Low
211	97-00-7	2,4-Dinitrochlorobenzen	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])Cl	100	Moderate-High	test	Moderate-High	Moderate-High	Moderate-High

Table S2. Atom-based descriptors used for input graph of GCN-based models

Name of atom-based descriptor	Software for calculation
Number of bonded neighbor atoms	RDKit
Number of bonded hydrogens	RDKit
Aromatic or not (1 for yes, 0 for no)	RDKit
Carbon or not (1 for yes, 0 for no)	RDKit
Nitrogen or not (1 for yes, 0 for no)	RDKit
Oxygen or not (1 for yes, 0 for no)	RDKit
Fluorine or not (1 for yes, 0 for no)	RDKit
Silicon or not (1 for yes, 0 for no)	RDKit
Phosphorus or not (1 for yes, 0 for no)	RDKit
Sulfur or not (1 for yes, 0 for no)	RDKit
Chlorine or not (1 for yes, 0 for no)	RDKit
Bromine or not (1 for yes, 0 for no)	RDKit
Iodine or not (1 for yes, 0 for no)	RDKit
Hydrogen or not (1 for yes, 0 for no)	RDKit
atomic charge (from GasteigerCharge)	RDKit
Atomic contribution to MolLogP	RDKit
Solvent Accesible Surface Area	RDKit
Mulliken charge	Gaussian 16
Atomic contribution to HOMO	Gaussian 16
Atomic contribution to HOMO-1	Gaussian 16
Atomic contribution to HOMO-2	Gaussian 16
Atomic contribution to LUMO	Gaussian 16
Atomic contribution to LUMO+1	Gaussian 16
Atomic contribution to LUMO+2	Gaussian 16

HOMO: Highest Ocuppied Molecular Orbital, LUMO: Lowest Unocuppied Molecular Orbital