

## Supporting Information

The development of an in silico profiler for mitochondrial toxicity

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Table S1: The complete Zhang *et al* dataset.<sup>1</sup>

ID	Name	Mitochondrial toxicity	SMILES
1	Menadione	1	<chem>O=C\2c1c(cccc1)C(=O)/C(=C/2)C</chem>
2	Pentamidine	1	<chem>[H]/N=C(\N)/c1ccc(cc1)OCCCCOc2ccc(cc2)/C(=N/[H])/N</chem>
3	Nalidixic acid	1	<chem>CCn1cc(c(=O)c2c1nc(cc2)C)C(=O)O</chem>
4	Diazepam	1	<chem>CN1c2ccc(cc2C(=NCC1=O)c3ccccc3)Cl</chem>
5	Clofibric acid	1	<chem>Clc1ccc(OC(C(=O)O)(C)C)cc1</chem>
6	Niclofolan	1	<chem>Clc2cc(c(O)c(c1c(O)c([N+][O-])=O)cc(Cl)c1)c2)[N+][O-]=O</chem>
7	Lonidamine	1	<chem>Clc1ccc(c(Cl)c1)Cn3nc(c2ccccc23)C(=O)O</chem>
8	Sulofenur	1	<chem>Clc1ccc(cc1)NC(=O)NS(=O)(=O)c2ccc3c(c2)CCC3</chem>
9	Ciprofloxacin	1	<chem>c1c2c(cc(c1F)N3CCNCC3)n(cc(c2=O)C(=O)O)C4CC4</chem>
10	Tolcapone	1	<chem>[O-][N+](=O)c2cc(C(=O)c1ccc(cc1)C)cc(O)c2O</chem>
11	Hexachlorophene	1	<chem>Clc1c(c(O)c(Cl)cc1Cl)Cc2c(O)c(Cl)cc(Cl)c2Cl</chem>
12	Buquinolate	1	<chem>CCOC(=O)c1cnc2cc(c(cc2c1O)OCC(C)C)OCC(C)C</chem>
13	Menoctone	1	<chem>O=C1c3ccccc3C(\O)=C(/C1=O)CCCCCCCC2CCCCC2</chem>
14	Amquinatate	1	<chem>O=C\2c1c(cc(c(c1)CCC)N(CC)CC)N/C=C/2C(=O)OC</chem>

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15	Decoquinatate	1	<chem>O=C\2c1c(cc(OCC)c(OCCCCCCCCC)c1)N/C=C/2C(=O)OCC</chem>
16	Tioxaprofen	1	<chem>Clc3ccc(c2oc(SC(C(=O)O)C)nc2c1ccc(Cl)cc1)cc3</chem>
17	Cyhalothrin	1	<chem>CC1([C@@H]([C@H]1C(=O)OC(C#N)c2cccc(c2)Oc3ccccc3)/C=C(\C(F)(F)F)/Cl)C</chem>
18	Myxothiazol	1	<chem>O=C(N)\C=C(\OC)[C@H](C)[C@@H](OC)/C=C/c1nc(sc1)c2nc(sc2)[C@H](\C=C\C=C\C(C)C)C</chem>
19	Haloperidol	1	<chem>c1cc(ccc1C(=O)CCCN2CCC(CC2)(c3ccc(cc3)Cl)O)F</chem>
20	Indomethacin	1	<chem>Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O</chem>
21	Phenytoin	1	<chem>c1ccc(cc1)C2(C(=O)NC(=O)N2)c3ccccc3</chem>
22	Lindane	1	<chem>Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H]1Cl</chem>
23	Procaine	1	<chem>O=C(OCCN(CC)CC)c1ccc(N)cc1</chem>
24	Methionine	1	<chem>CSCCC(C(=O)O)N</chem>
25	Fluphenazine	1	<chem>c1ccc2c(c1)N(c3cc(ccc3S2)C(F)(F)F)CCCN4CCN(CC4)CCO</chem>
26	Salicylic acid	1	<chem>c1ccc(c(c1)C(=O)O)O</chem>
27	Valproic acid	1	<chem>O=C(O)C(CCC)CCC</chem>
28	Phenformin	1	<chem>N(=C(/N=C(\N)N)N)\CCc1ccccc1</chem>
29	Lidocaine	1	<chem>CCN(CC)CC(=O)Nc1c(cccc1C)C</chem>
30	Butacaine	1	<chem>O=C(OCCCN(CCCC)CCC)c1ccc(N)cc1</chem>
31	Metformin	1	<chem>[H]/N=C(/N=C(N)N)\N(C)C</chem>

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32	Buformin	1	<chem>N(=C(/N)N)\C(=N\CCCC)N</chem>
33	Porfiromycin	1	<chem>O=C\1C/2=C\C(=O)/C(N)=C/1C)[C@H]([C@]3(OC)N\2C[C@@H]4N([C@H]34)C)COC(=O)N</chem>
34	Anthralin	1	<chem>O=C2c1c(O)cccc1Cc3c2c(O)ccc3</chem>
35	Propofol	1	<chem>Oc1c(cccc1C(C)C)C(C)C</chem>
36	Flutamide	1	<chem>O=C(Nc1cc(c(cc1)[N+])([O-])=O)C(F)(F)C(C)C</chem>
37	Ibuprofen	1	<chem>CC(C)Cc1ccc(cc1)C(C)C(=O)O</chem>
38	Zidovudine	1	<chem>Cc1cn(c(=O)[nH]c1=O)[C@H]2C[C@@H]([C@H](O2)CO)N=[N+]=[N-]</chem>
39	Ropivacaine	1	<chem>O=C(Nc1c(cccc1C)C)[C@H]2N(CCC)CCCC2</chem>
40	Etidocaine	1	<chem>O=C(Nc1c(cccc1C)C)C(N(CC)CCC)CC</chem>
41	Nabumetone	1	<chem>O=C(C)CCc1ccc2c(c1)ccc(OC)c2</chem>
42	Nimesulide	1	<chem>[O-][N+](=O)c2cc(Oc1ccccc1)c(cc2)NS(=O)(=O)C</chem>
43	Ciprofibrate	1	<chem>CC(C)(C(=O)O)Oc1ccc(cc1)C2CC2(Cl)Cl</chem>
44	Fluoxetine	1	<chem>CNCCC(c1ccccc1)Oc2ccc(cc2)C(F)(F)F</chem>
45	Idarubicin	1	<chem>O=C2c1c(O)c5c(c(O)c1C(=O)c3ccccc23)C[C@@](O)(C(=O)C)[C@@H]5O[C@@H]4O[C@H]([C@@H](O)[C@@H](N)C4)C</chem>
46	Nicorandil	1	<chem>c1cc(cnc1)C(=O)NCCO[N+](=O)[O-]</chem>
47	Carvedilol	1	<chem>COc1ccccc1OCCNCC(COc2cccc3c2c4ccccc4[nH]3)O</chem>

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48	Nefazodone	1	<chem>Clc4cccc(N3CCN(CCCN1/N=C(\N(C1=O)CCOc2cccc2)CC)CC3)c4</chem>
49	Didanosine	1	<chem>c1nc2c(c(n1)O)ncn2[C@H]3CC[C@H](O3)CO</chem>
50	Stavudine	1	<chem>O=C1/C(=C\N(C(=O)N1)[C@@H]/2O[C@@H](\C=C\2)CO)C</chem>
51	Nevirapine	1	<chem>Cc1ccnc2c1NC(=O)c3cccnc3N2C4CC4</chem>
52	Entacapone	1	<chem>[O-][N+](=O)c1cc(\C=C/C#N)C(=O)N(CC)CC)cc(O)c1O</chem>
53	Lamivudine	1	<chem>c1cn(c(=O)nc1N)[C@@H]2CS[C@@H](O2)CO</chem>
54	Diclofenac	1	<chem>c1ccc(c(c1)CC(=O)O)Nc2c(cccc2Cl)Cl</chem>
55	Chloramphenicol	1	<chem>c1cc(ccc1[C@H]([C@@H](CO)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]</chem>
56	Minocycline	1	<chem>CN(C)c1ccc(c2c1C[C@H]3C[C@H]4[C@@H](C(=C(C(=O)[C@]4(C(=C3C2=O)O)O)C(=O)N)O)N(C)C)O</chem>
57	Naproxen	1	<chem>C[C@@H](c1ccc2cc(ccc2c1)OC)C(=O)O</chem>
58	Butylated Hydroxy	1	No SMILES possible
59	Linezolid	1	<chem>O=C1O[C@@H](CNC(=O)C)CN1c3cc(F)c(N2CCOCC2)cc3</chem>
60	Celecoxib	1	<chem>O=S(=O)(c3ccc(n1nc(cc1c2ccc(cc2)C)C(F)(F)F)cc3)N</chem>
61	Efavirenz	1	<chem>FC(F)(F)[C@@]3(C#CC1CC1)OC(=O)Nc2ccc(Cl)cc23</chem>
62	Rosiglitazone	1	<chem>O=C1NC(=O)SC1Cc3ccc(OCCN(c2ncccc2)C)cc3</chem>
63	Chlorpromazine	1	<chem>CN(C)CCCN1c2cccc2Sc3c1cc(cc3)Cl</chem>
64	Mefenamic acid	1	<chem>O=C(O)c2c(Nc1cccc(c1)C)cccc2</chem>

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65	Flufenamic acid	1	<chem>FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)O</chem>
66	Tolfenamic acid	1	<chem>Clc2cccc(Nc1ccccc1C(=O)O)c2C</chem>
67	Fenofibrate	1	<chem>O=C(c1ccc(Cl)cc1)c2ccc(OC(C(=O)OC(C)C)(C)C)cc2</chem>
68	Atovaquone	1	<chem>c1cc2c(cc1)C(=O)C(=C(C2=O))[C@H]3CC[C@@H](CC3)c4ccc(cc4)Cl)O</chem>
69	Troglitazone	1	<chem>O=C1NC(=O)SC1Cc4ccc(OCC3(Oc2c(c(c(O)c(c2CC3)C)C)C)cc4</chem>
70	Tamoxifen	1	<chem>O(c1ccc(cc1)/C(c2ccccc2)=C(\c3ccccc3)CC)CCN(C)C</chem>
71	Tetracycline	1	<chem>C[C@]1(c2cccc(c2C(=O)C3=C([C@]4([C@@H](C[C@@H]31)[C@@H](C=C(C4=O)C(=O)N)O)N(C)C)O)O)O</chem>
72	Dieldrin	1	<chem>ClC5(Cl)[C@]3(Cl)C(\Cl)=C(\Cl)[C@@]5(Cl)[C@H]4[C@H]1C[C@H]([C@@H]2O[C@H]12)[C@@H]34</chem>
73	Sulindac	1	<chem>O=S(c1ccc(cc1)\C=C3/c2ccc(F)cc2\C(=C3C)CC(=O)O)C</chem>
74	Amiodarone	1	<chem>lc1cc(cc(l)c1OCCN(CC)CC)C(=O)c2c3ccccc3oc2CCCC</chem>
75	Saquinavir	1	<chem>O=C(N)C[C@H](NC(=O)c1nc2c(cc1)cccc2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN5[C@H](C(=O)NC(C)C)C[C@@H]4CCCC[C@@H]4C5</chem>
76	Daunorubicin	1	<chem>C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](Cc3c2c(c4c(c3O)C(=O)c5cccc(c5C4=O)OC)O)C(=O)C)O)N)O</chem>
77	Nelfinavir	1	<chem>O=C(c1cccc(O)c1C)N[C@@H](CSc2ccccc2)[C@H](O)CN4[C@H](C(=O)NC(C)(C)C)[C@@H]3CCCC[C@@H]3C4</chem>
78	Doxorubicin	1	<chem>C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](Cc3c2c(c4c(c3O)C(=O)c5cccc(c5C4=O)OC)O)C(=O)CO)O)N)O</chem>

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79	Epirubicin	1	<chem>O=C2c1c(O)c5c(c(O)c1C(=O)c3cccc(OC)c23)C[C@@](O)(C(=O)CO)C[C@@H]5O[C@@H]4O[C@H]([C@H](O)[C@@H](N)C4)C</chem>
80	Ritonavir	1	<chem>CC(C)c1nc(cs1)CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc2cccc2)C[C@@H]([C@H](Cc3cccc3)N C(=O)OCc4cnsc4)O</chem>
81	2,4-Dichlorophenoxyacetic acid	1	<chem>Clc1cc(Cl)ccc1OCC(=O)O</chem>
82	2-Methylamine	1	<chem>O(C=2/C=C\C1=C3/C=C\N(\C=C3\N=C1C=2)C)C</chem>
83	Aldicarb	1	<chem>O=C(O\N=C\SC)(C)C)NC</chem>
84	Betulinic acid	1	<chem>O=C(O)[C@@]54[C@@H]([C@@H]3[C@@]([C@]1([C@@H]([C@]2(C)[C@@H](CC1)C(C)(C)[C@@H](O)CC2)CC3)C(C)CC4)[C@H](C=C)\C)CC5</chem>
85	CCCP	1	<chem>Clc1cc(N\N=C(/C#N)C#N)ccc1</chem>
86	DAPI	1	<chem>[H]/N=C(/c1ccc(cc1)c2cc3ccc(cc3[nH]2)/C(=N/[H])/N)\N</chem>
87	DASPEI	1	<chem>c2(\C=C\c1[n](cccc1)CC)ccc(N(C)C)cc2</chem>
88	DDD	1	<chem>Oc4ccc3cc(SSc2ccc1c(ccc(O)c1)c2)ccc3c4</chem>
89	DDT	1	<chem>Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl</chem>
90	Dequalinium	1	<chem>c12cccc1c(cc([n+]2CCCCCCCC[n+]4c3cccc3c(N)cc4C)C)N</chem>
91	Diethylstilbestrol	1	<chem>CC/C(=C/CC)\c1ccc(cc1)O)/c2ccc(cc2)O</chem>
92	Ellipticine	1	<chem>Cc1c2ccncc2c(c3c1[nH]c4c3cccc4)C</chem>

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93	Ethidium bromide	1	<chem>CC[n]1c2cc(ccc2c3ccc(cc3c1c4cccc4)N)N</chem>
94	FCCP	1	<chem>FC(F)(F)Oc1ccc(cc1)N/N=C(\C#N)C#N</chem>
95	JC 1	1	<chem>Clc1cc2N(/C(N(c2cc1Cl)CC)=C\C=C\c4[n](c3cc(Cl)c(Cl)cc3n4CC)CC)CC</chem>
96	Methyltriphenylphosphonium	1	<chem>c1(ccccc1)[P+](c2ccccc2)(c3ccccc3)C</chem>
97	MPCU	1	<chem>Clc2ccc(NC(=O)NS(=O)(=O)c1ccc(cc1)C)cc2</chem>
98	Nitroxynil	1	<chem>Ic1cc(C#N)cc([N+])([O-])=O)c1O</chem>
99	Nonylacridine Orange	1	<chem>c3(ccc2cc1ccc(N(C)C)cc1[n+](c2c3)CCCCCCCC)N(C)C</chem>
100	o-Phenanthroline	1	<chem>c1cc2ccc3cccnc3c2nc1</chem>
101	Perfluorodecanoic acid	1	<chem>FC(F)(C(F)(F)C(=O)O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F</chem>
102	Perfluorooctane-sulfonamide	1	<chem>FC(F)(C(F)(F)S(=O)(=O)N)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F</chem>
103	Perfluorooctanoic acid	1	<chem>FC(F)(C(F)(F)C(=O)O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F</chem>
104	PK 11195	1	<chem>Clc3ccccc3c2nc(cc1cccc12)C(=O)N(C(C)CC)C</chem>
105	Rhein	1	<chem>O=C2c1cccc(O)c1C(=O)c3c2cc(cc3O)C(=O)O</chem>
106	Rhodamine 6G	1	<chem>CCOC(=O)c4cccc4C=1c3cc(C)c(cc3O/C/2=C/C(=N/CC)C/C)=C\C=1\2)NCC</chem>
107	Rhodamine 123	1	<chem>O=C(OC)c4cccc4C=1c3c(OC=2C=1\C=C/C(=[NH2])/C=2)cc(cc3)N</chem>



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108	Rhodamine B	1	<chem>CCN(CC)c1ccc2c(c1)oc-3cc(=[N])(CC)CCccc3c2c4cccc4C(=O)O</chem>
109	TBTP	1	<chem>O=P(SCCCC)(SCCCC)SCCCC</chem>
110	Tebufenpyrad	1	<chem>Clc2c(nn(c2C(=O)NCc1ccc(cc1)C(C)(C)C)C)CC</chem>
111	Trichlorophen- Oxyacetic acid	1	<chem>Clc1cc(OCC(=O)O)c(Cl)cc1Cl</chem>
112	TTFB	1	<chem>FC(F)(F)c2nc1c(Cl)c(Cl)c(Cl)c(Cl)c1n2</chem>
113	Victoria blue B	1	<chem>C/[N](C)=C1\C=C/C(C=C1)=C(\c4ccc(Nc2cccc2)c3cccc34)c5ccc(cc5)N(C)C</chem>
114	Zalcitabine	1	<chem>O=C1/N=C(/N)\C=C/N1[C@@H]2O[C@@H](CC2)CO</chem>
115	2,4-Dinitrophenol	1	<chem>c1cc(c(cc1[N+](=O)[O-])[N+](=O)[O-])O</chem>
116	Amytal	1	<chem>O=C1NC(=O)NC(=O)C1(CCC(C)C)CC</chem>
117	Antimycin A	1	<chem>O=CNC1cccc(c1O)C(=O)N[C@@H]2C(=O)O[C@H]([C@H](OC(=O)CC(C)C)[C@H](C(=O)O[C@@H]2C)CCC CCC)C</chem>
118	Azidothymidine	1	<chem>Cc1cn(c(=O)[nH]c1=O)[C@H]2C[C@@H]([C@H](O2)CO)N=[N+]=[N-]</chem>
119	Carbaryl	1	<chem>O=C(Oc2cccc1cccc12)NC</chem>
120	Chenodeoxycholic acid	1	<chem>C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C</chem>
121	Cholic acid	1	<chem>C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)O)C</chem>

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122	Deguelin	1	<chem>O=C2c5c(O[C@@H]3COc1cc(OC)c(OC)cc1[C@H]23)c4\C=C/C(Oc4cc5)(C)C</chem>
123	Deoxycholic acid	1	<chem>C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C</chem>
124	Diazinon	1	<chem>S=P(OCC)(OCC)Oc1nc(nc(c1)C)C(C)C</chem>
125	Diphenylamine	1	<chem>c1ccc(cc1)Nc2ccccc2</chem>
126	Glycocholic	1	<chem>C[C@H](CCC(=O)NCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)O)C</chem>
127	Lithocholic	1	<chem>O=C(O)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]4[C@H]2CC[C@@H]3C[C@H](O)CC[C@@]34C)C</chem>
128	Mitomycin C	1	<chem>CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H]([C@@]3([C@H]2COC(=O)N)OC)N4)N</chem>
129	MPTP	1	<chem>c2c(/C1=C/CN(C)CC1)cccc2</chem>
130	Naproxen	1	<chem>C[C@@H](c1ccc2cc(ccc2c1)OC)C(=O)O</chem>
131	Paraquat	1	<chem>C[n+]1ccc(cc1)c2cc[n+](cc2)C</chem>
132	Pentachlorophenol	1	<chem>Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl</chem>
133	Perhexiline	1	<chem>N3C(CC(C1CCCC1)C2CCCC2)CCCC3</chem>
134	Rotenone	1	<chem>CC(=C)[C@H]1Cc2c(ccc3c2O[C@@H]4COc5cc(c(cc5[C@@H]4C3=O)OC)OC)O1</chem>
135	Ranolazine	1	<chem>O=C(Nc1c(cccc1C)C)CN3CCN(CC(O)COc2ccccc2OC)CC3</chem>
136	Chloroquine	1	<chem>Clc1cc2nccc(c2cc1)NC(C)CCCN(CC)CC</chem>

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137	Atenolol	1	<chem>CC(C)NCC(COc1ccc(cc1)CC(=O)N)O</chem>
138	Amineptine	1	<chem>O=C(O)CCCCCNC3c1cccc1CCc2c3cccc2</chem>
139	Tianeptine	1	<chem>Clc1cc2c(cc1)C(c3c(N(C)S2(=O)=O)cccc3)NCCCCC(=O)O</chem>
140	Quinidine	1	<chem>O(c4cc1c(nccc1[C@H])(O)[C@@H]2N3CC[C@@H](C2)[C@@H](/C=C)C3)cc4)C</chem>
141	Abacavir	1	<chem>n3c1c(ncn1[C@H]2/C=C\[C@@H](CO)C2)c(nc3N)NC4CC4</chem>
142	Cerivastatin	1	<chem>O=C(O)C[C@H](O)C[C@H](O)/C=C/c1c(nc(c1c2ccc(F)cc2)COC)C(C)C(C)C</chem>
143	Cinnarizine	1	<chem>c1c(cccc1)C(c2ccccc2)N3CCN(CC3)C/C=C\c4ccccc4</chem>
144	Flunarizine	1	<chem>c1ccc(cc1)/C=C/CN2CCN(CC2)C(c3ccc(cc3)F)c4ccc(cc4)F</chem>
145	Ketoconazole	1	<chem>O=C(N5CCN(c4ccc(OC[C@@H]1O[C@](OC1)(c2ccc(Cl)cc2Cl)Cn3ccnc3)cc4)CC5)C</chem>
146	Bupivacaine	1	<chem>CCCCN1CCCCC1C(=O)Nc2c(cccc2)C</chem>
147	Clofibrate	1	<chem>Clc1ccc(OC(C(=O)OCC)(C)C)cc1</chem>
148	Prilocaine	1	<chem>O=C(Nc1ccccc1)C(NCCC)C</chem>
149	Gemfibrozil	1	<chem>Cc1ccc(c(c1)OCCCC(C)C(=O)O)C</chem>
150	Fenoprofen	1	<chem>O=C(O)C(c2cc(Oc1ccccc1)ccc2)C</chem>
151	Risperidone	1	<chem>Cc1c(c(=O)n2c(n1)CCCC2)CCN3CCC(CC3)c4c5ccc(cc5on4)F</chem>
152	Amphetamine	1	<chem>CC(Cc1ccccc1)N</chem>
153	Deoxycholic acid	1	<chem>C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2CC[C@H]4[C@@]3(CC[C@H]</chem>

### Supporting Information

			(C4)O)C)O)C
154	Taurocholic	1	<chem>C[C@H](CCC(=O)NCCS(=O)(=O)O)[C@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@@H]4[C@@]3(CC[C@H](C4)O)C)O)O)C</chem>
155	Phentolamine	-1	<chem>Oc3cc(N(c1ccc(cc1)C)CC/2=N/CCN\2)ccc3</chem>
156	Dopamine	-1	<chem>c1cc(c(cc1CCN)O)O</chem>
157	Guanethidine	-1	<chem>N(=C(\N)N)\CCN1CCCCCCC1</chem>
158	Diphenhydramine	-1	<chem>O(CCN(C)C)C(c1cccc1)c2cccc2</chem>
159	Promethazine	-1	<chem>S2c1cccc1N(c3c2cccc3)CC(N(C)C)C</chem>
160	Oxymetazoline	-1	<chem>Oc1c(c(c(cc1C(C)(C)C)C)CC/2=N/CCN\2)C</chem>
161	Tropicamide	-1	<chem>CCN(Cc1ccncc1)C(=O)C(CO)c2cccc2</chem>
162	Warfarin	-1	<chem>CC(=O)CC(c1cccc1)c2c(c3cccc3oc2=O)O</chem>
163	Phenindione	-1	<chem>O=C2c1cccc1C(=O)C2c3cccc3</chem>
164	Trimeprazine	-1	<chem>S2c1cccc1N(c3c2cccc3)CC(C)CN(C)C</chem>
165	Tripelennamine	-1	<chem>n1cccc1N(CCN(C)C)Cc2cccc2</chem>
166	Bromodiphen-Hydramine	-1	<chem>Brc1ccc(cc1)C(OCCN(C)C)c2cccc2</chem>
167	Trimethobenzamide	-1	<chem>O=C(c1cc(OC)c(OC)c(OC)c1)NCc2ccc(OCCN(C)C)cc2</chem>
168	Diphenylpyraline	-1	<chem>O(C(c1cccc1)c2cccc2)C3CCN(C)CC3</chem>

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169	Benzphetamine	-1	<chem>N(C)(Cc1cccc1)[C@@H](C)Cc2cccc2</chem>
170	Metoclopramide	-1	<chem>Clc1cc(c(OC)cc1N)C(=O)NCCN(CC)CC</chem>
171	Methoxamine	-1	<chem>O(c1ccc(OC)cc1C(O)C(N)C)C</chem>
172	Phenprocoumon	-1	<chem>OC=1c3cccc3OC(=O)C=1C(CC)c2cccc2</chem>
173	Crotamiton	-1	<chem>O=C(N(c1cccc1C)CC)/C=C/C</chem>
174	Alprostadil	-1	<chem>O=C1C[C@@H](O)[C@H](/C=C/[C@@H](O)CCCC)[C@H]1CCCCC(=O)O</chem>
175	Diphenidol	-1	<chem>OC(c1cccc1)(c2cccc2)CCCN3CCCC3</chem>
176	Methdilazine	-1	<chem>S2c1cccc1N(c3c2cccc3)CC4CCN(C)C4</chem>
177	Disopyramide	-1	<chem>O=C(N)C(c1ncccc1)(c2cccc2)CCN(C(C)C)C(C)C</chem>
178	Azatadine	-1	<chem>n4c3\C=C1/CCN(C)CC1)c2cccc2CCc3ccc4</chem>
179	Pentoxifylline	-1	<chem>CC(=O)CCCCn1c(=O)c2c(ncn2C)n(c1=O)C</chem>
180	Dobutamine	-1	<chem>Oc1ccc(cc1O)CCNC(C)CCc2ccc(O)cc2</chem>
181	Alprenolol	-1	<chem>O(c1cccc1C\C=C)CC(O)CNC(C)C</chem>
182	Naltrexone	-1	<chem>O=C4[C@@H]5Oc1c2c(ccc1O)C[C@H]3N(CC[C@]25[C@@]3(O)CC4)CC6CC6</chem>
183	Prazosin	-1	<chem>O=C(N3CCN(c2nc1cc(OC)c(OC)cc1c(n2)N)CC3)c4occc4</chem>
184	Minaprine	-1	<chem>n2nc(NCCN1CCOCC1)c(cc2c3cccc3)C</chem>
185	Guanfacine	-1	<chem>Clc1cccc(Cl)c1CC(=O)\N=C(/N)N</chem>

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186	Tocainide	-1	<chem>O=C(Nc1c(cccc1C)C)C(N)C</chem>
187	Nadolol	-1	<chem>OC(CNC(C)(C)C)COc1cccc2c1C[C@H](O)[C@H](O)C2</chem>
188	Midodrine	-1	<chem>O=C(NCC(O)c1cc(OC)ccc1OC)CN</chem>
189	Flecainide	-1	<chem>FC(F)(F)COc2cc(C(=O)NCC1NCCCC1)c(OCC(F)(F)F)cc2</chem>
190	Fenoldopam	-1	<chem>Clc1c3c(cc(O)c1O)C(c2ccc(O)cc2)CNCC3</chem>
191	Dapiprazole	-1	<chem>n1nc(n2c1CCCC2)CCN4CCN(c3ccccc3C)CC4</chem>
192	Enalapril	-1	<chem>O=C(O)[C@H]2N(C(=O)[C@@H](N[C@H](C(=O)OCC)CCc1cccc1)C)CCC2</chem>
193	Lisinopril	-1	<chem>c1ccc(cc1)CC[C@@H](C(=O)O)N[C@@H](CCCCN)C(=O)N2CCC[C@H]2C(=O)O</chem>
194	Quinapril	-1	<chem>O=C(OCC)[C@@H](N[C@H](C(=O)N2[C@H](C(=O)O)Cc1c(cccc1)C2)C)CCc3ccccc3</chem>
195	Ondansetron	-1	<chem>O=C3c2c1cccc1n(c2CCC3Cn4ccnc4C)C</chem>
196	Ridogrel	-1	<chem>FC(F)(F)c2cccc(C(=N\OCCCC(=O)O)/c1ccnc1)c2</chem>
197	Benazepril	-1	<chem>O=C(OCC)[C@@H](N[C@@H]2C(=O)N(c1cccc1CC2)CC(=O)O)CCc3ccccc3</chem>
198	Ramipril	-1	<chem>CCOC(=O)[C@H](CCc1cccc1)N[C@@H](C)C(=O)N2[C@H]3CCC[C@H]3C[C@H]2C(=O)O</chem>
199	Trandolapril	-1	<chem>O=C(OCC)[C@@H](N[C@H](C(=O)N1[C@H](C(=O)O)C[C@H]2CCCC[C@H]12)C)CCc3ccccc3</chem>
200	Granisetron	-1	<chem>CN4[C@@H]1CCC[C@H]4C[C@H](C1)NC(=O)c3nn(C)c2ccccc23</chem>
201	Acamprosate	-1	<chem>O=S(=O)(O)CCCN(C(=O)O)C</chem>
202	Moexipril	-1	<chem>O=C(OCC)[C@@H](N[C@H](C(=O)N2[C@H](C(=O)O)Cc1c(cc(OC)c(OC)c1)C2)C)CCc3ccccc3</chem>

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203	Dofetilide	-1	<chem>O=S(=O)(Nc1ccc(cc1)CCN(CCOc2ccc(cc2)NS(=O)(=O)C)C)C</chem>
204	Brimonidine	-1	<chem>Brc2c1nccnc1ccc2N/C3=N/CCN3</chem>
205	Losartan	-1	<chem>Clc1nc(n(c1CO)Cc4ccc(c2ccccc2c3nnnn3)cc4)CCCC</chem>
206	Arbutamine	-1	<chem>Oc1ccc(cc1O)[C@@H](O)CNCCCCc2ccc(O)cc2</chem>
207	Valsartan	-1	<chem>CCCCC(=O)N(Cc1ccc(cc1)c2ccccc2c3[nH]nnn3)[C@@H](C(C)C)C(=O)O</chem>
208	Atropine	-1	<chem>CN3[C@H]1CC[C@@H]3C[C@@H](C1)OC(=O)C(CO)c2ccccc2</chem>
209	Levorphanol	-1	<chem>Oc3ccc4C[C@H]1N(C)CC[C@@]2(CCCC[C@@H]12)c4c3</chem>
210	Pilocarpine	-1	<chem>O=C2OC[C@H](Cc1n(cnc1)C)[C@@H]2CC</chem>
211	Triamcinolone	-1	<chem>C[C@]12C[C@@H]([C@]3([C@H]([C@@H]1C[C@H]([C@@]2(C(=O)CO)O)O)CCC4=CC(=O)C=C[C@@]43C)F)O</chem>
212	Spironolactone	-1	<chem>O=C5O[C@@]4([C@@]3([C@H]([C@@H]2[C@H](SC(=O)C)/C1=C/C(=O)CC[C@]1(C)[C@H]2CC3)CC4)C)CC5</chem>
213	Fluocinonide	-1	<chem>O=C(OCC(=O)[C@]45OC(O[C@@H]5C[C@@H]2[C@@]4(C[C@H](O)[C@]3(F)[C@]/1/C=C\C(=O)\C=C\1[C@@H](F)C[C@@H]23)C)C)C)C</chem>
214	Betamethasone	-1	<chem>O=C(CO)[C@]3(O)[C@]2(C[C@H](O)[C@]4(F)[C@@]/1\C(=C/C(=O)\C=C\1)CC[C@H]4[C@@H]2[C@]3)C)C</chem>
215	Fluorometholone	-1	<chem>O=C(C)[C@]3(O)[C@]2(C[C@H](O)[C@]4(F)[C@@]/1\C(=C/C(=O)\C=C\1)[C@@H](C)C[C@H]4[C@@H]2)CC3)C)C</chem>
216	Methyldopa	-1	<chem>O=C(O)[C@@](N)(Cc1cc(O)c(O)cc1)C</chem>

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217	Nicergoline	-1	<chem>Cn1cc2c3c1cccc3[C@]4(C[C@H](CN([C@@H]4C2)C)COC(=O)c5cc(cnc5)Br)OC</chem>
218	Captopril	-1	<chem>C[C@H](CS)C(=O)N1CCC[C@H]1C(=O)O</chem>
219	Olopatadine	-1	<chem>O=C(O)Cc2ccc1OCc3c(C(\c1c2)=C\CCN(C)C)cccc3</chem>
220	Tirofiban	-1	<chem>O=S(=O)(N[C@H](C(=O)O)Cc2ccc(OCCCC1CCNCC1)cc2)CCCC</chem>
221	Palonosetron	-1	<chem>O=C5N([C@H]2C1CCN(CC1)C2)C[C@@H]4c3c5cccc3CCC4</chem>
222	Scopolamine	-1	<chem>OC[C@H](c1cccc1)C(=O)O[C@@H]2C[C@H]3N(C)[C@@H](C2)[C@@H]4O[C@H]34</chem>
223	Desloratadine	-1	<chem>c1cc2c(nc1)C(=C3CCNCC3)c4ccc(cc4CC2)Cl</chem>
224	Betanidine	-1	<chem>N(=C(/NCc1cccc1)NC)\C</chem>
225	Sibutramine	-1	<chem>Clc1ccc(cc1)C2(C(N(C)C)CC(C)C)CCC2</chem>
226	Thiethylperazine	-1	<chem>S(c2cc1N(c3c(Sc1cc2)cccc3)CCCN4CCN(C)CC4)CC</chem>
227	Mequitazine	-1	<chem>c1ccc2c(c1)N(c3cccc3S2)CC4CN5CCC4CC5</chem>
228	Terfenadine	-1	<chem>OC(c1cccc1)(c2cccc2)C4CCN(CCCC(O)c3ccc(cc3)C(C)(C)CC4</chem>
229	Nabilone	-1	<chem>O=C3CC[C@@H]1[C@H](c2c(OC1(C)C)cc(cc2O)C(C)(C)CCCCC)C3</chem>
230	Acitretin	-1	<chem>Cc1cc(c(c(c1/C=C/C(=C/C=C/C(=C/C(=O)O)/C)/C)C)OC</chem>
231	Azelastine	-1	<chem>Clc1ccc(cc1)CC\3=N\N(C(=O)c2cccc2/3)C4CCCN(C)CC4</chem>
232	Famotidine	-1	<chem>c1c(nc(s1)N=C(N)N)CSCC/C(=N/S(=O)(=O)N)/N</chem>
233	Loratadine	-1	<chem>CCOC(=O)N1CCC(=C2c3ccc(cc3CCc4c2nccc4)Cl)CC1</chem>



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234	Sibutramine	-1	<chem>Clc1ccc(cc1)C2(C(N(C)C)CC(C)C)CCC2</chem>
235	Remikiren	-1	<chem>O=S(=O)(C(C)(C)C)C[C@H](C(=O)N[C@H](C(=O)N[C@@H](CC1CCCC1)[C@@H](O)[C@@H](O)C2CC2)Cc3cncn3)Cc4ccccc4</chem>
236	Deserpidine	-1	<chem>O=C(OC)[C@H]6[C@H]4C[C@@H]3c2nc1cccc1c2CCN3C[C@H]4C[C@@H](OC(=O)c5cc(OC)c(OC)c(OC)c5)[C@@H]6OC</chem>
237	Irbesartan	-1	<chem>CCCCC1=NC2(CCCC2)C(=O)N1Cc3ccc(cc3)c4ccccc4c5[nH]nnn5</chem>
238	Fexofenadine	-1	<chem>O=C(O)C(c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4)(C)C</chem>
239	Eprosartan	-1	<chem>CCCCc1ncc(n1Cc2ccc(cc2)C(=O)O)/C=C(\Cc3cccs3)/C(=O)O</chem>
240	Dipyridamole	-1	<chem>C1CCN(CC1)c2c3c(c(nc(n3)N(CCO)CCO)N4CCCC4)nc(n2)N(CCO)CCO</chem>
241	Fosinopril	-1	<chem>O=C(CP(=O)(CCCCc1cccc1)OC(OC(=O)CC)C(C)C)N2C[C@@H](C[C@H]2C(O)=O)C3CCCCC3</chem>
242	Candoxatril	-1	<chem>O=C(N[C@H]1CC[C@H](CC1)C(O)=O)C4(C[C@@H](COCCOC)C(=O)Oc2cc3CCCCc3cc2)CCCC4</chem>
243	Lactulose	-1	<chem>O[C@H]2[C@H](O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O)[C@H](O[C@]2(O)CO)CO</chem>
244	Rescinnamine	-1	<chem>O=C(OC)[C@H]6[C@H]4C[C@@H]3c2nc1cc(OC)ccc1c2CCN3C[C@H]4C[C@@H](OC(=O)\C=C\c5cc(OC)c(OC)c(OC)c5)[C@@H]6OC</chem>
245	Tobramycin	-1	<chem>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)CO)O)N)O)O)[C@@H]3[C@@H](C[C@@H]([C@H](O3)CN)O)N)N</chem>
246	Argatroban	-1	<chem>O=C(O)[C@@H]3N(C(=O)[C@@H](NS(=O)(=O)c1cccc2c1NCC(C2)C)CCC/N=C(\N)N)CC[C@@H](C)C3</chem>
247	Trimethaphan	-1	<chem>O=C2N(C4C[S+]1CCCC1C4N2Cc3ccccc3)Cc5ccccc5</chem>

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248	Bretylum	-1	<chem>Brc1cccc1C[N+](CC)(C)C</chem>
249	Clidinium	-1	<chem>O=C(OC2C1CC[N+](CC1)(C)C2)C(O)(c3cccc3)c4cccc4</chem>
250	Marinol	-1	<chem>CCCCC1cc(c2c(c1)OC([C@H]3[C@H]2C=C(CC3)C)(C)C)O</chem>
251	Methantheline	-1	<chem>O=C(OCC[N+](CC)(CC)C)C2c3c(Oc1c2cccc1)cccc3</chem>
252	Oxyphenonium	-1	<chem>O=C(OCC[N+](CC)(CC)C)C(O)(c1cccc1)C2CCCC2</chem>
253	Propantheline	-1	<chem>O=C(OCC[N+](C(C)C)(C(C)C)C)C2c3c(Oc1c2cccc1)cccc3</chem>
254	Meperidine	1	<chem>O=C(OCC)C2(c1cccc1)CCN(C)CC2</chem>
255	Isoniazid	1	<chem>O=C(NN)c1ccncc1</chem>
256	Acetaminophen	1	<chem>CC(=O)Nc1ccc(cc1)O</chem>
257	Propranolol	1	<chem>CC(C)NCC(COc1cccc2c1cccc2)O</chem>
258	Clozapine	1	<chem>CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl</chem>
259	Piroxicam	1	<chem>CN1C(=C(c2cccc2S1(=O)=O)O)C(=O)Nc3cccn3</chem>
260	Ribavirin	1	<chem>c1nc(nn1[C@H]2[C@@H]([C@@H]([C@H](O2)CO)O)O)C(=O)N</chem>
261	Pioglitazone	1	<chem>O=C1NC(=O)SC1Cc3ccc(OCCc2ncc(cc2)CC)cc3</chem>
262	Xanthomegnin	1	<chem>COC=2C(=O)c1c6C(=O)OC(C)Cc6cc(O)c1C(=O)C=2\C5=C(/OC)C(=O)c4c(c(O)cc3CC(C)OC(=O)c34)C5=O</chem>
263	Malachite green	1	<chem>OC(c1ccc(N(C)C)cc1)(c2cccc2)c3ccc(N(C)C)cc3</chem>
264	Methyl benzoquate	1	<chem>O=C\3c2c(cc(OCc1cccc1)c(c2)CCCC)N/C=C/3C(=O)OC</chem>

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265	MKT-077	1	<chem>O=C2C(\S/C(=C\c1cccc[n+]1CC)N2CC)=C3/Sc4cccc4N3C</chem>
266	MTT	1	<chem>Cc1c(sc(n1)[n+]2nc(nn2c3cccc3)c4cccc4)C</chem>
267	Safranin O	1	<chem>n1c4c([n+](c2c1cc(c(N)c2)C)c3cccc3)cc(c(c4)C)N</chem>
268	Vacor	1	<chem>[O-][N+](=O)c1ccc(cc1)NC(=O)NCc2cccnc2</chem>
269	Aspirin	1	<chem>CC(=O)Oc1cccc1C(=O)O</chem>
270	Meloxicam	1	<chem>Cc1cnc(s1)NC(=O)C2=C(c3cccc3S(=O)(=O)N2C)O</chem>
271	Cysteamine	-1	<chem>SCCN</chem>
272	Phentermine	-1	<chem>NC(Cc1cccc1)(C)C</chem>
273	Triprolidine	-1	<chem>n3c(\C(=C\CN1CCCC1)c2ccc(cc2)C)cccc3</chem>
274	Flucytosine	-1	<chem>FC=1\C=N/C(=O)NC=1N</chem>
275	Tolmetin	-1	<chem>O=C(c1ccc(n1C)CC(=O)O)c2ccc(cc2)C</chem>
276	Timolol	-1	<chem>O[C@H](COc1nsc1N2CCOCC2)CNC(C)(C)C</chem>
277	Cisapride	-1	<chem>Clc1cc(c(OC)cc1N)C(=O)NC3CCN(CCCOc2ccc(F)cc2)CC3OC</chem>
278	Dexmedetomidine	-1	<chem>n1cc(nc1)C(c2c(c(ccc2)C)C)C</chem>
279	Mannitol	-1	<chem>C([C@H])([C@H])([C@@H])([C@@H](CO)O)O)O)O</chem>
280	Clotrimazole	-1	<chem>c1ccc(cc1)C(c2cccc2)(c3cccc3Cl)n4ccnc4</chem>
281	Levothyroxine	-1	<chem>c1c(cc(c(c1)Oc2cc(c(c(c2)I)O)I)I)C[C@@H](C(=O)O)N</chem>

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282	Telmisartan	-1	<chem>CCCC1nc2c(cc(cc2n1Cc3ccc(cc3)c4ccccc4C(=O)O)c5nc6ccccc6n5C)C</chem>
283	Natamycin	-1	<chem>OC(=O)[C@@H]3[C@@H](O)C[C@@]2(O)C[C@@H](O)C[C@H]4O[C@@H]4/C=C/C(=O)O[C@H](C)C\C=C\C=C\C=C\C=C\C[C@H](OC1O[C@H](C)[C@@H](O)[C@H](N)[C@@H]1O)C[C@@H]3O2</chem>
284	Dolasetron	-1	<chem>O=C5CN4[C@@H]1C[C@H]5C[C@H]4C[C@H](C1)OC(=O)c3cnc2ccccc23</chem>
285	Ramelteon	-1	<chem>O=C(NCC[C@H]3c2c(ccc1OCCc12)CC3)CC</chem>
286	Tolazoline	-1	<chem>N\1=C(\NCC/1)Cc2ccccc2</chem>
287	Levocarnitine	-1	<chem>[O-]C(=O)C[C@@H](O)C[N+](C)(C)C</chem>
288	Apraclonidine	-1	<chem>Clc1c(c(Cl)cc(N)c1)N/C2=N/CCN2</chem>

## Supporting Information

Table S2: Shows the structural alerts developed for this paper

Name	Structural alert
2-(Dialkylamino)-N-(2,6-dimethylphenyl)acetamides	<chem>c1([CH3])cccc([CH3])c1[NX3H][CX3](=[OX1])[CH2][NX3]([CH2,CH3])[CH2,CH3]</chem>
Thiazolinediones	<chem>[SX2]1[CX3](=[OX1])[NX3H][CX3](=[OX1])[CX4]1</chem>
2-Anilinobenzoic acids	<chem>c1cccc([CX3](=[OX1])[OH])c1[NX3H]c1cccc1</chem>
Salicylates	<chem>c1cccc([CX3](=[OX1])[OH])c1[OH]</chem>
Anthranilic acids	<chem>c1cccc([CX3](=[OX1])[OH])c1[NH2]</chem>
Anthracene-9,10-diones	<chem>[OX1]=C1c2cccc2C(=[OX1])c2cccc12</chem>
Naphthoquinones	<chem>c1ccc2c(c1)C(=[OX1])C=CC2=[OX1]</chem>
Perfluorinated-carboxylic-acids	<chem>[\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX3](=[OX1])[OH]),\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX3](=[OX1])[OH]),\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX3](=[OX1])[OH]),\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX3](=[OX1])[OH])]</chem>
Perfluorinated-sulphonamides	<chem>[\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[SX4](=[OX1])(=[OX1])([NH2])),\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[SX4](=[OX1])(=[OX1])([NH2])),\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[SX4](=[OX1])(=[OX1])([NH2])),\$([CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[CX4](F)(F)[SX4](=[OX1])(=[OX1])([NH2]))]</chem>
Bile acids	<chem>[OH]C1CCC2C(CCC3C4CCC([CH2][CH2][CH2][CX3](=[OX1])[OH,NX3H])C4CCC23)C1</chem>
Phenothiazines	<chem>[NX3]([CH2,CH3])([CH2,CH3])[CX4][CX4][CX4]N1c2cccc2Sc2ccc([\$(C(F)(F)(F)),Cl])cc12</chem>
Fluoromethylsulphanilides	<chem>c1cccc1[NX3H][SX4](=[OX1])(=[OX1])[CX4](F)F</chem>
Nitrophenols	<chem>c1cccc([NX3+][OX1-]=O)c1[CX3](=[OX1])[OH]</chem>
Nitrosulphonanilides	<chem>c1cccc1[NX3H][SX4](=[OX1])(=[OX1])[CX4]</chem>
Phenylhydrazones	<chem>c1cccc1[NX3H][NX2]=[CX3](#[6])#[6]</chem>
Thiadiazinedione dioxides	<chem>[NX3]1([CX4])CX3(=O)[CH]([CX3](=O)[CX4])[CX3](=O)[NX3]([CX4])[SX4]1(=O)=O</chem>
Acyindolones	<chem>c1ccc2c(c1)[CH]([CX3](=O)[NX3]2)[CX3](=O)[CX4]</chem>

## Supporting Information

### References

1. Zhang H, Chen QY, Xiang ML, Ma CY, Huang Q, Yang SY (2009). In silico prediction of mitochondrial toxicity by using GA-CG-SVM approach. *Toxicol In Vitro* 23:134-140