Experimental and calculated with CORAL toxicity to Tetrahymena pyriformis

A.A. Toropov, A.P. Toropova and E. Benfenati QSAR modelling of the toxicity to *Tetrahymena pyriformis* by balance of correlations. Mol. Divers. 14(2010) 821-827

CAS	SMILES	DCW	pIGC50 Expr	pIGC50 CORAL	pIGC50 Expr-Calc	
156-38-7	c1(CC(=O)O)ccc(O)cc1	1.4454314	-1.500	-0.248	-1.252	**Subtraining set**
620-24-6	c(cc(O)c1)cc1CO	1.3196812	-1.040	-0.980	-0.060	
4383-06-6	Oc1c(OC)ccc(CO)c1	1.5276396	-0.990	0.230	-1.220	
7149-10-2	NCc1cc(OC)c(O)cc1	1.3246078	-0.970	-0.951	-0.019	
99-06-9	c(cc(O)c1)cc1C(=O)O	1.4107324	-0.810	-0.450	-0.360	
619-57-8	Oc1ccc(C(=O)N)cc1	1.4549722	-0.780	-0.193	-0.587	
498-00-0	OCc1cc(OC)c(O)cc1	1.3726471	-0.700	-0.672	-0.028	
91-10-1	c(cc(OC)c1O)cc1OC	1.4588672	-0.600	-0.170	-0.430	
90-72-2	Oc1c(CN(C)C)cc(CN(C)C)cc1CN(C)C	1.4130187	-0.520	-0.437	-0.083	
69-72-7	c(ccc1C(=O)O)cc1O	1.4618571	-0.510	-0.152	-0.358	
90-05-1	c1c(OC)c(O)ccc1	1.4465842	-0.510	-0.241	-0.269	
14191-95-8	Oc(ccc1CC#N)cc1	1.4249851	-0.380	-0.367	-0.013	
121-71-1	c(cc(O)c1)cc1C(=O)C	1.4502765	-0.380	-0.220	-0.160	
99-93-4	Oc(ccc1C(=O)C)cc1	1.4908909	-0.300	0.016	-0.316	
95-48-7	c(ccc1C)cc1O	1.5402239	-0.300	0.304	-0.604	
2380-78-1	OCCc1cc(OC)c(O)cc1	1.4513594	-0.180	-0.214	0.034	
621-42-1	c(ccc1NC(=O)C)c(O)c1	1.3994274	-0.160	-0.516	0.356	
621-59-0	Oc(cc(c1)C=O)c(c1)OC	1.4631262	-0.140	-0.145	0.005	
498-02-2	CC(=O)c1cc(OC)c(O)cc1	1.5041191	-0.120	0.093	-0.213	
500-99-2	Oc(cc(c1)OC)cc1OC	1.4711806	-0.090	-0.098	0.008	
108-39-4	c(cc(c1)O)cc1C	1.5339218	-0.060	0.267	-0.327	
19438-10-9	c(ccc1C(=O)OC)c(O)c1	1.4551744	-0.050	-0.191	0.141	
121-33-5	Oc(ccc1C=O)c(c1)OC	1.4868766	-0.030	-0.007	-0.023	
121-32-4	c1c(C=O)cc(OCC)c(O)c1	1.5213738	0.020	0.194	-0.174	
394-32-1	CC(=O)c1c(O)ccc(F)c1	1.5295520	0.040	0.241	-0.201	
95-87-4	c(cc(c1O)C)c(c1)C	1.4976356	0.080	0.056	0.024	
99-76-3	Oc(ccc1C(=O)OC)cc1	1.4523426	0.080	-0.208	0.288	
108-68-9	c(c(cc1C)O)c(c1)C	1.5108021	0.110	0.132	-0.022	
526-75-0	c(cc(O)c1C)cc1C	1.5518568	0.120	0.371	-0.251	
90-00-6	c(ccc1CC)cc1O	1.5027004	0.160	0.085	0.075	
620-17-7	c(cc(O)c1)cc1CC	1.4531953	0.230	-0.203	0.433	
2316-64-5	c1c(O)c(CO)cc(Br)c1	1.5412546	0.340	0.310	0.030	
148-53-8	c(cc(OC)c1O)cc1C=O	1.5537479	0.380	0.382	-0.002	
89-73-6	c1c(C(=O)NO)c(O)ccc1	1.5542892	0.380	0.385	-0.005	
97-53-0	Oc1c(OC)cc(CC=C)cc1	1.6222862	0.420	0.781	-0.361	
106-48-9	Clc(ccc1O)cc1	1.6606327	0.550	1.004	-0.454	
120-47-8	Oc(ccc1C(=O)OCC)cc1	1.4776637	0.570	-0.060	0.630	
2973-76-4	Brc(cc(c1)C=O)c(O)c1OC	1.6144057	0.620	0.735	-0.115	
402-45-9	c1cc(O)ccc1C(F)(F)F	1.5945393	0.620	0.620	0.000	
585-34-2	c(ccc1C(C)(C)C)c(O)c1	1.6437722	0.730	0.906	-0.176	
87-65-0	Clc(ccc1)c(O)c1Cl	1.5567535	0.740	0.400	0.340	
65262-96-6	c1(O)cc(Cl)cc(OC)c1	1.6326729	0.760	0.842	-0.082	
88-69-7	c(ccc1C(C)C)cc1O	1.6407801	0.800	0.889	-0.089	
392-71-2	c1c(Cl)c(O)c(Cl)cc1(F)	1.6244842	0.800	0.794	0.006	
98-54-4	Oc(ccc1C(C)(C)C)cc1	1.6405734	0.910	0.888	0.022	
527-54-8	Oc(cc(c1C)C)cc1C	1.5934919	0.930	0.614	0.316	
131-55-5	Oc1cc(O)c(C(=O)c2c(O)cc(O)cc2)cc1	1.7385113	0.959	1.458	-0.499	
99-71-8	Oc(ccc1C(C)CC)cc1	1.6306647	0.980	0.830	0.150	
1137-42-4	O=C(c1ccccc1)(c2ccc(O)cc2)	1.6652424	1.020	1.031	-0.011	
120-83-2	Clc(ccc1O)cc1Cl	1.6021596	1.040	0.664	0.376	
2437-49-2	Oc1c(Br)c(O)c(Br)cc1(Br)	1.6925351	1.060	1.190	-0.130	
583-78-8	Clc(ccc1Cl)cc1O	1.6563875	1.130	0.980	0.150	
2613-23-2	c1c(F)c(Cl)cc(O)c1	1.6221328	1.130	0.780	0.350	
591-20-8	Brc(ccc1)cc1O	1.6081836	1.150	0.699	0.451	
1879-09-0	Oc(c(cc1C)C)c(c1)C(C)(C)C	1.6967982	1.160	1.215	-0.055	
80-46-6	Oc(ccc1C(C)(C)CC)cc1	1.6552690	1.230	0.973	0.257	
7530-27-0	c1(Br)cc(Cl)c(O)c(C)c1	1.6417189	1.280	0.894	0.386	
88-18-6	c(ccc1C(C)(C)C)cc1O	1.6655371	1.300	1.033	0.267	
2409-55-4	c(cc(O)c1C(C)(C)C)c(c1)C	1.6465918	1.300	0.923	0.377	
580-51-8	Oc1cc(c2ccccc2)ccc1	1.7332901	1.350	1.427	-0.077	
18979-53-8	Oc1ccc(OCCCCC)cc1	1.7473181	1.360	1.509	-0.149	
615-58-7	Brc(cc(Br)c1O)cc1	1.7403617	1.400	1.468	-0.068	

88-06-2	Clc(cc(Cl)c1O)cc1Cl	1.7268273	1.410	1.390	0.020	
131-57-7	c1ccccc1C(=O)c2c(O)cc(OC)cc2	1.7135287	1.420	1.312	0.108	
90-60-8	C(=O)c1c(O)c(Cl)cc(Cl)c1	1.6639393	1.550	1.024	0.526	
591-35-5	Clc(cc(Cl)c1)cc1O	1.7621526	1.570	1.595	-0.025	
1138-52-9	c1c(C(C)(C)C)cc(C(C)(C)C)cc1(O)	1.7940758	1.640	1.781	-0.141	
95-77-2	Clc(ccc1O)c(Cl)c1	1.7619403	1.750	1.594	0.156	
3217-15-0	c1(Br)cc(Cl)c(O)c(Cl)c1	1.7128810	1.780	1.308	0.472	
13037-86-0	Oc(ccc1OCCCCCCC)cc1	1.8273943	2.030	1.975	0.055	
140-66-9	Oc(ccc1C(C)(C)CC(C)(C)C)cc1	1.7899422	2.100	1.757	0.343	
29558-77-8	Oc1ccc(c2ccc(Br)cc2)cc1	1.8826668	2.310	2.297	0.013	
2631-77-8	C(=O)c1c(O)c(I)cc(I)c1	1.8965844	2.340	2.378	-0.038	
103-90-2	Oc(ccc1NC(=O)C)cc1	1.3967041	-0.820	-0.532	-0.288	
452-86-8	Oc1c(O)cc(C)cc1	1.5768961	0.370	0.517	-0.147	
533-73-3	Oc1c(O)cc(O)cc1	1.5309000	0.440	0.249	0.191	
123-31-9	Oc1ccc(O)cc1	1.5264702	0.470	0.224	0.246	
120-80-9	Oc1c(O)cccc1	1.4973275	0.750	0.054	0.696	
95-85-2	Clc(ccc1O)cc1N	1.5754275	0.780	0.508	0.272	
2138-22-9	Oc1c(O)cc(Cl)cc1	1.6452484	1.060	0.915	0.145	
583-69-7	Oc1c(Br)cc(O)cc1	1.6263687	1.680	0.805	0.875	
1020-31-1	Oc1c(O)c(C(C)(C)C)cc(C(C)(C)C)c1	1.8751377	2.110	2.253	-0.143	
824-46-4	Oc1c(OC)cc(O)cc1	1.5440794	2.200	0.326	1.874	
488-47-1	Oc1c(O)c(Br)c(Br)c(Br)c1(Br)	1.7751817	0.980	1.671	-0.691	
527-18-4	Oc1c(C)c(C)c(O)c(C)c1C	1.6446837	1.280	0.912	0.368	
29663-11-4	Oc(c(cc1N(=O)=O)N(=O)=O)c(c1)N(=O)=O	1.6388535	-0.160	0.878	-1.038	
577-71-9	c1c(N(=O)=O)c(N(=O)=O)cc(O)c1	1.6118943	0.270	0.721	-0.451	
618-80-4	Clc(cc(c1)N(=O)=O)c(O)c1Cl	1.6847186	0.630	1.145	-0.515	
329-71-5	c1c(N(=O)=O)cc(O)c(N(=O)=O)c1	1.6118943	0.950	0.721	0.229	
51-28-5	Oc(ccc1N(=O)=O)c(c1)N(=O)=O	1.6647108	1.080	1.028	0.052	
534-52-1	Oc(c(cc1N(=O)=O)C)c(c1)N(=O)=O	1.7062616	1.720	1.270	0.450	
87-86-5	Clc(c(Cl)c(Cl)c1O)c(Cl)c1Cl	1.9508780	2.050	2.694	-0.644	
935-95-5	Clc(cc(Cl)c1Cl)c(Cl)c1O	1.8941863	2.220	2.364	-0.144	
704-13-2	C(=O)c1cc(O)c(N(=O)=O)cc1	1.5502787	0.270	0.362	-0.092	
42454-06-8	c1c(N(=O)=O)c(C=O)cc(O)c1	1.5694055	0.330	0.473	-0.143	
119-33-5	Oc1c(N(=O)=O)cc(C)cc1	1.6692894	0.570	1.055	-0.485	
3011-34-5	C(=O)c1cc(N(=O)=O)c(O)cc1	1.5502787	0.610	0.362	0.248	
104-91-6	c(cc(c1)N=O)c(c1)O	1.5995898	0.650	0.649	0.001	
601-89-8	Oc1c(N(=O)=O)c(O)ccc1	1.5953275	0.660	0.624	0.036	
3947-58-8	BrCC(=O)Nc1c(O)ccc(N(=O)=O)c1	1.6378938	0.874	0.872	0.002	
403-19-0	Oc1c(F)cc(N(=O)=O)cc1	1.7005827	1.073	1.237	-0.164	
446-36-6	c1(O)c(N(=O)=O)ccc(F)c1	1.6470892	1.130	0.926	0.204	
6358-07--2	Clc(cc(c1O)N)c(c1)N(=O)=O	1.6489352	1.170	0.936	0.234	
394-33-2	Oc1c(N(=O)=O)cc(F)cc1	1.7005827	1.384	1.237	0.147	
7147-89-9	Clc(cc(c1O)N(=O)=O)c(c1)C	1.6063779	1.640	0.689	0.951	
99-96-7	Oc(ccc1C(=O)O)cc1	1.4399462	-1.020	-0.280	-0.740	**Calibration set**
501-94-0	Oc(ccc1CCO)cc1	1.4615509	-0.830	-0.154	-0.676	
504-15-4	Oc1cc(O)cc(C)c1	1.5768961	-0.390	0.517	-0.907	
94-71-3	c1c(OCC)c(O)ccc1	1.4718050	-0.360	-0.095	-0.265	
65383-57-5	c1c(OC)c(OCC)cc(O)c1	1.4887836	-0.300	0.004	-0.304	
65-45-2	c(ccc1C(=O)N)cc1O	1.4252596	-0.240	-0.365	0.125	
108-95-2	c(ccc1O)cc1	1.4870533	-0.210	-0.006	-0.204	
106-44-5	c1cc(C)ccc1O	1.4968899	-0.180	0.051	-0.231	
87-28-5	c1(C(=O)OCCO)c(O)cccc1	1.4289880	-0.080	-0.344	0.264	
4421-08--3	N#Cc1cc(OC)c(O)cc1	1.4691914	-0.030	-0.110	0.080	
371-41-5	Fc(ccc1O)cc1	1.5232701	0.020	0.205	-0.185	
611-20-1	c(ccc1C#N)cc1O	1.5544298	0.030	0.386	-0.356	
105-67-9	c(cc(O)c1C)c(c1)C	1.5227041	0.070	0.202	-0.132	
582-24-1	CC(=O)c1c(O)cccc1	1.4533941	0.080	-0.202	0.282	
70-70-2	Oc1cc(C(=O)CC)ccc1	1.5589714	0.115	0.413	-0.298	
95-65-8	c(cc(c1C)C)c(O)c1	1.5886964	0.120	0.586	-0.466	
134-96-3	C(=O)c1cc(OC)c(O)c(OC)c1	1.4708208	0.170	-0.100	0.270	
936-02-7	c(ccc1C(=O)NN)cc1O	1.4532900	0.180	-0.202	0.382	
95-57-8	Clc(ccc1)c(c1)O	1.6150898	0.180	0.739	-0.559	
875-59-2	CC(=O)c1c(C)cc(O)cc1	1.5306280	0.190	0.248	-0.058	
123-07-9	c(cc(c1)CC)c(c1)O	1.5294435	0.210	0.241	-0.031	
94-67-7	c(ccc1C=NO)cc1O	1.5320695	0.250	0.256	-0.006	
2416-94-6	Oc1c(C)c(C)ccc1(C)	1.5994231	0.280	0.648	-0.368	
527-60-6	Oc1c(C)cc(C)cc1(C)	1.6247589	0.280	0.796	-0.516	
1450-72-2	CC(=O)c1c(O)ccc(C)c1	1.5014060	0.310	0.078	0.232	
95-56-7	Brc(ccc1)c(c1)O	1.5886636	0.330	0.586	-0.256	
697-82-5	Oc(cc(c1)C)c(c1C)C	1.5635571	0.360	0.439	-0.079	
615-74-7	Oc1c(Cl)ccc(C)c1	1.6623260	0.390	1.014	-0.624	
90-02-8	c(ccc1C=O)cc1O	1.5603726	0.420	0.421	-0.001	
28177-48-2	c1cc(F)c(O)c(F)c1	1.5895350	0.470	0.591	-0.121	

7781-98-8	CCOC(=O)c1cccc(O)c1	1.5180035	0.480	0.174	0.306	
767-00-0	c(cc(c1)C#N)c(c1)O	1.5290446	0.520	0.239	0.281	
18979-50-5	Oc1ccc(OCCC)cc1	1.6245601	0.522	0.794	-0.272	
700-38-9	Oc1c(N(=O)=O)ccc(C)c1	1.6374201	0.586	0.869	-0.283	
6627-55-0	c1c(C)cc(Br)c(O)c1	1.5740113	0.600	0.500	0.100	
367-27-1	c1c(F)cc(F)c(O)c1	1.5838867	0.600	0.558	0.042	
618-45-1	c(cc(O)c1)cc1C(C)C	1.5721597	0.610	0.489	0.121	
5446-06--6	COc1cc(O)c(C(=O)OC)cc1	1.5158611	0.620	0.162	0.458	
106-41-2	Brc(ccc1O)cc1	1.6334613	0.680	0.846	-0.166	
1124-04-5	c1(C)c(C)cc(Cl)c(O)c1	1.6602820	0.690	1.002	-0.312	
122-94-1	Oc(ccc1OCCCC)cc1	1.6382416	0.700	0.874	-0.174	
1570-64-5	Clc(ccc1O)cc1C	1.6688930	0.700	1.052	-0.352	
97-54-1	Oc1ccc(C=CC)cc1OC	1.5554430	0.750	0.392	0.358	
35421-08-0	Clc(ccc1O)c(c1)C	1.6375418	0.800	0.870	-0.070	
540-38-5	Ic(ccc1O)cc1	1.6123415	0.850	0.723	0.127	
1806-29-7	c1cc(O)c(c2c(O)cccc2)cc1	1.6280680	0.884	0.815	0.069	
101-18-8	Oc1cc(Nc2ccccc2)ccc1	1.6595081	1.014	0.998	0.016	
2491-32-9	c1ccc(CC(=O)c2ccc(O)cc2)cc1	1.6914080	1.069	1.183	-0.114	
14143-32-9	c1c(Cl)c(CC)cc(O)c1	1.6065462	1.080	0.690	0.390	
90-43-7	Oc1c(c2ccccc2)cccc1	1.7001989	1.090	1.235	-0.145	
88-04-0	Clc(c(cc1O)C)c(c1)C	1.6784144	1.200	1.108	0.092	
117-99-7	c1cc(O)c(C(=O)c2ccccc2)cc1	1.6502507	1.225	0.944	0.281	
7463-51-6	c1(C)c(Br)c(C)cc(O)c1	1.6412298	1.270	0.891	0.379	
1518-83-8	C2CCCC2c1ccc(O)cc1	1.7315285	1.290	1.417	-0.127	
28994-41-4	Oc1ccccc1Cc2ccccc2	1.7394917	1.311	1.463	-0.152	
94-26-8	Oc1ccc(C(=O)OCCCC)cc1	1.6471425	1.333	0.926	0.407	
6521-30-8	Oc1ccc(C(=O)OCCC(C)C)cc1	1.6919191	1.480	1.186	0.294	
1131-60-8	Oc1ccc(C2CCCCC2)cc1	1.7925302	1.558	1.772	-0.214	
90-59-5	c1(C=O)cc(Br)cc(Br)c1(O)	1.6967517	1.640	1.215	0.425	
128-37-0	Oc(c(cc1C)C(C)(C)C)c(c1)C(C)(C)C	1.8348503	1.800	2.018	-0.218	
89-68-9	Clc(cc(c1O)C(C)C)c(c1)C	1.7816391	1.850	1.709	0.141	
118-79-6	Brc(cc(Br)c1O)cc1Br	1.7986239	2.030	1.807	0.223	
933-78-8	Oc1c(Cl)c(Cl)cc(Cl)c1	1.8760039	2.370	2.258	0.112	
104-40-5	Oc(ccc1CCCCCCCCC)cc1	1.9100312	2.470	2.456	0.014	
38713-56-3	Oc1ccc(C(=O)OCCCCCCCCCC)cc1	1.9761581	2.633	2.841	-0.208	
591-27-5	c(cc(c1)O)cc1N	1.4480152	-0.520	-0.233	-0.287	
123-30-8	c(cc(c1)N)c(c1)O	1.5344477	-0.080	0.270	-0.350	
488-17-5	Oc1c(O)c(C)ccc1	1.5523067	0.280	0.374	-0.094	
1199-46-8	c1c(O)c(N)cc(C(C)(C)C)c1	1.6627602	0.370	1.017	-0.647	
87-66-1	Oc1c(O)c(O)ccc1	1.5070279	0.850	0.110	0.740	
95-55-6	c(ccc1N)cc1O	1.6047696	0.940	0.679	0.261	
615-67-8	Oc1c(Cl)cc(O)cc1	1.6452484	1.260	0.915	0.345	
2835-96-3	Oc1c(C)cc(N)cc1	1.6365399	1.310	0.864	0.446	
608-43-5	Oc1c(C)c(C)c(O)cc1	1.6093047	1.410	0.706	0.704	
3096-69-3	c1(O)c(C)c(C)c(N)cc1	1.6491216	1.440	0.937	0.503	
1198-55-6	Oc1c(O)c(Cl)c(Cl)c(Cl)c1(Cl)	1.8509092	1.700	2.112	-0.412	
1079-21-6	Oc1c(c2ccccc2)cc(O)cc1	1.7383201	2.010	1.457	0.553	
87-87-6	Oc1c(Cl)c(Cl)c(O)c(Cl)c1Cl	1.7932666	2.110	1.776	0.334	
573-56-8	c1cc(N(=O)=O)c(O)c(N(=O)=O)c1	1.6176425	0.540	0.754	-0.214	
609-93-8	Oc(c(cc1C)N(=O)=O)c(c1)N(=O)=O	1.6588505	1.230	0.994	0.236	
320-76-3	Oc1c(F)cc(Br)cc1N(=O)=O	1.8492835	1.619	2.102	-0.483	
771-61-9	Fc(c(F)c(F)c1O)c(F)c1F	1.7674092	1.640	1.626	0.014	
609-89-2	c1(O)c(Cl)cc(Cl)cc1(N(=O)=O)	1.7981044	1.750	1.804	-0.054	
608-71-9	Brc(c(Br)c(Br)c1O)c(Br)c1Br	1.9856221	2.660	2.896	-0.236	
4901-51-3	Clc(c(Cl)c(Cl)c1O)c(Cl)c1	2.0220782	2.710	3.108	-0.398	
99-57-0	Oc(ccc1N(=O)=O)c(c1)N	1.6058538	0.480	0.686	-0.206	
2042-14-0	c1c(O)cc(N(=O)=O)c(C)c1	1.5684267	0.740	0.468	0.272	
2973-19-5	c1(O)c(CCl)cc(N(=O)=O)cc1	1.7157474	0.750	1.325	-0.575	
119-34-6	c(cc(O)c1N(=O)=O)c(c1)N	1.6344720	0.880	0.852	0.028	
3316-09--4	Oc1c(O)cc(N(=O)=O)cc1	1.6205984	1.170	0.771	0.399	
100-02-7	c(cc(c1)N(=O)=O)c(c1)O	1.5651543	1.420	0.449	0.971	
619-08-9	Clc(cc(c1)N(=O)=O)c(O)c1	1.7462049	1.590	1.502	0.088	
2581-34-2	Oc(ccc1N(=O)=O)cc1C	1.6203693	1.730	0.770	0.960	
7693-52-9	Oc1c(N(=O)=O)cc(Br)cc1	1.7216608	1.869	1.360	0.509	
108-73-6	Oc1cc(O)cc(O)c1	1.5309000	-1.264	0.249	-1.513	
89-64-5	Clc(ccc1O)cc1N(=O)=O	1.7994332	2.050	1.812	0.238	**Test set**
90-01-7	c(ccc1CO)cc1O	1.3343485	-0.954	-0.895	-0.059	
108-46-3	Oc1cc(O)ccc1	1.5264702	-0.652	0.224	-0.876	
5471-51-2	CC(=O)CCc1ccc(O)cc1	1.4037600	-0.497	-0.491	-0.006	
150-19-6	c(cc(O)c1)cc1OC	1.4235544	-0.326	-0.375	0.049	
60563-13-5	CCOC(=O)Cc1cc(OC)c(O)cc1	1.4643789	-0.230	-0.138	-0.092	
150-76-5	c(cc(c1)OC)c(c1)O	1.5212936	-0.143	0.193	-0.336	
873-62-1	c(cc(O)c1)cc1C#N	1.5536185	-0.064	0.382	-0.446	

622-62-8	c(cc(c1)OCC)c(c1)O	1.5478169	0.013	0.348	-0.335
70-70-2	Oc(ccc1C(=O)CC)cc1	1.5042458	0.053	0.094	-0.041
100-83-4	c(cc(O)c1)cc1C=O	1.5161386	0.085	0.163	-0.078
95-88-5	Oc1cc(O)c(Cl)cc1	1.6511156	0.125	0.949	-0.824
367-12-4	Fc(ccc1)c(c1)O	1.4814943	0.185	-0.038	0.223
123-08-0	c(cc(c1)C=O)c(c1)O	1.5168110	0.266	0.167	0.099
1745-81-9	c(ccc1CC=C)cc1O	1.5191515	0.334	0.181	0.153
372-20-3	Fc(ccc1)cc1O	1.4996975	0.381	0.068	0.313
99-89-8	Oc(ccc1C(C)C)cc1	1.6161875	0.473	0.746	-0.273
552-41-0	CC(=O)c1c(O)cc(OC)cc1	1.4987743	0.550	0.062	0.488
4920-77-8	Oc1c(N(=O)=O)c(C)ccc1	1.6432593	0.610	0.903	-0.293
645-56-7	Oc(ccc1CCC)cc1	1.5350830	0.643	0.274	0.369
36436-65-4	CC(=O)c1c(O)cc(C)c(C)c1	1.5565349	0.707	0.399	0.308
5460-31-1	Oc1c(C)c(N(=O)=O)ccc1	1.6432593	0.779	0.903	-0.124
108-43-0	Clc(ccc1)cc1O	1.6349345	0.871	0.855	0.016
137-19-9	Oc1cc(O)c(Cl)cc1(Cl)	1.6441820	0.967	0.909	0.058
103-16-2	c1ccccc1COc2ccc(O)cc2	1.6296933	1.038	0.824	0.214
626-02-8	Ic(ccc1)cc1O	1.5873906	1.119	0.578	0.541
2374-05--2	Oc1c(C)cc(Br)cc1C	1.6835661	1.167	1.138	0.029
576-24-9	Clc(ccc1)c(Cl)c1O	1.7346744	1.276	1.435	-0.159
500-66-3	Oc1cc(O)cc(CCCCC)c1	1.7747218	1.306	1.668	-0.362
92-69-3	Oc1ccc(c2ccccc2)cc1	1.7332901	1.393	1.427	-0.034
94-18-8	Oc1ccc(C(=O)OCc2ccccc2)cc1	1.5586986	1.547	0.411	1.136
18979-55-0	Oc(ccc1OCCCCCC)cc1	1.7620335	1.638	1.595	0.043
136-77-6	Oc1cc(O)c(CCCCCC)cc1	1.8471169	1.798	2.090	-0.292
95-95-4	Clc(cc(Cl)c1O)c(Cl)c1	1.8990410	2.097	2.392	-0.295
5153-25-3	CCCCC(CC)COC(=O)c1ccc(O)cc1	1.8399431	2.507	2.048	0.459
95-86-3	c1c(O)c(N)cc(N)c1	1.5492676	0.127	0.356	-0.229
1687-53-2	c1(OC)c(O)cc(N)cc1	1.5822826	0.450	0.548	-0.098
41458-65-5	Oc1c(C)cc(C)cc1(N)	1.6183951	0.886	0.759	0.127
700-13-0	Oc1c(C)c(C)c(O)c(C)c1	1.6365432	1.342	0.864	0.478
95-71-6	Oc1c(C)cc(O)cc1	1.5768961	1.858	0.517	1.341
771-63-1	Oc1c(F)c(F)c(O)c(F)c1F	1.7711223	1.844	1.647	0.197
66-56-8	c1cc(N(=O)=O)c(N(=O)=O)c(O)c1	1.6176425	0.463	0.754	-0.291
769-39-1	c1c(F)c(F)c(O)c(F)c1(F)	1.6045238	1.167	0.678	0.489
305-85-1	Ic(cc(c1)N(=O)=O)c(O)c1I	1.8302096	1.712	1.991	-0.279
576-55-6	Brc(c(Br)c(Br)c1C)c(Br)c1O	1.9900001	2.574	2.921	-0.347
554-84-7	c(cc(O)c1)cc1N(=O)=O	1.5904804	0.506	0.596	-0.090
88-75-5	c(ccc1N(=O)=O)cc1O	1.6368834	0.670	0.866	-0.196
394-41-2	Oc1cc(F)c(N(=O)=O)cc1	1.7066471	0.935	1.272	-0.337
99-28-5	Brc(cc(c1)N(=O)=O)c(O)c1Br	1.7751346	1.356	1.671	-0.315
88-30-2	Oc1cc(C(F)(F)F)c(N(=O)=O)cc1	1.8471168	1.652	2.090	-0.438