Experimental [1] and calculated with CORAL carcinogenicity (pTD50) values. The sub-training set, calibration set, and test set are indicated by '+', '-', and '#', respectively.

[1] A. P. Toropovaa, A.A. Toropova, R. Gonella Diaza, E. Benfenati, G. Gini Analysis of the co-evolutions of correlations as a tool for QSAR-modeling carcinogenicity: an unexpected good prediction based on a model that seems untrustworthy. Cent. Eur. J. Chem. 9(2011) 165-174

	SMILES	pTD50 Expr	pTD50 Calc	CAS No
+	CC=O	-0.541	-0.457	75-07-0
+	CC(N)=O	-0.484	0.053	60-35-5
+	CC(=O)NC1C=CC2=C3C=CC=CC3=CC2=C1	2.263	1.974	53-96-3
+	CN3c2c(c(cc1OC(C)(C)C=Cc12)OC)C(=O)c4ccccc34	2.804	3.041	7008-42-6
+	C=CC(N)=O	1.278	0.011	79-06-1
+	O=[N+]([O-])c2ccc(/C=C(\c1ccco1)C(N)=O)o2	0.926	1.035	3688-53-7
+	O=C2c1ccccc1C(=O)c3c2c(N)c(Br)cc3Br	0.918	0.127	81-49-2
+	Nc1nnc(o1)c2oc(cc2)[N+]([O-])=O	1.728	1.849	3775-55-1
+	Nc1cc(ccc1O)[N+]([O-])=O	-0.736	0.529	99-57-0
+	[O-][N+](=O)c1cnc(N)s1	0.513	1.074	121-66-4
+	Nc2ccc3C(=O)c1ccccc1C(=O)c3c2	0.344	0.190	117-79-3
+	Cc2cc(/N=N/c1ccccc1C)ccc2N	1.746	0.948	97-56-3
+	CCCCCN(N=O)C(N)=O	2.462	2.484	10589-74-9
+	CC(C)(C)c1ccc(OCC(C)OS(=O)OCCCl)cc1	0.539	0.504	140-57-8
+	Clc1nc(NCC)nc(NC(C)C)n1	0.833	0.317	1912-24-9
+	N#[N+]\C=C(/[O-])OCC(N)C(=O)O	2.339	1.227	115-02-6
+	CC(C)[N+](\[O-])=N/C(C)C	4.686	2.779	17967-53-9
+	c1cc2c3ccc4cccc5ccc(cc2cc1)c3c45	2.421	3.002	50-32-8
+	OCC(CBr)(CBr)CO	0.373	0.858	3296-90-0
+	ClCOCCl	4.507	1.714	542-88-1
+	Nc3ccc(N)c2C(=O)c1c(N)ccc(N)c1C(=O)c23	0.235	0.755	2475-45-8
+	BrC(Cl)Cl	0.354	1.173	75-27-4
+	OCC(=O)C53OC(OC5CC2C1CCC4=CC(=O)C=CC4(C)C1C(O)CC23C)CCC	3.170	2.776	51333-22-3
+	O=C1CC(C)O1	0.795	-0.312	3068-88-0
+	CNC(=O)Oc2cccc1ccccc12	1.154	0.587	63-25-2
+	ClC(Cl)(Cl)Cl	1.827	1.221	56-23-5
+	Oc1ccccc1O	0.114	-0.693	120-80-9
+	O=C(O)CCCc1ccc(cc1)N(CCCl)CCCl	2.531	2.478	305-03-3
+	ClC=1C(=O)OC(O)C=1C(Cl)Cl	2.572	1.728	77439-76-0
+	CC1CC(C)CN(C1)S(=O)(=O)c2cc(C(=O)O)c(Cl)cc2	1.835	1.687	37087-94-8
+	Nc1cc(Cl)ccc1N	-0.176	0.164	95-83-0
+	Clc1ccc(NC(=O)N(C)C)cc1	0.181	0.904	150-68-5
+	Clc1ccc(NC(=O)N(C)C)cc1	1.512	0.904	10473-70-8
+	Clc1c(C#N)c(Cl)c(C#N)c(Cl)c1Cl	-0.931	0.500	1897-45-6
+	Nc1ccc(OC)cc1C	-0.535	-0.147	102-50-1
+	Nc1ccc(cc1)S(=O)(=O)c2ccc(N)cc2	1.045	1.194	80-08-0
+	Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl	0.622	0.605	50-29-3
+	O=C2CCC1C3CC=C4CC(O)CCC4(C)C3CCC12C	0.538	0.564	53-43-0
+	CC(=O)OC2CCC3(C)C4CCC1(C)C(CCC1=O)C4CC=C3C2	1.022	1.629	853-23-6
+	CC(=O)N(C(C)=O)C2C=CC=C1c3ccccc3C=C12	1.145	1.209	63019-65-8
+	C=CCN(CC=C)N=O	0.571	2.138	16338-97-9
+	O=[N+]([O-])c1ccc(o1)c2nc(N)nc(N)n2	2.114	1.537	720-69-4
+	Nc1cc(N)c(C)cc1	1.694	0.102	95-80-7
+	BrC(CBr)CCl	2.960	2.600	96-12-8
+	OC(C(O)CBr)C(O)C(O)CBr	1.566	1.841	10318-26-0
+	BrCCBr	2.092	0.750	106-93-4
+	CC(Cl)(Cl)F	-1.653	-0.788	1717-00-6
+	ClCCCl	1.090	1.846	107-06-2
+	COP(=O)(OC)O\C=C(\Cl)Cl	1.725	1.523	62-73-7
+	Oc1ccc(cc1)C(\CC)=C(\CC)c2ccc(O)cc2	3.080	2.187	56-53-1
+	c1ccc(cc1OCC2CO2)OCC3CO3	1.769	1.704	101-90-6
+	COc2ccc(cc2/C=C/c1ccc(N)cc1)OC	2.549	1.987	5803-51-0
+	O=[N+]([O-])c1ccc(o1)c2nc(C)cc(C)n2	2.198	1.623	59-35-8
+	CN(C)CNc2nnc(/C=C/c1ccc(o1)[N+]([O-])=O)o2	1.096	1.862	55738-54-0
+	CN(C)c1ccccc1	-0.013	0.158	121-69-7
+	CN(C)Nc1nc(cs1)c2ccc(o2)[N+]([O-])=O	2.793	2.597	26049-69-4
+	C/C(C)=C\Cl	0.455	0.848	513-37-1
+	O=NN1CCCN(CC1)N=O	3.410	4.208	55557-00-1
+	ClCC1CO1	1.495	1.166	106-89-8

+	C=CC(=O)OCC	-0.075	-0.362	140-88-5
+	CCO	-2.296	-0.412	64-17-5
+	[O-]\[N+](CC)=N\CC	3.667	3.192	16301-26-1
+	[O-]\[N+](CC)=N\C	3.669	2.707	57497-29-7
+	C1CO1	0.316	0.101	75-21-8
+	O=NN(CC)C(=O)NCCO	2.490	2.407	96724-44-6
+	OC(Cn1cncn1)(Cn2cncn2)c3ccc(F)cc3F	0.579	0.483	86386-73-4
+	FC(F)(F)C(=O)NC1C=CC2=C3C=CC=CC3=CC2=C1	2.233	2.028	363-17-7
+	O=CNNc1nc(cs1)c2ccc(o2)[N+]([O-])=O	1.701	1.651	3570-75-0
+	c1ccco1	2.235	0.604	110-00-9
+	O=Cc1ccco1	-0.852	0.370	98-01-1
+	Cc1cccn2c3nc(N)ccc3nc12	1.626	1.893	67730-11-4
+	NCC(=O)O	-2.534	0.011	56-40-6
+	Cl/C(Cl)=C(/Cl)\C(\Cl)=C(/Cl)Cl	0.598	0.409	87-68-3
+	ClC(Cl)(Cl)C(Cl)(Cl)Cl	0.631	0.917	67-72-1
+	CN(C)P(=O)(N(C)C)N(C)C	3.717	3.321	680-31-9
+	NNc1nc(cs1)c2ccc(cc2)[N+]([O-])=O	1.867	2.214	26049-70-7
+	CC(=O)N(O)C1C=CC2=C3C=CC=CC3=CC2=C1	2.384	2.247	53-95-2
+	FC(F)(F)C\N=C(/N)Nc1ccn(CCCCC(N)=O)n1	-0.582	-0.409	84545-30-2
+	O=C2Nc1ccc(cc1C2(C)C)C=3CCC(=O)NN=3	2.107	2.499	100643-96-7
+	Nc3nc2c(ccc1ncccc12)n3C	2.388	1.730	76180-96-6
+	[O-][N+]13CC=C2COC(=O)[C@@](O)(CO)[C@H](C)C/C(=C\C)C(=O)OC(CC1)C23	2.710	2.951	15503-86-3
+	C=C(C)C	-1.801	-0.156	115-11-7
+	CC(C)CON=O	0.280	0.645	542-56-3
+	O=C(NN)c1ccncc1	-0.039	0.599	54-85-3
+	CC(C)(O)C(O)(C(C)OC)C(=O)OCC1=CCN2CCC(OC(=O)C(\C)=C\C)C12	3.024	2.368	303-34-4
+	OCc3nc(NCCCOc2cc(CN1CCCCC1)ccc2)n(C)n3	-0.125	0.676	76956-02-0
+	Nc1nc(N)nc(N)n1	-0.765	-0.384	108-78-1
+	O=C(O)C(N)Cc1ccc(cc1)N(CCCl)CCCl	3.512	3.321	148-82-3
+	S=C1NC=CN1C	2.001	0.779	60-56-0
+	COc1cc2c3ccccc3oc2cc1N	0.866	1.012	5834-17-3
+	COc1c3occc3cc2C=CC(=O)Oc12	0.824	1.120	298-81-7
+	CC(C)(C)OC	-0.901	0.104	1634-04-4
+	Clc1ccc(cc1)c2ccc(OC(C)(C)C(=O)OC)cc2	1.805	1.050	21340-68-1
+	O=NN(C)c1ccc(cc1)N=O	2.104	3.783	99-80-9
+	O=[N+]([O-])c2ccc(/C=N/N1CC(C)NC1=O)o2	1.649	0.932	21638-36-8
+	O=C(N(C)N=O)c1ccccc1	1.706	1.760	63412-06-6
+	CC1CCCCN1N=O	0.987	1.498	14026-03-0
+	OC(CCCN(C)N=O)c1cccnc1	3.308	2.633	76014-81-8
+	O=C(CCCN(C)N=O)c1cccnc1	3.317	2.454	64091-91-4
+	CN(C)c1ccc(cc1)C(=O)c2ccc(cc2)N(C)C	1.677	1.891	90-94-8
+	ClC13C5(Cl)C2(Cl)C4C(Cl)(C(Cl)(Cl)C12Cl)C3(Cl)C4(Cl)C5(Cl)Cl	2.544	2.428	39801-14-4
+	NC(=O)OCC3C=1C(=O)C(N)=C(C)C(=O)C=1N4CC2NC2C34OC	5.509	5.058	50-07-7
+	O=[N+]([O-])c1ccc(s1)c3nc(N2CCOCC2)c4ccccc4n3	1.833	1.984	58139-48-3
+	O=C(O)C2=CN(CC)c1nc(C)ccc1C2=O	0.063	0.116	389-08-2
+	Nc2cccc1c2cccc1N	0.357	0.171	2243-62-1
+	Nc1ccc2ccccc2c1	0.366	0.334	91-59-8
+	O=C(Nc1ncc(s1)[N+]([O-])=O)NCC	0.218	0.770	139-94-6
+	Nc1cc(ccc1OC)[N+]([O-])=O	0.494	0.788	99-59-2
+	O=[N+]([O-])c1ccc(/C=N/NC(N)=O)o1	1.453	0.902	59-87-0
+	O=[N+]([O-])c1ccc(o1)c2cnc3ccccn23	1.227	1.203	75198-31-1
+	[O-][N+](=O)c1ccc(o1)c2nc(CNC(C)=O)on2	0.627	1.202	36133-88-7
+	CC\C=C(/CC)[N+]([O-])=O	1.174	0.612	4812-22-0
+	O=[N+]([O-])c2ccc(/C=N/N1CCNC1=O)o2	1.630	0.696	555-84-0
+	ClCCN(C)CCCl	4.137	2.804	51-75-2
+	CC(C)Oc1ccccc1OC(=O)N(C)N=O	2.816	2.321	38777-13-8
+	FC(F)(F)CCCN(CCCC(F)(F)F)N=O	2.551	1.040	83335-32-4
+	O=NN(CCO)CC(O)CO	1.439	1.957	89911-78-4
+	CC1CN(N=O)CC(C)N1C(=O)c2ccccc2	1.408	2.699	61034-40-0
+	O=C(NCCCl)N(N=O)CC(C)O	2.380	3.498	96806-35-8
+	CC(C)CN(N=O)C(=O)N	1.487	2.321	760-60-1
+	O=NN(C)c1ccc(F)cc1	2.781	2.446	937-25-7
+	CN(CCc1ccccc1)N=O	4.216	2.261	13256-11-6
+	O=C1OCCN1N=O	2.479	1.200	38347-74-9
+	O=NN1CCCN(N=O)C1	2.939	4.184	15973-99-6
+	O=NN2CCCCC2c1cccnc1	1.206	2.218	1133-64-8
+	CCN(CC)N=O	3.586	2.253	55-18-5
+	CN(C)N=O	2.888	2.295	62-75-9
+	O=Nc2ccc(Nc1ccccc1)cc2	-0.006	1.137	156-10-5
+	OC(C(C)N(C)N=O)c1ccccc1	0.310	2.290	17608-59-2
+	O=C1NC(=O)CN1N=O	0.469	1.652	42579-28-2
+	CN(N=O)CC(O)CO	2.317	1.817	86451-37-8
+	CN(N=O)CCCO	1.852	1.721	70415-59-7

+	O=NN(C)c1ccccn1	2.807	1.774	16219-98-0
+	O=NN1CCOCC1	3.028	1.672	59-89-2
+	O=NN1CCNCC1	1.118	2.539	5632-47-3
+	O=NN1CCCC1	2.098	1.785	930-55-2
+	CC1SC(C)SC(C)N1N=O	2.600	2.730	81795-07-5
+	CC(=O)Nc2ccc3c1ccccc1C(=O)c3c2	1.585	0.576	3096-50-2
+	Nc1ccc(cc1)Oc2ccc(N)cc2	1.323	1.146	101-80-4
+	CN1CCC2OC(=O)C3(CC(C)C(C)(O)C(=O)OCC(=CC1)C2=O)OC3C	2.617	1.955	60102-37-6
+	CCOc1ccc(cc1)NC(C)=O	-0.843	-0.039	62-44-2
+	O=C2C=C(C)N(C)N2c1ccccc1	-0.815	0.375	60-80-0
+	Oc1ccc(cc1)C3(OC(=O)c2ccccc23)c4ccc(O)cc4	-0.452	0.422	77-09-8
+	O=C3C=Cc1ccccc1/C3=N\Nc2ccccc2	0.927	0.008	842-07-9
+	O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2	-0.575	0.326	50-33-9
+	c2ccc(OCC1CO1)cc2	0.533	0.475	122-60-1
+	CCCc1cc2OCOc2cc1COCCOCCOCCCC	-0.272	0.227	51-03-6
+	O=C1OCC1(C)C	-0.324	-0.568	1955-45-9
+	ClCCN(CCCl)c1ccc(cc1)CCCC(=O)OCC(=O)C5(O)CCC4C3CCC2=CC(=O)C=CC2(C)C3C(O)CC45C~	1.527	3.007	29069-24-7
+	NC(=O)N(CCC)N=O	1.541	2.121	816-57-9
+	CC1CO1	-0.107	0.127	75-56-9
+	O=S(=O)(Nc1ccccn1)c3ccc(N\N=C2/C=CC(=O)C(=C2)C(=O)O)cc3	-0.601	-0.798	599-79-1
+	O=C1OC2CCN(C)CC=C(COC(=O)C(C)(O)C(C)C\C1=C\C)C2=O	2.332	2.218	2318-18-5
+	Oc2cccc3Oc1c4C5C=COC5Oc4cc(OC)c1C(=O)c23	3.329	3.593	10048-13-2
+	OC1OC(CO)C(O)C(O)C1NC(=O)N(C)N=O	2.440	3.170	18883-66-4
+	c1ccccc1C2CO2	0.336	0.222	96-09-3
+	C=C(Cl)CSC(=S)N(CC)CC	0.933	1.089	95-06-7
+	Oc1cc(cc(O)c1)C(O)CNC(C)(C)C	-0.260	0.379	23031-25-6
+	Cl/C(Cl)=C(\Cl)Cl	0.215	0.801	127-18-4
+	F/C(F)=C(\F)F	-0.029	-0.424	116-14-3
+	O=[N+]([O-])C([N+]([O-])=O)([N+](=O)[O-])[N+]([O-])=O	2.642	2.497	509-14-8
+	Nc1ccc(cc1)Sc2ccc(N)cc2	1.766	0.042	139-65-1
+	NC(N)=S	-0.112	0.574	62-56-6
+	O=C1C=C(C(=O)C(=C1N2CC2)N3CC3)N4CC4	4.662	4.347	68-76-8
+	O=C(CCCCCCC)OC(COC(=O)CCCCCCC)COC(=O)CCCCCCC	-1.067	-1.071	538-23-8
+	Clc1cc(Cl)cc(Cl)c1O	-0.312	0.379	88-06-2
+	ClCC(Cl)CCl	2.038	1.958	96-18-4
+	CN(C)C(=S)NC	0.661	1.098	2489-77-2
+	NC(=O)OCC	0.334	-0.053	51-79-6
+	BrC=C	0.762	0.190	593-60-2
-	C\C(C)=N\Nc1ncc(s1)c2ccc(o2)[N+]([O-])=O	1.644	1.349	18523-69-8
-	CC(=O)OC(C=C)c1ccc2OCOc2c1	0.945	-0.131	34627-78-6
-	O=C(C)Nc1ccc(cc1)c2ccccc2	2.253	0.843	4075-79-0
-	C=CC#N	0.497	-0.162	107-13-1
-	O=C2Oc1c4C5C=COC5Oc4cc(OC)c1C=3CCC(=O)C2=3	4.991	4.619	1162-65-8
-	NC(=O)N(CC=C)N=O	2.578	2.065	760-56-5
-	O=C3c1ccccc1C(=O)c2c3ccc(C)c2N	0.603	1.367	82-28-0
-	Nc1nnc(s1)c2oc(cc2)[N+]([O-])=O	2.506	1.741	712-68-5
-	O=[N+]([O-])c1cc(N)ccc1O	-0.302	0.106	119-34-6
-	NCC1(CC(=O)O)CCCCC1	-1.533	-0.317	60142-96-3
-	Nc1nncn1	0.927	0.192	61-82-5
-	[O-]\[N+](C)=N\C	3.201	2.894	25843-45-2
-	CC1=CN(C(=O)NC1=O)C2CC(/N=[N+]=[N-])C(CO)O2	-1.637	-0.729	30516-87-1
-	Nc1nc(c(CCOCC)c2ncnn12)c3ccccc3	-0.286	0.009	88133-11-3
-	c1ccccc1	-0.335	-0.566	71-43-2
-	Nc1ccc(cc1)c2ccc(N)cc2	2.027	0.987	92-87-5
-	c1cccc2occc12	-0.555	0.047	271-89-6
-	NC(=O)Cc2c([O-])on[n+]2Cc1ccccc1	-0.260	0.387	14504-15-5
-	CNc1ccc(cc1[N+]([O-])=O)N(CCO)CCO	-0.439	0.487	2784-94-3
-	C=CC=C	-0.683	-0.317	106-99-0
-	CC(C)(C)O	0.060	-0.158	75-65-0
-	ClC2(Cl)C1(Cl)C(Cl)=C(Cl)C2(Cl)C(C1C(=O)O)C(=O)O	0.979	0.982	115-28-6
-	Clc2ccc(Oc1ccc(N)cc1)cc2	0.767	0.932	101-79-1
-	Nc1ccc(Cl)c(N)c1	-0.344	0.264	5131-60-2
-	ClCC(F)(F)F	0.133	-0.084	75-88-7
-	Cc2cccc(Nc1cc(Cl)nc(SCC(=O)NCCO)n1)c2C	1.752	1.461	65089-17-0
-	COCCl	1.166	0.864	107-30-2
-	C=C(Cl)C=C	-0.150	-0.499	126-99-8
-	ClC2(Cl)CC2c1ccc(OC(C)(C)C(=O)O)cc1	2.123	0.974	52214-84-3
-	Clc1ccc(OC(C)(C)C(=O)OCC)cc1	0.157	0.061	637-07-0
-	Nc1cc(C)ccc1OC	0.146	0.186	120-71-8
-	C\C=C\C=O	1.222	-0.024	123-73-9
-	O=P1(NCCCO1)N(CCCl)CCCl	2.072	2.843	50-18-0
-	Brc2c(Oc1c(Br)c(Br)c(Br)c(Br)c1Br)c(Br)c(Br)c(Br)c2Br	-0.542	-1.014	1163-19-5

-	Nc1ccc2c3ccccc3oc2c1	1.869	1.544	4106-66-5
-	O=C(NCCCC)N(CCCC)N=O	1.672	2.702	56654-52-5
-	ClC#CCl	1.423	1.617	7572-29-4
-	Clc1ccc(Cl)cc1	-0.642	0.035	106-46-7
-	Nc1ccc(cc1Cl)c2ccc(N)c(Cl)c2	0.955	1.100	91-94-1
-	OCCOCCO	-1.194	-0.737	111-46-6
-	O=NN1CC=CCO1	0.100	1.768	3276-41-3
-	O=C1CCc2ccccc2O1	-1.302	-0.238	119-84-6
-	CCCc1ccc2OCOc2c1	0.060	0.440	94-58-6
-	COc1cc(ccc1/N=C=O)c2ccc(\N=C=O)c(OC)c2	-0.740	-0.486	91-93-0
-	COc5c(OC)cc(O)c2c5Oc1c3C4C=COC4Oc3cc(OC)c1C2=O	3.024	2.645	65176-75-2
-	CN(C)c2ccc(/N=N/c1ccccc1)cc2	1.833	2.165	60-11-7
-	O=[N+]([O-])c1cnc(C)n1C	0.919	0.673	551-92-8
-	Cc1c(cccc1[N+](=O)[O-])[N+]([O-])=O	2.795	0.731	606-20-2
-	C1COCCO1	-0.481	-0.045	123-91-1
-	Oc3cc4CCC2C(CCC1(C)C2CCC1(O)C#C)c4cc3	3.171	1.775	57-63-6
-	CCOc1ccc(cc1)NC(N)=O	-0.474	0.254	150-69-6
-	CCc1ccccc1	-1.612	-0.228	100-41-4
-	S=C1NCCN1	1.099	1.370	96-45-7
-	CCC(CCCC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	-0.263	-0.945	117-81-7
-	O=C(NCC(C)=O)N(CC)N=O	2.981	2.548	110559-84-7
-	N#CN(CC)N=O	1.430	2.222	38434-77-4
-	NC(=O)N(CCF)N=O	3.034	1.968	69112-98-7
-	O=C(O)CC(O)CC(O)/C=C/c2c(c1ccccc1n2C(C)C)c3ccc(F)cc3	0.517	0.773	93957-54-1
-	OCC1CO1	1.238	-0.052	556-52-5
-	Oc2cc3CC4(O)COc1c(O)c(O)ccc1C4c3cc2O	-0.520	0.331	517-28-2
-	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	1.868	0.882	118-74-1
-	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	1.414	1.369	319-84-6
-	N(Nc1ccccc1)c2ccccc2	1.518	1.057	122-66-7
-	ClC(Cl)C(F)(F)F	-1.190	0.213	306-83-2
-	O=C3c1ccccc1C(=O)c2c3cccc2O	0.380	0.607	129-43-1
-	O=[N+]([O-])c1ccc(s1)c2nc(NCCO)c3ccccc3n2	2.228	1.581	33389-36-5
-	O=C(N)N(N=O)CCCO	2.177	2.224	71752-70-0
-	C=CC(O)c1ccc2OCOc2c1	0.986	0.017	5208-87-7
-	O=C2CN(CC(C)N1CC(=O)NC(=O)C1)CC(=O)N2	1.399	0.820	21416-87-5
-	Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC	2.493	2.060	53-86-1
-	CS(=O)c3ccc(c1nc2cnccc2n1)c(OC)c3	0.610	1.058	86315-52-8
-	O=C1C=C(C)CC(C)(C)C1	-0.942	0.256	78-59-1
-	O=P1(NCCCl)OCCCN1CCCl	2.548	3.061	3778-73-2
-	O=C2C1(Cl)C3(Cl)C5(Cl)C1(Cl)C4(Cl)C2(Cl)C3(Cl)C4(Cl)C5(Cl)Cl	2.219	1.817	143-50-0
-	CC1=CCC(CC1)C(C)=C	-0.175	-0.109	5989-27-5
-	Cc1nc3c(nc1)ccc2c3nc(N)n2C	2.109	2.409	77500-04-0
-	S=C1Nc2ccccc2S1	-0.313	0.459	149-30-4
-	CC1CN1P(=O)(N2CC2C)N3CC3C	1.684	2.176	57-39-6
-	COc1cccc(O)c1O	0.459	-0.688	934-00-9
-	Oc1ccc(OC)cc1	-0.724	-0.526	150-76-5
-	[O-]\[N+](C)=N\CC	0.884	3.378	57497-34-4
-	NC(=O)OC	0.123	0.143	598-55-0
-	CN(C)c2ccc(/N=N/c1cc(C)ccc1)cc2	1.863	2.358	55-80-1
-	O=[N+]([O-])\N=C(\N)N(C)N=O	2.263	3.102	70-25-7
-	[O-][N+](=O)c3c(C)ccc2C(=O)c1ccccc1C(=O)c23	0.499	0.113	129-15-7
-	NC(CCCNC(=O)N(C)N=O)C(=O)O	2.443	2.902	63642-17-1
-	Cc1cc(O)c(O)cc1	-0.301	-0.348	452-86-8
-	Cc2ccc3cc1c5ccccc5ccc1c4CCc2c34	2.738	2.423	56-49-5
-	Nc2ccc(Cc1ccc(N)c(Cl)c1)cc2Cl	1.141	1.109	101-14-4
-	Cc2cc(Cc1ccc(N)c(C)c1)ccc2N	1.487	0.866	838-88-0
-	[O-][N+](=O)CN	0.641	0.539	598-57-2
-	N#CN(C)N=O	2.249	2.408	33868-17-6
-	Cc1ncc([N+]([O-])=O)n1CCO	-0.501	-0.082	443-48-1
-	O=C(O)C(C)(C)Oc1ccc(cc1)C3CCCc2ccccc23	1.451	0.078	3771-19-5
-	OC(=O)CN(CC(=O)O)CC(=O)O	-0.967	-0.152	139-13-9
-	O=C(C)Nc1nnc(s1)c2ccc(o2)[N+]([O-])=O	1.459	1.717	2578-75-8
-	O=C(C)Nc1nc(cs1)c2ccc(o2)[N+]([O-])=O	1.153	1.667	531-82-8
-	O=CNc1nc(cs1)c2ccc(o2)[N+]([O-])=O	1.750	1.068	24554-26-5
-	COc1ccccc1[N+]([O-])=O	0.992	-0.664	91-23-6
-	[O-][N+](=O)c1ccccc1	0.684	-0.122	98-95-3
-	CC(CC)[N+]([O-])=O	-0.443	0.514	600-24-8
-	Clc2cc(Cl)ccc2Oc1ccc(cc1)[N+]([O-])=O	-0.170	0.392	1836-75-5
-	[O-][N+](=O)C1C=CC2=C3C=CC=CC3=CC2=C1	2.870	2.547	607-57-8
-	O=[N+]([O-])c2ccc(/C=N/N1CC(=O)NC1=O)o2	0.165	0.361	67-20-9
-	[O-][N+](C)=O	0.179	0.726	75-52-5
-	CCC(CC)[N+]([O-])=O	0.694	0.498	551-88-2
-	[O-][N+](=O)c4ccc1ccc2cccc3ccc4c1c23	1.871	1.716	5522-43-0

-	[O-][N+](=O)c1cccc2cccnc12	1.249	1.142	607-35-2
-	O=C1NC(=O)N(N=O)CC1	3.163	2.135	16813-36-8
-	O=NN(CC(C)O)CC(O)CO	3.523	2.102	89911-79-5
-	OC(CNCC(C)=O)C(O)N=O	3.699	1.915	92177-50-9
-	CC(O)CN(CCO)N=O	1.181	1.959	56222-35-6
-	CN(CCCCCCCCCCCC)N=O	2.629	1.940	55090-44-3
-	CN(CCCCCCCCCCCCCC)N=O	2.192	1.906	75881-20-8
-	CN(CCCCCCCCCC)N=O	2.201	1.974	75881-22-0
-	NC(=O)N(C)N=O	3.046	2.324	684-93-5
-	O=NN1CC=CCC1	3.271	1.786	55556-92-8
-	FC(F)(F)CN(CC)N=O	1.792	1.991	82018-90-4
-	CC1CN(N=O)CC(C)N1C	3.018	2.553	75881-18-4
-	CC(O)CN(CC=C)N=O	2.216	2.052	91308-70-2
-	C=CCN(N=O)CCO	2.423	1.841	91308-69-9
-	CN(N=O)C(=O)Nc1nc2ccccc2s1	2.320	2.503	51542-33-7
-	O=C(C)CN(CC(=O)C)N=O	2.508	1.992	60599-38-4
-	CCCCN(CCCC)N=O	2.360	2.185	924-16-3
-	OCCN(N=O)CCO	1.627	1.703	1116-54-7
-	O=NN(c1ccccc1)c2ccccc2	0.074	2.122	86-30-6
-	CCCN(CCC)N=O	2.845	2.219	621-64-7
-	CCN(C)N=O	3.244	2.439	10595-95-6
-	O=NN(CC)C(=O)OCC	3.209	2.113	614-95-9
-	O=NN1CCCCCCC1	3.575	1.734	20917-49-1
-	CN(N=O)CCO	1.907	1.738	26921-68-6
-	CC(=O)CN(C)N=O	3.829	2.109	55984-51-5
-	O=NN(C)c1ccccc1	2.982	1.778	614-00-6
-	CN(CCCCCCCCCCC)N=O	1.956	1.957	68107-26-6
-	O=NN2CCCC2c1c[n+]([O-])ccc1	2.344	2.382	78246-24-9
-	O=C(O)C(Cc1ccccc1)NC(=O)c2cc(Cl)c3CC(C)OC(=O)c3c2O	3.593	2.387	303-47-9
-	O=C(O)C2=CN(CC)c1cc3OCOc3cc1C2=O	0.194	0.542	14698-29-4
-	S=C(SN1CCOCC1)N2CCOCC2	0.437	0.482	13752-51-7
-	Clc1c(OC)c(Cl)c(Cl)c(Cl)c1Cl	1.053	0.710	1825-21-4
-	OCC(=O)C4(O)CCC3C2CCC1=CC(=O)C=CC1(C)C2C(O)CC34C	2.372	1.917	50-24-8
-	CC(C)NC(=O)c1ccc(CNNC)cc1	1.742	0.787	671-16-9
-	O=S1(=O)CCCO1	1.503	-0.520	1120-71-4
-	O=C1CCO1	1.693	-0.272	57-57-8
-	N/C(=N/[N+]([O-])=O)N(CCC)N=O	2.126	3.314	13010-07-6
-	S=C1NC(CCC)=CC(=O)N1	1.094	0.691	51-52-5
-	O=C2c1ccccc1C(=O)c3c2c(O)cc(O)c3O	-0.423	0.452	81-54-9
-	[O-][N+](=O)c3cc(C)ccc3N\\N=C1\c2ccccc2C=CC1=O	-0.581	-0.666	2425-85-6
-	CC=1CCCC(C)(C)C=1/C=CC(\C)=C\C=C\C(\C)=C\COC(C)=O	0.420	1.486	127-47-9
-	O=C1OCC3=CCN2CCC(OC(=O)C(/CC(C)C1(O)CO)=C\C)C23	-0.390	0.878	480-54-6
-	OCc1cc(ccc1O)C(O)CNC(C)(C)C	0.777	0.391	18559-94-9
-	Oc1ccc2OCOc2c1	-0.990	0.004	533-31-3
-	O=S(=O)(c1ccc(NC(C)=O)cc1)c2ccc(NC(C)=O)cc2	0.777	0.883	77-46-3
-	FCC(F)(F)F	-2.467	-1.003	811-97-2
-	O=NN1CCCCO1	0.679	1.750	40548-68-3
-	C1CCCO1	-0.752	-0.306	109-99-9
-	S=P(N1CC1)(N2CC2)N3CC3	3.062	2.580	52-24-4
-	CC(N)=S	0.815	0.307	62-55-5
-	NC=3Nc2c(ncn2C1CC(O)C(CO)O1)C(=S)N=3	2.130	2.291	789-61-7
-	O=C1C=CNC(=S)N1	1.032	0.427	141-90-2
-	Cc1ccccc1S(=O)(N)=O	-1.364	-0.666	88-19-7
-	OCC(=O)C54OC(C)(C)OC5CC3C2CCC1=CC(=O)C=CC1(C)C2(F)C(O)CC34C	3.914	4.274	76-25-5
-	BrC(Br)Br	-0.409	0.499	75-25-2
-	Cc1cc(C)c(N)cc1C	0.605	0.000	137-17-7
-	Cc1cc(C)c(C)cc1	-1.559	-0.135	95-63-6
-	O=[N+]([O-])OC(CO[N+]([O-])=O)CO[N+](=O)[O-]	0.094	0.680	55-63-0
-	BrCC(Br)COP(=O)(OCC(Br)CBr)OCC(Br)CBr	2.260	2.814	126-72-7
-	O=C1C=CNC(=O)N1	-0.777	0.337	66-22-8
-	CC(=O)OC=C	-0.598	-0.237	108-05-4
-	C=CF	0.362	-0.181	75-02-5
-	O=C2C=CC(C)=C\C2=N\Nc1ccc(NC(C)=O)cc1	-0.149	-0.066	2832-40-8
#	O=C2Oc1c4C5C=COC5Oc4cc(OC)c1C=3CCC(O)C2=3	5.102	4.820	29611-03-8
#	C=CC\N=C=S	0.014	0.616	57-06-7
#	CC(C)CC(=O)OCC=C	0.063	-0.198	2835-39-4
#	Nc1nc(cs1)c2oc(cc2)[N+]([O-])=O	1.558	1.691	38514-71-5
#	Nc1ccc(cc1O)[N+]([O-])=O	0.143	0.529	121-88-0
#	O=C(O)CCCCCCCCCCN	-0.737	-0.250	2432-99-7
#	N(=N/c1ccccc1)\c2ccccc2	0.879	1.320	103-33-3
#	O=[N+]([O-])c1ccc(s1)c2nc(N(CCO)CCO)c3ccccc3n2	2.060	1.626	33372-39-3
#	BrCC	-0.136	0.259	74-96-4
#	O=C(OCc1ccccc1)c2ccccc2C(=O)OCCCC	-0.522	0.267	85-68-7

#	O=C(N)N(CCCC)N=O	2.448	2.577	869-01-2
#	Oc1ccc(/C=C/C(=O)O)cc1O	-0.217	-0.180	331-39-5
#	O=C(N)N(N=O)CC(=O)O	1.533	2.266	60391-92-6
#	Cc2cccc(Nc1cc(Cl)nc(SCC(=O)O)n1)c2C	1.871	0.926	50892-23-4
#	Clc1ccccc1	-0.341	-0.292	108-90-7
#	ClCF	0.396	0.783	593-70-4
#	OC1OC(CO)C(O)C(O)C1NC(=O)N(CCCl)N=O	3.923	3.764	54749-90-5
#	Oc3cccc2C(=O)c1cccc(O)c1C(=O)c23	-0.009	-0.950	117-10-2
#	O\N=C1\CCCC1	0.385	0.182	1192-28-5
#	ClC(Cl)C(=O)O	-0.096	0.951	79-43-6
#	CCN(CC)C(C)=O	1.115	0.718	685-91-6
#	CCNC(=S)NCC	0.741	0.834	105-55-5
#	CN(C)[N+]([O-])=O	2.217	1.350	4164-28-7
#	CCCCCN(CCCCC)N=O	1.665	2.152	13256-06-9
#	CCC1CO1	-0.484	0.110	106-88-7
#	OC(=O)C(N)CCSCC	1.517	1.170	13073-35-3
#	O=C(C)Nc1ccc(cc1)c2ccc(F)cc2	2.356	1.512	398-32-3
#	O=CNNc1nc(C)cs1	1.038	0.338	32852-21-4
#	Nc1ccc2nc3ccccn3c2n1	0.639	0.749	67730-10-3
#	CCCCCCN(N=O)C(N)=O	2.529	2.467	18774-85-1
#	NNc1nc(cs1)c2ccc(N)cc2	2.302	1.614	26049-71-8
#	NNc1nc(cs1)c2oc(cc2)[N+]([O-])=O	1.851	2.274	26049-68-3
#	O=C(NCC)N(N=O)CCO	2.458	2.399	96724-45-7
#	NC(=O)N(N=O)CCO	2.737	1.767	13743-07-2
#	CC(O)c1ccccc1	-0.574	-0.626	98-85-1
#	CN(C)c2ccc(Cc1ccc(cc1)N(C)C)cc2	1.191	2.099	101-61-1
#	ClC53C1(Cl)C4(Cl)C2(Cl)C1(Cl)C(Cl)(Cl)C5(Cl)C2(Cl)C3(Cl)C4(Cl)Cl	2.489	2.701	2385-85-5
#	O=C1OCC3=CCN2CCC(OC(=O)C(C)C(C)(O)C1(C)O)C23	2.539	1.536	315-22-0
#	O=C1NN=C(O1)c2oc(cc2)[N+]([O-])=O	1.360	2.328	2122-86-3
#	[O-][N+](=O)c1ccc(o1)c2cscn2	1.407	1.903	53757-28-1
#	O=[N+]([O-])c1ccc(o1)c2nc(NC(C)=O)nc(NC(C)=O)n2	1.337	1.679	51325-35-0
#	[O-][N+](=O)c1ccc2CCc3cccc1c23	1.361	0.354	602-87-9
#	O=[N+]([O-])c1ccc(cc1)C(=O)O	-0.235	-0.016	62-23-7
#	O=C(NCCCl)N(N=O)CCO	2.740	3.179	96806-34-7
#	OC1CCN(N=O)C1	2.162	2.365	75896-33-2
#	O=C(N=O)CCNCCO	1.910	1.713	92177-49-6
#	O=NN(CC=C)CC(O)CO	2.288	1.842	88208-16-6
#	C=CCN(CC(=O)C)N=O	2.628	2.197	91308-71-3
#	O=NN(CCCCC)C(=O)OCC	2.270	2.063	64005-62-5
#	CC(O)CN(CC(C)O)N=O	2.283	2.104	53609-64-6
#	O=NN1CCCCCCCCCCC1	1.290	1.650	40580-89-0
#	O=NN1CCCCC1	1.902	1.768	100-75-4
#	O=NN1CCSCC1	1.390	2.539	26541-51-5
#	Cc1ccccc1N=O	0.378	0.576	611-23-4
#	CN(C)/N=N/c1ccccc1	1.810	1.113	7227-91-0
#	Oc2ccccc2c1ccccc1	-0.134	-0.259	90-43-7
#	C=CCc1ccc2OCOc2c1	-0.434	0.415	94-59-7
#	CC(C)C(O)(C(C)O)C(=O)OCC1=CCN2CCC(OC(=O)C(\C)=C\C)C12	2.300	2.201	22571-95-5
#	O=C(Nc1nc(cs1)c2ccc(o2)[N+]([O-])=O)C(F)(F)F	1.656	0.769	42011-48-3
#	C=CCl	1.010	0.549	75-01-4
#	O=C1CCCN1C=C	0.967	0.632	88-12-0