QSAR models for the prediction of dietary biomagnification factor in fish

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Supplementary materials

Table S1 – Dataset 1: based on good quality data (high and medium). Chemicals are reported with CAS numbers, names, splitting category (Training or Prediction set), experimental and predicted Log BMF_L, standardized residuals, HAT values and values of the molecular descriptors included in the model.

Table S2 – Dataset 2: Dataset based only on low quality data with experimental Log BMF_L (low) and predicted Log BMF_L (by Equation 2).

Table S3 – Dataset 3: Consistent dataset based on high quality data (Dataset 1) and verified low quality data from Dataset 2. Chemicals are reported with CAS numbers, names, splitting category (Training or Prediction set), experimental and predicted Log BMF_L, standardized residuals, HAT values and values of the molecular descriptors included in the model.

Table S4 - List of the excluded molecules.

Table S5 – List of the molecules outside the Applicability Domain (AD) of equations 1 and 3. with CAS numbers, SMILES, Structures, chemicals common names, and information on the AD.

Table S1 – Dataset 1: based on good quality data (high and medium). Chemicals are reported with CAS numbers, names, splitting category (Training or Prediction set), experimental and predicted Log BMF_L, standardized residuals, HAT values and values of the molecular descriptors included in the model.

CAS	Chemical Name	Split Eq. 1	Exp Log BMF_L highQuality	Pred Log BMF_L	Pred. Mod. Eq.Res.	Std.Pred. Mod. Eq. Res.	HAT i/i (h*=0.209)	AATS5i	BCUTw-1l	Pubchem FP257	C3SP2	MATS1i	GATS5m	GGI5
10394-57-7	9-n butylphenanthrene	Training	-1.854	-1.174	0.680	1.610	0.022	152.312	11.890	1	5	0.053	1.095	0.389
104-72-3	Decyl benzene	Prediction	-0.745	-0.776	-0.031	-0.073	0.026	163.684	11.890	0	1	0.000	0.935	0.090
107534-96-3	Tebuconazole	Training	-1.921	-1.923	-0.002	-0.005	0.136	169.903	11.890	1	1	-0.078	0.494	0.893
111-84-2	n-nonane	Training	-0.893	-1.195	-0.302	-0.722	0.038	167.659	11.890	0	0	-0.079	0.919	0.056
112281-77-3	Tetraconazole	Prediction	-2.046	-1.411	0.634	1.635	0.173	170.118	11.988	1	1	-0.118	1.037	0.847
112-40-3	n-dodecane	Prediction	-0.878	-1.056	-0.179	-0.425	0.031	166.549	11.890	0	0	-0.059	0.946	0.056
112-41-4	1-dodecene	Training	-0.941	-0.996	-0.055	-0.131	0.031	165.927	11.890	0	0	-0.057	0.933	0.056
118-74-1	Hexachlorobenzene	Training	0.306	0.549	0.243	0.678	0.293	168.159	11.999	0	0	0.000	0.000	0.000
118-82-1	Binox M	Prediction	0.155	-1.265	-1.420	-4.417	0.433	157.787	11.890	1	6	0.064	1.427	2.542
120068-37-3	Fipronil	Training	-1.699	-1.697	0.002	0.007	0.412	180.878	11.999	1	1	-0.016	1.159	1.567
120-12-7	Anthracene	Training	-1.875	-1.651	0.224	0.538	0.049	155.231	11.850	1	4	0.055	0.962	0.111
123-48-8	2,2,4,4,6,6 pentamethyl-3-heptene	Prediction	-1.284	-0.390	0.894	2.446	0.267	150.833	11.890	0	1	-0.057	1.997	0.500
125116-23-6	Metconazole	Training	-1.721	-1.726	-0.005	-0.012	0.126	169.212	11.890	1	1	-0.034	0.467	0.858
126690-66-2	2,4,6 Trimethyl-3-heptene	Prediction	-1.041	-0.769	0.272	0.688	0.143	156.295	11.890	0	1	-0.069	1.679	0.222
13029-08-8	2,2'-Dichlorophenyl	Prediction	0.663	0.097	-0.566	-1.369	0.062	152.071	11.999	1	2	0.035	1.340	0.194
13150-81-7	2,6-Dimethyldecane	Training	-1.319	-0.993	0.326	0.774	0.028	166.327	11.890	0	0	-0.059	0.951	0.222

13151-34-3	3-methyl decane	Prediction	-1.699	-1.179	0.520	1.238	0.033	168.836	11.890	0	0	-0.064	0.835	0.111
13475-82-6	2,2,4,6,6-pentamethylheptane	Training	-0.728	-0.608	0.120	0.304	0.143	157.726	11.890	0	0	-0.059	1.652	0.500
14233-37-5	9,10-Anthracenedione, 1,4-bis[(1-methylethyl)amino]-	Training	-0.500	-0.857	-0.357	-0.883	0.103	152.222	11.890	1	4	0.017	1.124	1.389
15254-25-8	2,3,6,7-Tetramethylanthracene	Training	-1.757	-2.096	-0.339	-0.838	0.102	160.517	11.890	1	8	0.053	0.819	0.444
15968-05-5	2,2',6,6'-Tetrachlorobiphenyl	Training	0.623	0.420	-0.203	-0.488	0.046	149.757	11.999	1	2	0.035	1.106	0.250
1610-22-6	1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydrochrysene	Training	-0.770	-0.496	0.273	0.663	0.068	159.450	11.900	0	4	0.089	1.072	0.361
16435-49-7	2-methyl-1-dodecene	Prediction	-1.200	-1.102	0.099	0.234	0.029	165.756	11.890	0	1	-0.053	0.940	0.111
16606-02-3	2,4',5-Trichlorobiphenyl	Training	0.525	0.404	-0.121	-0.291	0.049	152.367	11.999	1	2	0.035	0.829	0.389
1678-98-4	iso-butyl cyclohexane	Training	-0.652	-0.695	-0.044	-0.104	0.024	165.164	11.900	0	0	0.000	1.036	0.118
16958-92-2	Diisotridecyl adipate	Training	-1.959	-1.017	0.942	2.251	0.040	165.093	11.890	0	0	-0.085	1.023	0.222
1705-85-7	6-methylchyrsene	Training	-1.398	-1.251	0.148	0.353	0.039	150.424	11.890	1	7	0.061	1.148	0.618
1706-50-9	1,1':3',1"Tercyclohexane	Training	-0.357	-0.223	0.134	0.323	0.062	163.993	11.900	0	0	0.068	0.937	0.500
17088-22-1	1-ethylpyrene	Training	-1.699	-1.424	0.275	0.657	0.040	152.141	11.890	1	7	0.067	1.162	0.458
17301-23-4	2,6-Dimethyl undecane	Training	-1.027	-0.950	0.077	0.183	0.028	166.145	11.890	0	0	-0.054	0.956	0.278
17312-44-6	2,3 Dimethyldecane	Prediction	-1.585	-1.196	0.389	0.928	0.034	169.888	11.890	0	0	-0.059	0.774	0.167
1732-13-4	1,2,3,6,7,8 Hexahydropyrene	Training	-1.252	-1.471	-0.219	-0.527	0.051	154.831	11.900	1	6	0.086	1.229	0.111
1795-15-9	n - Octyl Cyclohexane	Training	-1.222	-0.752	0.470	1.114	0.025	166.787	11.900	0	0	0.000	0.887	0.090

18094-01-4	2 methyl 1-Tridecene	Prediction	-0.921	-1.081	-0.160	-0.381	0.028	165.618	11.890	0	1	-0.049	0.945	0.111
1836-75-5	2,4-Dichloro-1-(4-nitrophenoxy) benzene	Training	-0.821	-0.485	0.336	0.910	0.254	154.242	11.850	1	0	0.168	0.854	0.417
1839-63-0	1,3,5-Trimethyl cyclohexane	Training	-0.456	-0.954	-0.498	-1.192	0.044	166.510	11.900	0	0	0.000	1.254	0.000
18516-37-5	2-methyl-1-undecene	Training	-1.456	-1.126	0.330	0.785	0.031	165.927	11.890	0	1	-0.057	0.933	0.111
1889-67-4	Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethaneDiyl)bis-	Training	-0.777	-1.424	-0.646	-1.553	0.050	162.220	11.890	1	2	0.030	0.911	0.625
191-24-2	Benzo(ghi)perylene	Training	-1.495	-1.618	-0.123	-0.305	0.111	145.804	11.850	1	10	0.070	1.085	0.736
193-39-5	Indeno 1,2,3-cd pyrene	Training	-1.538	-1.634	-0.096	-0.239	0.112	146.060	11.850	1	10	0.070	1.124	0.820
194-69-4	Benzo(c)chrysene	Training	-1.301	-1.600	-0.299	-0.723	0.061	148.346	11.850	1	8	0.064	1.079	0.542
19780-74-6	5-ethyl-1-nonene	Training	-0.461	-0.984	-0.523	-1.244	0.030	166.134	11.890	0	0	-0.063	0.909	0.167
20279-21-4	1,2,3,10b-Tetrahydrofluoranthene	Training	-1.638	-1.252	0.386	0.920	0.033	154.143	11.900	1	5	0.080	1.217	0.219
204256-07-5	2,3 Dimethy-5(4methylpentyl) naphthalene	Training	-1.367	-1.748	-0.381	-0.909	0.034	160.151	11.890	1	5	0.031	0.951	0.514
2050-68-2	4,4'-Dichlorobiphenyl	Training	0.519	0.460	-0.058	-0.144	0.110	153.991	11.999	1	2	0.035	0.471	0.361
2051-30-1	2,6-Dimethyl octane	Prediction	-1.854	-1.201	0.652	1.555	0.034	169.400	11.890	0	0	-0.071	0.814	0.222
206-44-0	Fluoranthene	Training	-1.553	-1.585	-0.032	-0.077	0.057	149.167	11.850	1	6	0.065	1.303	0.219
207-08-9	Benzo(k)fluoranthene	Prediction	-1.979	-1.614	0.365	0.881	0.060	148.762	11.850	1	8	0.067	1.091	0.594
214-17-5	Benzo[b]chrysene	Training	-1.745	-1.721	0.023	0.056	0.058	150.131	11.850	1	8	0.064	1.034	0.528
217-59-4	Triphenylene	Training	-1.658	-1.311	0.346	0.835	0.056	146.996	11.850	1	6	0.061	1.175	0.375
218-01-9	Chrysene	Prediction	-1.538	-1.598	-0.061	-0.145	0.041	150.909	11.850	1	6	0.061	1.125	0.361
2189-60-8	n-octyl benzene	Prediction	-1.648	-0.759	0.888	2.109	0.026	163.529	11.890	0	1	0.000	0.927	0.090
22907-72-8	1,4 Diisopropyl cyclohexane	Prediction	-0.479	-1.009	-0.530	-1.262	0.032	170.097	11.890	0	0	0.000	0.844	0.361

23342-25-8	2,2,5,7-Tetramethyltetraline	Prediction	-1.301	-0.796	0.505	1.220	0.060	159.824	11.890	0	4	0.041	1.207	0.535
243-17-4	Benzo(b)fluorene	Training	-1.602	-1.197	0.405	0.963	0.028	153.527	11.900	1	6	0.066	0.978	0.445
2435-85-0	Hexadecahydropyrene	Training	0.009	-0.295	-0.304	-0.738	0.071	164.555	11.900	0	0	0.108	1.010	0.111
2437-56-1	1-Tridecene	Training	-0.963	-0.972	-0.009	-0.022	0.030	165.756	11.890	0	0	-0.053	0.940	0.056
2541-69-7	7-Methylbenz(a)anthracene	Training	-2.097	-1.364	0.733	1.750	0.038	151.919	11.890	1	7	0.061	1.121	0.583
25569-80-6	2,3'-Dichlorobiphenyl	Training	0.267	0.099	-0.169	-0.406	0.055	152.564	11.999	1	2	0.035	1.340	0.333
26186-00-5	1-Heptadecyne	Training	-0.086	-0.863	-0.777	-1.847	0.029	164.854	11.890	0	0	-0.039	0.948	0.056
2732-58-3	6-ethylchyrsene	Prediction	-1.495	-1.200	0.295	0.705	0.041	150.325	11.890	1	7	0.062	1.119	0.708
2974-92-7	3,4-Dichlorobiphenyl	Training	0.477	0.362	-0.115	-0.277	0.061	153.530	11.999	1	2	0.035	0.722	0.361
2980-71-4	2-methyl-1-nonene	Prediction	-1.367	-1.194	0.173	0.413	0.035	166.432	11.890	0	1	-0.069	0.916	0.111
3074-71-3	2,3-Dimethylheptane	Prediction	-0.792	-1.397	-0.605	-1.454	0.050	171.973	11.890	0	0	-0.079	0.689	0.111
319-84-6	(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	Training	-1.516	-0.834	0.682	1.789	0.203	176.439	11.999	0	0	0.000	1.358	0.000
32774-16-6	3,3',4,4',5,5'-Hexachlorobiphenyl	Training	0.496	0.434	-0.061	-0.146	0.036	151.311	11.999	1	2	0.035	1.031	0.583
33025-41-1	2,3,4,4'-Tetrachlorobiphenyl	Training	0.688	0.353	-0.335	-0.799	0.035	152.146	11.999	1	2	0.035	1.015	0.500
3321-50-4	Cyclohexane, 1,1'-(1,2-EthaneDiyl)Bis-	Training	-1.301	-0.581	0.721	1.726	0.044	167.485	11.900	0	0	0.045	0.779	0.181
33460-02-5	3 Phenyl bicyclohexyl	Training	-1.046	-1.102	-0.056	-0.133	0.029	165.756	11.890	0	1	-0.053	0.940	0.111
34883-43-7	2,4'-Dichlorobiphenyl	Training	0.574	0.180	-0.394	-0.942	0.041	153.025	11.999	1	2	0.035	1.090	0.278

35065-27-1	2,2',4,4',5,5'-Hexachlorobiphenyl	Training	0.614	0.661	0.047	0.114	0.058	150.336	11.999	1	2	0.035	0.813	0.694
37680-65-2	2,2',5-Trichlorobiphenyl	Training	0.580	0.364	-0.216	-0.516	0.039	151.413	11.999	1	2	0.035	1.029	0.361
38380-01-7	2,2',4,4',5-Pentachlorobiphenyl	Prediction	0.868	0.535	-0.333	-0.799	0.045	150.995	11.999	1	2	0.035	0.891	0.583
38444-73-4	2,2',6-Trichlorobiphenyl	Prediction	0.568	0.205	-0.363	-0.876	0.058	150.908	11.999	1	2	0.035	1.323	0.222
38444-77-8	2,4',6-Trichlorobiphenyl	Training	0.580	0.105	-0.475	-1.151	0.066	151.851	11.999	1	2	0.035	1.417	0.306
38444-78-9	2,2',3-Trichlorobiphenyl	Prediction	0.477	0.207	-0.270	-0.650	0.051	151.401	11.999	1	2	0.035	1.323	0.361
38444-85-8	2,3,4'-Trichlorobiphenyl	Prediction	0.352	0.247	-0.105	-0.251	0.037	152.355	11.999	1	2	0.035	1.123	0.389
38444-86-9	2,3',4'-Trichlorobiphenyl	Prediction	0.519	0.263	-0.255	-0.609	0.036	152.355	11.999	1	2	0.035	1.123	0.444
3891-98-3	2,6,10-Trimethyl dodecane	Training	-0.002	-0.946	-0.944	-2.244	0.028	167.226	11.890	0	0	-0.046	0.894	0.389
40458-98-8	2,7-Diisopropyl naphthalene	Training	-1.438	-1.594	-0.156	-0.372	0.031	160.496	11.890	1	4	0.034	0.940	0.583
41411-64-7	2,3,3',4,4',5,6-Heptachlorobiphenyl	Training	0.894	0.527	-0.367	-0.878	0.044	149.655	11.999	1	2	0.035	1.194	0.750
41464-39-5	2,2',3,5'-Tetrachlorobiphenyl	Training	0.789	0.407	-0.382	-0.912	0.037	150.743	11.999	1	2	0.035	1.106	0.472
41464-49-7	2,3,3',5'-Tetrachlorobiphenyl	Prediction	0.238	0.241	0.003	0.007	0.052	151.224	11.999	1	2	0.035	1.360	0.500
4175-54-6	1,2,3,4-Tetrahydro-1,4-Dimethyl naphthalene (1,4-Dimethyl Tetralin)	Training	-0.801	-0.831	-0.029	-0.070	0.031	163.515	11.890	0	2	0.046	1.079	0.125
4292-75-5	n-hexyl cyclohexane	Training	-1.377	-0.783	0.594	1.409	0.026	167.334	11.900	0	0	0.000	0.864	0.090
43121-43-3	Triadimefon	Prediction	-1.921	-2.023	-0.102	-0.266	0.188	167.398	11.890	1	0	-0.183	0.697	0.871
4316-65-8	3,5,5' Trimethyl hexene	Training	-1.201	-1.019	0.181	0.439	0.065	162.847	11.890	0	0	-0.077	1.284	0.000

438-22-2	5α(H)-androstane	Prediction	-0.172	-0.245	-0.073	-0.178	0.090	165.899	11.900	0	0	0.094	0.935	0.667
4390-04-9	2,2,4,4,6,8,8-heptamethyl nonane	Prediction	0.004	-0.340	-0.344	-0.910	0.216	154.865	11.890	0	0	-0.043	1.814	0.778
475-03-6	1,1,6 Trimethyl Tetralin	Training	-0.484	-0.858	-0.374	-0.894	0.039	162.053	11.890	0	3	0.043	1.163	0.319
488-23-3	1,2,3,4 Tetramethyl benzene	Training	-1.292	-1.774	-0.481	-1.189	0.100	171.512	11.890	0	4	0.000	0.777	0.000
4920-95-0	3,3',4,4' Tetramethyl 1,1'-biphenyl	Training	-2.046	-2.069	-0.023	-0.057	0.080	164.109	11.890	1	6	0.032	0.708	0.528
496-10-6	Bicyclo[4.3.0]nonane	Training	-1.102	-1.056	0.047	0.114	0.079	174.319	11.900	0	0	0.068	0.694	0.000
50-32-8	Benzo[a]pyrene	Training	-1.745	-1.657	0.088	0.212	0.062	148.080	11.850	1	8	0.067	1.151	0.375
50876-32-9	cis 1,1,3,5 Tetramethyl cyclohexane	Training	-0.265	-0.801	-0.536	-1.310	0.082	162.838	11.900	0	0	0.000	1.510	0.000
51655-65-3	2-butyl-1-decene	Prediction	-0.975	-1.037	-0.063	-0.149	0.029	164.953	11.890	0	1	-0.049	0.961	0.111
52663-59-9	2,2',3,4-Tetrachlorobiphenyl	Training	0.218	0.328	0.111	0.264	0.038	151.192	11.999	1	2	0.035	1.187	0.472
526-73-8	1,3,5-Trimethylbenzene	Training	-1.602	-1.720	-0.118	-0.288	0.084	172.994	11.890	0	3	0.000	0.729	0.000
52886-35-8	3-methyl-1-hexyl cyclohexane	Training	-1.181	-0.739	0.441	1.046	0.023	166.495	11.900	0	0	0.000	0.936	0.146
5325-97-3	1,2,3,4,5,6,7,8-octahydrophenanthrene	Training	-0.893	-0.633	0.260	0.629	0.062	159.370	11.900	0	4	0.076	1.132	0.125
53-70-3	Dibenzo[a,h]anthracene	Training	-2.155	-1.721	0.434	1.046	0.058	150.131	11.850	1	8	0.064	1.034	0.528
541-02-6	Decamethylcyclopentasiloxane	Training	0.532	1.007	0.475	1.380	0.350	155.496	11.998	0	0	-0.178	1.027	1.944
556-67-2	Octamethylcyclotetrasiloxane	Training	0.602	0.374	-0.228	-0.584	0.160	160.019	11.998	0	0	-0.178	0.994	0.944
55702-45-9	2,3,6-Trichlorobiphenyl	Training	0.470	0.191	-0.279	-0.672	0.054	151.401	11.999	1	2	0.035	1.323	0.306
55712-37-3	2,3',4-Trichlorobiphenyl	Training	0.556	0.263	-0.293	-0.699	0.036	152.355	11.999	1	2	0.035	1.123	0.444
5617-41-4	n-heptyl cyclohexane	Training	-1.699	-0.766	0.933	2.214	0.026	167.033	11.900	0	0	0.000	0.877	0.090

56-49-5	3-methylcholanthene	Training	-1.523	-1.700	-0.177	-0.433	0.086	152.912	11.890	1	9	0.074	1.141	0.601
56558-16-8	2,2',4,6,6'-Pentachlorobiphenyl	Training	0.393	0.500	0.107	0.257	0.043	149.548	11.999	1	2	0.035	1.048	0.361
5707-44-8	4-ethyl-1,1'-biphenyl	Prediction	-1.745	-1.390	0.354	0.843	0.029	158.741	11.890	1	3	0.034	0.947	0.313
57465-28-8	3,3',4,4',5-Pentachlorobiphenyl	Prediction	0.581	0.457	-0.124	-0.297	0.042	151.981	11.999	1	2	0.035	0.891	0.583
581-40-8	2,3-Dimethylnaphthalene	Training	-1.921	-1.894	0.027	0.066	0.054	163.525	11.890	1	4	0.040	0.861	0.167
608-93-5	Pentachlorobenzene	Prediction	-0.387	-0.272	0.115	0.286	0.107	170.886	11.999	0	0	0.000	1.128	0.000
6117-97-1	4-methyl dodecane	Training	-1.114	-1.019	0.095	0.225	0.029	166.090	11.890	0	0	-0.054	1.001	0.111
62338-09-4	2,2,3-Trimethyl decane	Training	-1.181	-1.200	-0.019	-0.046	0.036	170.617	11.890	0	0	-0.054	0.732	0.222
629-50-5	n-Tridecane	Training	-0.569	-1.027	-0.458	-1.090	0.030	166.327	11.890	0	0	-0.054	0.951	0.056
629-59-4	n-Tetradecane	Training	0.029	-1.002	-1.032	-2.453	0.029	166.145	11.890	0	0	-0.050	0.956	0.056
629-73-2	1-Hexadecene	Training	0.183	-0.920	-1.103	-2.621	0.029	165.408	11.890	0	0	-0.043	0.953	0.056
66246-88-6	1H-1,2,4-Triazole, 1-[2-(2,4-Dichlorophenyl)pentyl]-	Training	-2.000	-1.794	0.206	0.512	0.109	162.141	11.890	1	1	-0.124	0.951	0.569
68194-04-7	2,2',4,6'-Tetrachlorobiphenyl	Training	-0.854	0.326	1.180	2.825	0.043	150.699	11.999	1	2	0.035	1.187	0.333
68194-05-8	2,2',3,4',6-Pentachlorobiphenyl	Training	0.303	0.502	0.198	0.474	0.039	150.041	11.999	1	2	0.035	1.048	0.500
68194-15-0	2,2',3,4,5,6'-Hexachlorobiphenyl	Prediction	-0.523	0.565	1.088	2.608	0.045	149.371	11.999	1	2	0.035	1.180	0.778
68194-16-1	2,2',3,3',4,5,6-Heptachlorobiphenyl	Training	0.009	0.647	0.638	1.531	0.047	148.712	11.999	1	2	0.035	1.125	0.778

6975-98-0	2-methyl decane	Training	-1.444	-1.076	0.368	0.875	0.031	166.826	11.890	0	0	-0.064	0.939	0.111
702-79-4	1,3-Dimethyladamantane	Training	-1.174	-0.491	0.683	1.674	0.087	163.721	11.900	0	0	0.098	1.378	0.000
70356-09-1	1-(4-tert-butylphenyl)-3-(4-methoxyphenyl)propane-1,3-Dione	Training	-0.914	-1.508	-0.593	-1.439	0.067	161.118	11.890	1	3	-0.022	0.889	1.056
7045-71-8	2-methyl undecane	Training	-1.292	-1.040	0.252	0.600	0.030	166.549	11.890	0	0	-0.059	0.946	0.111
7116-96-3	4-pentyl-1,1'-Biphenyl	Prediction	-1.174	-1.379	-0.205	-0.487	0.029	158.588	11.890	1	3	0.031	0.942	0.340
71608-00-9	1-octylpyrene	Prediction	-1.108	-1.643	-0.535	-1.283	0.044	155.729	11.890	1	7	0.061	1.026	0.486
717-74-8	Benzene, 1,3,5-Tris(1-methylethyl)-	Training	-0.398	-0.492	-0.094	-0.233	0.097	159.698	11.890	0	3	0.000	0.969	1.042
72-43-5	Methoxy chlor	Training	-0.969	-0.703	0.266	0.668	0.126	158.028	11.996	1	2	-0.092	1.415	0.653
73575-52-7	2,3',4,5'-Tetrachlorobiphenyl	Training	0.218	0.330	0.112	0.268	0.038	151.685	11.999	1	2	0.035	1.187	0.611
74472-36-9	2,3,3',5,6-Pentachlorobiphenyl	Training	0.477	0.423	-0.054	-0.130	0.040	150.072	11.999	1	2	0.035	1.205	0.528
74472-38-1	2,3,4,4',6-Pentachlorobiphenyl	Training	0.857	0.396	-0.461	-1.100	0.036	150.983	11.999	1	2	0.035	1.122	0.528
74472-48-3	2,2',3,4,4',6,6'-Heptachlorobiphenyl	Training	0.928	0.703	-0.225	-0.541	0.049	148.681	11.999	1	2	0.035	0.980	0.694
74487-85-7	2,2',3,4',5,6,6'-Heptachlorobiphenyl	Training	0.884	0.807	-0.076	-0.184	0.061	148.231	11.999	1	2	0.035	0.912	0.806
781-17-9	4,5,9,10-Tetrahydropyrene	Training	-1.553	-1.486	0.067	0.162	0.050	154.874	11.900	1	6	0.080	1.214	0.111
81-15-2	Musk-xylene	Training	-0.210	-0.392	-0.182	-0.600	0.495	169.015	11.890	0	3	0.278	1.353	1.618
821-95-4	1-undecene	Prediction	-1.409	-1.026	0.383	0.912	0.033	166.145	11.890	0	0	-0.063	0.926	0.056

832-69-9	1-Methylphenanthrene	Training	-1.721	-1.408	0.314	0.744	0.026	154.746	11.890	1	5	0.055	1.138	0.299
84-15-1	o-Terphenyl	Training	-0.499	-1.087	-0.588	-1.429	0.072	148.112	11.850	1	4	0.046	1.027	0.333
85-01-8	Phenanthrene	Training	-1.122	-1.616	-0.494	-1.188	0.053	153.631	11.850	1	4	0.055	1.139	0.125
872-05-9	1-decene	Training	-0.991	-1.064	-0.072	-0.173	0.034	166.432	11.890	0	0	-0.069	0.916	0.056
88671-89-0	Myclobutanil	Training	-2.097	-1.536	0.561	1.390	0.105	162.237	11.890	1	1	-0.107	0.619	0.684
91-17-8	t-decalin	Training	-0.068	-0.897	-0.830	-2.004	0.060	171.594	11.900	0	0	0.062	0.764	0.000
91-20-3	Naphthalene	Training	-2.301	-2.034	0.267	0.656	0.090	162.291	11.850	1	2	0.042	1.043	0.000
91-57-6	2-Methylnaphthalene	Training	-2.000	-1.588	0.412	0.988	0.045	159.982	11.890	1	3	0.041	1.047	0.083
92-06-8	m-terphenyl	Training	-1.347	-1.266	0.081	0.196	0.057	151.381	11.850	1	4	0.046	0.969	0.500
92-51-3	Bicyclohexyl	Training	-0.770	-0.542	0.227	0.543	0.039	166.327	11.900	0	0	0.052	0.897	0.139
933-12-0	3,5,5 Trimethyl cyclohexene	Training	-1.137	-0.943	0.194	0.463	0.036	166.852	11.900	0	0	0.000	1.184	0.000
93-46-9	N,N′-Di-2-naphthyl-p-phenyleneDiamine	Training	-1.096	-1.512	-0.416	-0.998	0.047	155.106	11.850	1	4	0.074	0.966	0.361
94361-06-5	Cyproconazole	Training	-1.959	-1.405	0.554	1.354	0.081	164.796	11.900	1	1	-0.037	0.639	0.771
98-51-1	1-tert butyl-4-methyl benzene	Training	-1.018	-1.015	0.003	0.006	0.027	165.778	11.890	0	2	0.000	0.945	0.354

Table S2 – Dataset 2: Dataset based only on low quality with experimental Log BMF_L (low) and predicted Log BMF_L (by Equation 2).

CAS	Chemical Name	SMILES	Log_BMF_L LowQuality	Log_BMF_L Pred. by model eq.
1024-57-3	2,3,4,5,6,7,7-Heptachloro-1a,1b,5,5a,6,6a,-Hexahydro-(2a alpha, 1b beta, 2 alpha, 5 alpha, 5a beta, 6 beta, 6a alpha-2,5-methano-2H-indeno[1,2-b]oxirene	ClC1C2OC2C2C1C1(Cl)C(=C(C2(C1(Cl)Cl)Cl)Cl)Cl	0.415	0.319
10605-21-7	Carbendazim	COC(=O)Nc1nc2c([nH]1)cccc2	-3.745	-1.807
117-81-7	Di-2-Ethylhexyl phthalate	CCCCC(COC(=O)c1ccccc1C(=O)OCC(CCCC)CC)CC	-1.125	-1.041
120068-36-2	Fipronil sulfone	N#Cc1nn(c(c1S(=O)(=O)C(F)(F)F)N)c1c(Cl)cc(cc1Cl)C(F)(F)F	0.777	-1.418
129-00-0	Pyrene	c1cc2ccc3c4c2c(c1)ccc4ccc3	-2.301	-1.771
131860-33-8	Azoxystrobin	COC=C(c1ccccc1Oc1ncnc(c1)Oc1ccccc1C#N)C(=O)OC	-3.347	-2.205
15299-99-7	Napropamide	CCN(C(=O)C(Oc1cccc2c1cccc2)C)CC	-2.852	-2.203
1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]Dioxin	Clc1cc2Oc3cc(Cl)c(cc3Oc2cc1Cl)Cl	0.103	0.612
2051-24-3	Decachlorobiphenyl	Clc1c(c2c(Cl)c(Cl)c(c(c2Cl)Cl)Cl)c(Cl)c(c(c1Cl)Cl)Cl	0.319	1.048
205646-11-3	1,2,9,10-Tetrachlorodecane	ClCC(CCCCCCC(CCl)Cl)Cl	-0.658	0.035
208465-21-8	Mesosulfuron-methyl	COC(=O)c1ccc(cc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(n1)OC)CNS(=O)(=O)C	-5.699	-1.274
2136-99-4	2,2',3,3',5,5',6,6'-Octachlorobiphenyl	Clc1c(Cl)cc(c(c1c1c(Cl)c(Cl)cc(c1Cl)Cl)Cl)Cl	0.667	1.026
221155-23-3	1,2,13,14-Tetrachlorotetradecane	ClCC(CCCCCCCCCCC(CCl)Cl)Cl	0.100	0.194
2381-21-7	1-Methylpyrene	Cc1ccc2c3c1ccc1c3c(cc2)ccc1	-2.301	-1.489
2385-85-5	Mirex	ClC12C(Cl)(Cl)C3(C4(C1(Cl)C1(C2(Cl)C3(C4(C1(Cl)Cl)Cl)Cl)Cl)Cl)Cl	0.371	1.549
2437-79-8	2,2',4,4'-Tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccc(cc1Cl)Cl	0.833	0.370
2471-09-2	OctacosamethylTridecasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)C	-1.699	2.531
2471-10-5	Triacontamethyltetradecasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)C	-1.699	2.715
2652-13-3	Eicosamethylnonasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)C	-1.097	1.858
27575-78-6	Tris(4-chlorophenyl)methane	Clc1ccc(cc1)C(c1ccc(cc1)Cl)c1ccc(cc1)Cl	0.538	0.836
3010-80-8	Tris(4-chlorophenyl)methanol	OC(c1ccc(cc1)Cl)(c1ccc(cc1)Cl)c1ccc(cc1)Cl	-0.260	0.997
31508-00-6	2,3',4,4',5-Pentachlorobiphenyl	Clc1cc(Cl)c(cc1c1ccc(c(c1)Cl)Cl)Cl	0.776	0.531
32598-10-0	2,3',4,4'-Tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccc(c(c1)Cl)Cl	0.470	0.392
32598-11-1	2,3',4',5-Tetrachlorobiphenyl	Clc1ccc(c(c1)c1ccc(c(c1)Cl)Cl)Cl	0.771	0.446
32598-14-4	2,3,3',4,4'-Pentachlorobiphenyl	Clc1ccc(cc1Cl)c1ccc(c(c1Cl)Cl)Cl	0.740	0.406

32690-93-0	2,4,4',5-Tetrachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)c(cc1Cl)Cl	0.903	0.506
3322-93-8	Tetrabromoethylcyclohexane β	BrCC(C1CCC(C(C1)Br)Br)Br	-0.318	0.239
33284-50-3	2,4-Dichlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccccc1	0.703	0.170
33284-52-5	3,3',5,5'-Tetrachlorobiphenyl	Clc1cc(cc(c1)Cl)c1cc(Cl)cc(c1)Cl	0.457	0.291
34123-59-6	Isoproturon	O=C(N(C)C)Nc1ccc(cc1)C(C)C	-3.211	-0.719
34883-39-1	2,5-Dichlorobiphenyl	Clc1ccc(c(c1)c1ccccc1)Cl	-0.638	0.268
35065-28-2	2,2',3,4,4',5'-Hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1ccc(c(c1Cl)Cl)Cl)Cl	0.803	0.577
35065-29-3	2,2',3,4,4',5,5'-Heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl	0.842	0.701
35065-30-6	2,2',3,3',4,4',5-Heptachlorobiphenyl	Clc1c(Cl)ccc(c1Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.851	0.586
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl	Clc1ccc(cc1c1cc(Cl)ccc1Cl)Cl	0.481	0.549
35694-06-5	2,2',3,4,4',5-Hexachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.836	0.600
35694-08-7	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	Clc1cc(c(c(c1Cl)Cl)Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.958	0.669
35822-46-9	1,2,3,4,6,7,8-H7CDD	Clc1c(Cl)cc2c(c1Cl)Oc1c(O2)c(Cl)c(c(c1Cl)Cl)Cl	-0.469	0.644
36559-22-5	2,2',3,4'-Tetrachlorobiphenyl	Clc1ccc(c(c1)Cl)c1cccc(c1Cl)Cl	0.572	0.334
36734-19-7	Iprodione	CC(NC(=O)N1CC(=O)N(C1=O)c1cc(Cl)cc(c1)Cl)C	-2.673	-0.835
37680-66-3	2,2',4-Trichlorobiphenyl	Clc1ccc(c(c1)Cl)c1ccccc1Cl	0.204	0.250
37680-73-2	2,2',4,5,5'-Pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(cc1Cl)Cl)Cl	0.783	0.631
38379-99-6	2,2',3,5',6-Pentachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)ccc(c1Cl)Cl)Cl	0.734	0.605
38380-02-8	2,2',3,4,5'-Pentachlorobiphenyl	Clc1ccc(c(c1)c1ccc(c(c1Cl)Cl)Cl)Cl	0.760	0.506
38380-03-9	2,3,3',4',6-Pentachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)ccc(c1Cl)Cl	0.919	0.381
38380-04-0	2,2',3,4',5',6-Hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)ccc(c1Cl)Cl)Cl	0.792	0.674
38380-05-1	2,2',3,3',4,6'-Hexachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl	0.743	0.556
38380-07-3	2,2',3,3',4,4'-Hexachlorobiphenyl	Clc1c(ccc(c1Cl)Cl)c1ccc(c(c1Cl)Cl)Cl	0.769	0.459
38380-08-4	2,3,3',4,4',5-Hexachlorobiphenyl	Clc1ccc(cc1Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.869	0.528
38411-22-2	2,2',3,3',6,6'-Hexachlorobiphenyl	Clc1ccc(c(c1c1c(Cl)ccc(c1Cl)Cl)Cl)Cl	0.678	0.771
38411-25-5	2,2',3,3',4,5,6'-Heptachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl	0.830	0.705
38444-76-7	2,3',6-Trichlorobiphenyl	Clc1cccc(c1)c1c(Cl)cccc1Cl	-0.046	0.062
38444-81-4	2,3',5-Trichlorobiphenyl	Clc1ccc(c(c1)c1cccc(c1)Cl)Cl	0.653	0.333
38444-84-7	2,3,3'-Trichlorobiphenyl	Clc1cccc(c1)c1cccc(c1Cl)Cl	-0.222	0.173
38444-93-8	2,2',3,3'-Tetrachlorobiphenyl	Clc1c(Cl)cccc1c1cccc(c1Cl)Cl	0.514	0.274
39227-61-7	1,2,3,4,7-P5CDD	Clc1ccc2c(c1)Oc1c(O2)c(Cl)c(c(c1Cl)Cl)Cl	-1.092	0.703
39635-31-9	2,3,3',4,4',5,5'-Heptachlorobiphenyl	Clc1cc(cc(c1Cl)Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.631	0.514
40186-70-7	2,2',3,3',4,5',6-Heptachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl	0.778	0.705
40186-71-8	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	Clc1cc(Cl)c(c(c1Cl)Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl	0.803	0.954
40186-72-9	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	Clc1cc(c(c(c1Cl)Cl)Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl	0.531	0.804
41464-41-9	2,2',5,6'-Tetrachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)cccc1Cl)Cl	-0.398	0.437
41464-43-1	2,3,3',4'-Tetrachlorobiphenyl	Clc1cc(ccc1Cl)c1cccc(c1Cl)Cl	0.667	0.309
41464-46-4	2,3',4',6-Tetrachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)cccc1Cl	0.322	0.220
41464-47-5	2,2',3,6'-Tetrachlorobiphenyl	Clc1c(Cl)cccc1c1c(Cl)cccc1Cl	-0.398	0.299
41464-51-1	2,2',3',4,5-Pentachlorobiphenyl	Clc1cc(Cl)c(cc1c1cccc(c1Cl)Cl)Cl	0.842	0.506

42740-50-1	2,2',3,3',4,4',5,6'-Octachlorobiphenyl	Clc1cc(Cl)c(c(c1c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl)Cl	0.833	0.741
483-65-8	1-methyl-7-(1methylethyl)-phenanthrene	CC(c1ccc2c(c1)ccc1c2cccc1C)C	-1.553	-1.545
50-29-3	4,4'-DDT	ClC(C(c1ccc(cc1)Cl)c1ccc(cc1)Cl)(Cl)Cl	0.752	-0.009
50563-36-5	Dimethachlor	COCCN(c1c(C)cccc1C)C(=O)CCl	-4.462	-0.420
5103-74-2	1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-Hexahydro-4,7-methano-1H-indene	ClC1CC2C(C1Cl)C1(C(C2(Cl)C(=C1Cl)Cl)(Cl)Cl)Cl	0.326	0.645
51908-16-8	2,2',3,4',5,5'-Hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1cc(Cl)c(cc1Cl)Cl)Cl	0.916	0.649
52663-58-8	2,3,4',6-Tetrachlorobiphenyl	Clc1ccc(cc1)c1c(Cl)ccc(c1Cl)Cl	0.806	0.310
52663-60-2	2,2',3,3',6-Pentachlorobiphenyl	Clc1c(Cl)cccc1c1c(Cl)ccc(c1Cl)Cl	0.505	0.480
52663-61-3	2,2',3,5,5'-Pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)cc(c1Cl)Cl)Cl	0.744	0.579
52663-62-4	2,2',3,3',4-Pentachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1cccc(c1Cl)Cl	0.738	0.381
52663-65-7	2,2',3,3',4,6,6'-Heptachlorobiphenyl	Clc1cc(Cl)c(c(c1Cl)Cl)c1c(Cl)ccc(c1Cl)Cl	0.767	0.823
52663-66-8	2,2',3,3',4,5'-Hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1ccc(c(c1Cl)Cl)Cl)Cl	0.431	0.530
52663-68-0	2,2',3,4',5,5',6-Heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)c(Cl)cc(c1Cl)Cl)Cl	0.756	0.798
52663-69-1	2,2',3,4,4',5',6-Heptachlorobiphenyl	Clc1cc(Cl)c(cc1c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl	0.790	0.727
52663-70-4	2,2',3,3',4,5',6'-Heptachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl	0.796	0.682
52663-71-5	2,2',3,3',4,4',6-Heptachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)c1ccc(c(c1Cl)Cl)Cl)Cl	0.848	0.611
52663-72-6	2,3',4,4',5,5'-Hexachlorobiphenyl	Clc1cc(Cl)c(cc1c1cc(Cl)c(c(c1)Cl)Cl)Cl	0.732	0.552
52663-74-8	2,2',3,3',4,5,5'-Heptachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl	0.854	0.633
52663-75-9	2,2',3,3',4,5,5',6'-Octachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl	0.820	0.789
52663-77-1	2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	Clc1c(Cl)c(Cl)c(c(c1Cl)Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl	0.728	1.048
52663-78-2	2,2',3,3',4,4',5,6-Octachlorobiphenyl	Clc1ccc(c(c1Cl)Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl	0.641	0.717
52663-79-3	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	Clc1c(Cl)cc(c(c1Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl)Cl	0.799	0.975
52712-04-6	2,2',3,4,5,5'-Hexachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(c(c1Cl)Cl)Cl)Cl	0.839	0.649
52712-05-7	2,2',3,4,5,5',6-Heptachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl)Cl	0.845	0.798
52744-13-5	2,2',3,3',5,6'-Hexachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1c(Cl)ccc(c1Cl)Cl)Cl	0.724	0.651
53-19-0	o,p'-DDD	ClC(C(c1ccccc1Cl)c1ccc(cc1)Cl)Cl	0.380	0.056
541-01-5	Hexadecamethylheptasiloxane	C[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)C	-1.398	1.546
544-76-3	n-Hexadecane	CCCCCCCCCCCCCCCC	-0.314	-1.040
55215-18-4	2,2',3,3',4,5-Hexachlorobiphenyl	Clc1cccc(c1Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.839	0.530
556-69-4	Octadecamethyloctasiloxane	C[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)C	-0.796	1.698
556-70-7	Docosamethyldecasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)C	-1.222	2.023
56-55-3	Benzo[a]anthracene	c1ccc2c(c1)cc1c(c2)ccc2c1cccc2	-2.301	-1.614
60145-20-2	2,2',3,3',5-Pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1cccc(c1Cl)Cl)Cl	0.761	0.454
60145-23-5	2,2',3,4,4',5,6'-Heptachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.836	0.658
60233-25-2	2,2',3,4',6'-Pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)Cl)c1cccc(c1Cl)Cl	0.230	0.406
67129-08-2	Metazachlor	ClCC(=O)N(c1c(C)cccc1C)Cn1cccn1	-4.493	-0.884

68194-14-9	2,2',3,4,5',6-Hexachlorobiphenyl	Clc1ccc(c(c1)c1c(Cl)cc(c(c1Cl)Cl)Cl)Cl	0.799	0.674
7012-37-5	2,4,4'-Trichlorobiphenyl	Clc1ccc(cc1)c1ccc(cc1Cl)Cl	0.290	0.322
70362-45-7	2,2',3,6-Tetrachlorobiphenyl	Clc1ccccc1c1c(Cl)ccc(c1Cl)Cl	0.568	0.414
70362-46-8	2,2',3,5-Tetrachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1ccccc1Cl)Cl	0.829	0.435
70424-68-9	2,3,3',4',5-Pentachlorobiphenyl	Clc1cc(Cl)c(c(c1)c1ccc(c(c1)Cl)Cl)Cl	1.033	0.457
70424-70-3	2,3',4',5,5'-Pentachlorobiphenyl	Clc1ccc(c(c1)c1cc(Cl)c(c(c1)Cl)Cl)Cl	0.380	0.480
71888-89-6	Diisoheptyl phthalate	CC(CCCCOC(=O)c1ccccc1C(=O)OCCCCC(C)C)C	-2.509	-1.121
72-54-8	p,p'-DDD	ClC(C(c1ccc(cc1)Cl)c1ccc(cc1)Cl)Cl	0.602	0.023
74472-33-6	2,3,3',6-Tetrachlorobiphenyl	Clc1cccc(c1)c1c(Cl)ccc(c1Cl)Cl	0.720	0.274
74472-34-7	2,3,4',5-Tetrachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)cc(c1Cl)Cl	0.857	0.446
74472-37-0	2,3,4,4',5-Pentachlorobiphenyl	Clc1ccc(cc1)c1cc(Cl)c(c(c1Cl)Cl)Cl	0.829	0.531
74472-42-7	2,3,3',4,4',6-Hexachlorobiphenyl	Clc1ccc(cc1Cl)c1c(Cl)cc(c(c1Cl)Cl)Cl	0.826	0.459
74472-44-9	2,3,3',4',5,6-Hexachlorobiphenyl	Clc1cc(ccc1Cl)c1c(Cl)c(Cl)cc(c1Cl)Cl	0.929	0.507
74472-53-0	2,3,3',4,4',5,5',6-Octachlorobiphenyl	Clc1c(Cl)cc(cc1Cl)c1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl	0.806	0.552
779-02-2	9-Methylanthracene	Cc1c2ccccc2cc2c1cccc2	-2.398	-1.425
789-02-6	1-Chloro-2-(2,2,2-Trichloro-1-(4-chlorophenyl)ethyl)benzene (o,p'-DDT)	Clc1ccc(cc1)C(C(Cl)(Cl)Cl)c1ccccc1Cl	0.839	0.114
79277-27-3	Thifensulfuron-methyl	COc1nc(nc(n1)C)NC(=O)NS(=O)(=O)c1ccsc1C(=O)OC	-4.297	-1.816
81777-89-1	Clomazone	O=C1N(OCC1(C)C)Cc1ccccc1Cl	-3.699	0.543
83164-33-4	Diflufenican	Fc1ccc(c(c1)F)NC(=O)c1cccnc1Oc1cccc(c1)C(F)(F)F	-2.991	-0.847
84632-59-7	3,6-Bis-(4-tert-butyl-phenyl)-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione	CC(c1ccc(cc1)c1[nH]c(=O)c2c1c(=O)[nH]c2c1ccc(cc1)C(C)(C)C)(C)C	-1.413	-1.228

Table S3 – Dataset 3: Consistent dataset based on high quality data (Dataset 1) and verified low quality data from Dataset 2. Chemicals are reported with CAS numbers, names, splitting category (Training or Prediction set), experimental and predicted Log BMF_L, standardized residuals, HAT values and values of the molecular descriptors included in the model.

CAS	Chemical Name	Split. Eq. 3	Exp BMF_L	Pred BMF_L	Pred.Mod. Eq.Res.	Std.Pred. Mod.Eq. Res.	HAT i/i (h*=0.12)	PubchemFP503	SubFPC295	R_TpiPCTPC	MLFER_S	maxHother	GGI5	VE3_Dt
4390-04-9	2,2,4,4,6,8,8-heptamethyl nonane	Training	0.004	-0.513	-0.518	-1.247	0.093	0	0	1.000	-0.149	0	0.778	-4.765
1024-57-3	2,3,4,5,6,7,7-Heptachloro-1a,1b,5,5a,6,6a,-Hexahydro-(2a alpha, 1b beta, 2 alpha, 5 alpha, 5a beta, 6 beta, 6a alpha-2,5-methano-2H-indeno[1,2-b]oxirene	Training	0.415	-0.352	-0.767	-1.851	0.095	0	2	1.387	1.581	0	0.789	-7.426
10394-57-7	9-n butylphenanthrene	Training	-1.854	-1.512	0.342	0.795	0.024	0	0	15.938	1.237	0.4354 0529	0.389	-3.214
104-72-3	Decyl benzene	Prediction	-0.745	-1.246	-0.501	-1.180	0.049	0	0	2.553	0.553	0.4119 0382	0.090	-2.872
107534-96-3	Tebuconazole	Training	-1.921	-1.648	0.273	0.668	0.119	1	6	3.259	1.415	0.6867 8148	0.893	-3.078
111-84-2	n-nonane	Training	-0.893	-0.734	0.159	0.371	0.034	0	0	1.000	0.127	0	0.056	-30.905
112281-77-3	Tetraconazole	Prediction	-2.046	-2.215	-0.169	-0.425	0.169	1	7	3.957	1.406	0.7523 4702	0.847	-2.903
112-40-3	n-dodecane	Prediction	-0.878	-0.850	0.028	0.065	0.044	0	0	1.000	0.127	0	0.056	0.000
112-41-4	1-dodecene	Training	-0.941	-1.352	-0.410	-0.965	0.047	0	0	1.130	0.167	0.3712 5584	0.056	0.000
117-81-7	Di-2-Ethylhexyl phthalate	Prediction	-1.125	-2.541	-1.416	-3.463	0.119	0	6	3.007	1.313	0.5582 2961	0.917	-99.355

118-74-1	Hexachlorobenzene	Training	0.306	-0.461	-0.767	-1.810	0.054	0	0	3.571	0.889	0	0.000	-41.666
118-82-1	Binox M	Prediction	0.155	0.201	0.046	0.145	0.471	0	2	5.877	1.163	0.34168828	2.542	-110.478
120068-37-3	Fipronil	Training	-1.699	-0.896	0.803	1.979	0.133	1	7	11.297	3.629	0.72210054	1.567	-5.977
120-12-7	Anthracene	Training	-1.875	-1.871	0.004	0.009	0.036	0	0	18.797	1.261	0.45	0.111	-3.781
123-48-8	2,2,4,4,6,6 pentamethyl-3-heptene	Training	-1.284	-0.746	0.538	1.263	0.043	0	0	1.449	0.045	0.20298611	0.500	-44.916
125116-23-6	Metconazole	Training	-1.721	-1.571	0.151	0.365	0.103	1	6	2.956	1.526	0.68167944	0.858	-6.290
126690-66-2	2,4,6 Trimethyl-3-heptene	Prediction	-1.041	-0.971	0.070	0.162	0.027	0	0	1.436	0.125	0.24076389	0.222	-35.127
129-00-0	Pyrene	Training	-2.301	-1.862	0.439	1.046	0.071	0	0	24.028	1.503	0.45	0.111	-54.942
13029-08-8	2,2'-Dichlorophenyl	Training	0.663	0.208	-0.455	-1.064	0.035	1	0	11.992	1.285	0.43138203	0.194	-48.012
13150-81-7	2,6-Dimethyldecane	Prediction	-1.319	-0.762	0.557	1.306	0.042	0	0	1.000	0.049	0	0.222	-6.058
13151-34-3	3-methyl decane	Prediction	-1.699	-0.825	0.874	2.049	0.042	0	0	1.000	0.088	0	0.111	-2.673
13475-82-6	2,2,4,6,6-pentamethylheptane	Training	-0.728	-0.509	0.219	0.516	0.052	0	0	1.000	-0.07	0	0.500	-42.581
14233-37-5	9,10-Anthracenedione, 1,4-bis[(1-methylethyl)amino]-	Training	-0.500	-1.994	-1.493	-3.633	0.110	0	6	6.900	2.239	0.54155286	1.389	-82.012
15254-25-8	2,3,6,7-Tetramethylanthracene	Training	-1.757	-1.401	0.356	0.836	0.046	0	0	18.211	1.165	0.41611111	0.444	-63.229
15299-99-7	Napropamide	Training	-2.852	-3.083	-0.231	-0.554	0.089	0	6	7.742	1.935	0.52441397	0.486	-1.468
15968-05-5	2,2',6,6'-Tetrachlorobiphenyl	Training	0.623	0.441	-0.183	-0.427	0.036	1	0	11.576	1.475	0.40445169	0.250	-55.555

1610-22-6	1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydrochrysene	Training	-0.770	-0.569	0.200	0.472	0.049	0	0	3.137	0.853	0.3094 1185	0.361	-62.901
16435-49-7	2-methyl-1-dodecene	Training	-1.200	-1.275	-0.075	-0.176	0.041	0	0	1.124	0.143	0.3434 7806	0.111	-3.938
16606-02-3	2,4',5-Trichlorobiphenyl	Prediction	0.525	0.254	-0.271	-0.628	0.014	1	0	12.277	1.418	0.4142 1382	0.389	-4.806
1678-98-4	iso-butyl cyclohexane	Training	-0.652	-0.763	-0.111	-0.261	0.040	0	0	1.000	0.199	0	0.118	-1.567
16958-92-2	Diisotridecyl adipate	Training	-1.959	-2.172	-0.213	-0.573	0.273	0	6	1.114	0.989	0	0.222	-129.757
1705-85-7	6-methylchyrsene	Training	-1.398	-1.600	-0.202	-0.475	0.046	0	0	22.968	1.579	0.4460 9375	0.618	-6.362
1706-50-9	1,1':3',1''Tercyclohexane	Training	-0.357	-0.152	0.205	0.478	0.037	0	0	1.000	0.421	0	0.500	-64.879
17088-22-1	1-ethylpyrene	Training	-1.699	-1.750	-0.051	-0.120	0.045	0	0	22.804	1.479	0.4430 0733	0.458	-5.362
17301-23-4	2,6-Dimethyl undecane	Training	-1.027	-0.731	0.296	0.694	0.043	0	0	1.000	0.049	0	0.278	-4.472
17312-44-6	2,3 Dimethyldecane	Prediction	-1.585	-0.812	0.773	1.814	0.043	0	0	1.000	0.049	0	0.167	-2.336
1732-13-4	1,2,3,6,7,8 Hexahydropyrene	Training	-1.252	-0.986	0.266	0.625	0.043	0	0	8.114	1.123	0.3640 2778	0.111	-56.051
1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]Dioxin	Training	0.103	-0.391	-0.495	-1.182	0.078	1	4	7.554	2.419	0.5226 2086	0.444	-63.229
1795-15-9	n - Octyl Cyclohexane	Prediction	-1.222	-0.756	0.466	1.091	0.040	0	0	1.000	0.238	0	0.090	-2.449
18094-01-4	2 methyl 1-Tridecene	Prediction	-0.921	-1.270	-0.350	-0.819	0.041	0	0	1.110	0.143	0.3419 9877	0.111	-4.357
1836-75-5	2,4-Dichloro-1-(4-nitrophenoxy) benzene	Training	-0.821	-0.855	-0.034	-0.080	0.040	1	3	7.060	1.539	0.6406 5558	0.417	-4.690

1839-63-0	1,3,5-Trimethyl cyclohexane	Training	-0.456	-0.739	-0.283	-0.662	0.035	0	0	1.000	0.16	0	0.000	-34.311
18516-37-5	2-methyl-1-undecene	Training	-1.456	-1.280	0.176	0.413	0.041	0	0	1.141	0.143	0.3452 1417	0.111	-3.532
1889-67-4	Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethaneDiyl)bis-	Training	-0.777	-0.654	0.123	0.293	0.069	0	0	4.834	0.821	0.4089 6259	0.625	-63.275
191-24-2	Benzo(ghi)perylene	Prediction	-1.495	-1.362	0.133	0.323	0.110	0	0	29.450	2.087	0.45	0.736	-79.929
193-39-5	Indeno 1,2,3-cd pyrene	Prediction	-1.538	-1.560	-0.022	-0.053	0.083	0	0	29.487	2.087	0.45	0.820	-13.214
194-69-4	Benzo(c)chrysene	Training	-1.301	-1.655	-0.354	-0.839	0.059	0	0	26.325	1.945	0.45	0.542	-6.220
19780-74-6	5-ethyl-1-nonene	Prediction	-0.461	-1.149	-0.688	-1.618	0.048	0	0	1.152	0.128	0.3655 1158	0.167	-38.756
20279-21-4	1,2,3,10b-Tetrahydrofluoranthene	Training	-1.638	-1.187	0.451	1.055	0.038	0	0	9.009	1.208	0.4228 5147	0.219	-7.015
204256-07-5	2,3 Dimethy-5(4methylpentyl) naphthalene	Training	-1.367	-1.194	0.172	0.402	0.030	0	0	8.907	0.808	0.4009 2998	0.514	-3.379
2050-68-2	4,4'-Dichlorobiphenyl	Training	0.519	0.283	-0.235	-0.549	0.033	1	0	12.813	1.285	0.4272 2584	0.361	-50.864
2051-24-3	Decachlorobiphenyl	Training	0.319	0.392	0.073	0.177	0.107	0	0	11.633	1.701	0	1.139	-79.929
2051-30-1	2,6-Dimethyl octane	Prediction	-1.854	-0.770	1.084	2.542	0.043	0	0	1.000	0.049	0	0.222	-3.756
205646-11-3	1,2,9,10-Tetrachlorodecane	Training	-0.658	-0.285	0.372	0.871	0.038	0	0	1.000	0.677	0	0.167	-49.491
206-44-0	Fluoranthene	Training	-1.553	-1.894	-0.341	-0.801	0.047	0	0	22.751	1.503	0.45	0.219	-7.015
207-08-9	Benzo(k)fluoranthene	Prediction	-1.979	-1.696	0.282	0.669	0.062	0	0	26.583	1.845	0.45	0.594	-5.116
2136-99-4	2,2',3,3',5,5',6,6'-	Prediction	0.668	1.217	0.550	1.296	0.052	1	0	11.451	1.759	0.3348 2506	0.917	-76.246

	Octachlorobiphenyl													
214-17-5	Benzo[b]chrysene	Training	-1.745	-1.679	0.066	0.156	0.060	0	0	26.594	1.945	0.45	0.528	-6.755
217-59-4	Triphenylene	Training	-1.658	-1.517	0.141	0.333	0.060	0	0	22.798	1.603	0.45	0.375	-66.126
218-01-9	Chrysene	Training	-1.538	-1.577	-0.039	-0.093	0.063	0	0	23.536	1.603	0.45	0.361	-64.477
2189-60-8	n-octyl benzene	Prediction	-1.648	-1.265	0.383	0.900	0.048	0	0	2.788	0.553	0.4146 5862	0.090	-2.449
221155-23-3	1,2,13,14-Tetrachlorotetradecane	Training	0.100	-0.228	-0.328	-0.770	0.044	0	0	1.000	0.677	0	0.167	-64.879
22907-72-8	1,4 Diisopropyl cyclohexane	Training	-0.479	-0.495	-0.017	-0.039	0.034	0	0	1.000	0.121	0	0.361	-42.153
23342-25-8	2,2,5,7-Tetramethyltetraline	Training	-1.301	-0.916	0.385	0.903	0.041	0	0	3.528	0.552	0.3416 7092	0.535	-3.084
2381-21-7	1-Methylpyrene	Training	-2.301	-1.853	0.448	1.055	0.049	0	0	23.535	1.479	0.4460 9375	0.368	-6.606
243-17-4	Benzo(b)fluorene	Training	-1.602	-1.404	0.198	0.460	0.027	0	0	16.747	1.463	0.4448 9796	0.445	-5.006
2435-85-0	Hexadecahydropyrene	Training	0.009	-0.404	-0.412	-0.964	0.035	0	0	1.000	0.493	0	0.111	-54.942
2437-56-1	1-Tridecene	Training	-0.963	-1.177	-0.214	-0.505	0.050	0	0	1.114	0.167	0.3697 7655	0.056	-45.803
2437-79-8	2,2',4,4'-Tetrachlorobiphenyl	Training	0.833	0.520	-0.313	-0.729	0.029	1	0	12.168	1.475	0.3990 6998	0.417	-55.095
2541-69-7	7-Methylbenz(a)anthracene	Training	-2.097	-1.626	0.471	1.107	0.045	0	0	23.021	1.579	0.4460 9375	0.583	-6.404
25569-80-6	2,3'-Dichlorobiphenyl	Training	0.267	0.128	-0.140	-0.323	0.018	1	0	12.170	1.285	0.4334 064	0.333	-6.032
26186-00-5	1-Heptadecyne	Training	-0.086	-0.577	-0.491	-1.149	0.037	0	0	1.152	0.236	0	0.056	-59.027
2732-58-3	6-ethylchyrsene	Training	-1.495	-1.496	-0.001	-0.003	0.046	0	0	22.238	1.579	0.4430 0733	0.708	-5.357
27575-78-6	Tris(4-chlorophenyl)methane	Training	0.538	0.989	0.451	1.075	0.072	1	0	8.126	1.765	0.3970 7124	0.375	-78.404

2974-92-7	3,4-Dichlorobiphenyl	Training	0.477	0.080	-0.397	-0.920	0.019	1	0	12.466	1.242	0.4423167	0.361	-3.075
2980-71-4	2-methyl-1-nonene	Training	-1.367	-1.290	0.076	0.179	0.042	0	0	1.164	0.143	0.34978029	0.111	-2.769
3010-80-8	Tris(4-chlorophenyl) methanol	Training	-0.260	0.639	0.898	2.101	0.037	1	1	7.844	2.047	0.44334491	0.729	0.000
3074-71-3	2,3-Dimethylheptane	Prediction	-0.792	-0.850	-0.058	-0.137	0.044	0	0	1.000	0.049	0	0.111	-1.816
31508-00-6	2,3',4,4',5-Pentachlorobiphenyl	Training	0.776	0.500	-0.276	-0.637	0.011	1	0	12.328	1.56	0.39762022	0.611	-5.396
319-84-6	(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	Training	-1.516	-0.252	1.264	3.011	0.072	0	0	1.000	0.985	0	0.000	-41.666
32598-10-0	2,3',4,4'-Tetrachlorobiphenyl	Training	0.470	0.406	-0.064	-0.147	0.012	1	0	12.410	1.47	0.40525054	0.556	-7.469
32598-11-1	2,3',4',5-Tetrachlorobiphenyl	Prediction	0.771	0.408	-0.363	-0.839	0.011	1	0	12.196	1.508	0.40322617	0.500	-7.727
32598-14-4	2,3,3',4,4'-Pentachlorobiphenyl	Training	0.740	0.477	-0.263	-0.608	0.012	1	0	12.334	1.517	0.39762022	0.611	-5.638
32690-93-0	2,4,4',5-Tetrachlorobiphenyl	Training	0.903	0.356	-0.547	-1.264	0.012	1	0	12.341	1.47	0.40860787	0.500	-3.883
32774-16-6	3,3',4,4',5,5'-Hexachlorobiphenyl	Training	0.496	0.731	0.235	0.549	0.032	1	0	12.455	1.569	0.3704563	0.583	-62.383
33025-41-1	2,3,4,4'-Tetrachlorobiphenyl	Training	0.688	0.332	-0.357	-0.824	0.013	1	0	12.348	1.427	0.40860787	0.500	-3.993
3321-50-4	Cyclohexane, 1,1'-(1,2-	Training	-1.301	-0.463	0.838	1.952	0.029	0	0	1.000	0.349	0	0.181	-48.355

	EthaneDiyl)Bis-													
3322-93-8	Tetrabromoethylcyclohexane β	Training	-0.318	-0.146	0.172	0.410	0.071	0	0	1.000	1.065	0	0.319	-2.222
33284-50-3	2,4-Dichlorobiphenyl	Prediction	0.703	0.041	-0.663	-1.537	0.021	1	0	12.304	1.247	0.4410028	0.278	-3.177
33284-52-5	3,3',5,5'-Tetrachlorobiphenyl	Prediction	0.457	0.496	0.039	0.090	0.031	1	0	12.125	1.475	0.39323045	0.361	-55.555
33460-02-5	3 Phenyl bicyclohexyl	Training	-1.046	-1.275	-0.229	-0.537	0.041	0	0	1.124	0.143	0.34347806	0.111	-3.938
34883-39-1	2,5-Dichlorobiphenyl	Prediction	-0.638	0.077	0.715	1.657	0.020	1	0	12.078	1.285	0.440102	0.278	-3.122
34883-43-7	2,4'-Dichlorobiphenyl	Prediction	0.574	0.077	-0.497	-1.152	0.020	1	0	12.335	1.285	0.43472029	0.278	-5.408
35065-27-1	2,2',4,4',5,5'-Hexachlorobiphenyl	Training	0.614	0.899	0.285	0.665	0.034	1	0	12.085	1.655	0.3609184	0.694	-65.396
35065-28-2	2,2',3,4,4',5'-Hexachlorobiphenyl	Training	0.803	0.638	-0.165	-0.382	0.012	1	0	12.091	1.612	0.38045201	0.694	-9.494
35065-29-3	2,2',3,4,4',5,5'-Heptachlorobiphenyl	Training	0.842	0.767	-0.075	-0.173	0.016	1	0	12.031	1.664	0.35328809	0.806	-5.902
35065-30-6	2,2',3,3',4,4',5-Heptachlorobiphenyl	Training	0.851	0.715	-0.136	-0.315	0.016	1	0	12.036	1.621	0.3728217	0.806	-5.703
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl	Training	0.481	0.640	0.158	0.369	0.030	1	0	11.865	1.551	0.39241253	0.472	-58.779
35694-06-5	2,2',3,4,4',5-Hexachlorobiphenyl	Training	0.836	0.629	-0.206	-0.477	0.014	1	0	12.037	1.574	0.38535682	0.750	-4.217
35694-08-7	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	Training	0.958	1.076	0.118	0.277	0.045	1	0	11.997	1.673	0.34230043	0.861	-72.663

35822-46-9	1,2,3,4,6,7,8-H7CDD	Training	-0.469	-0.352	0.117	0.274	0.041	1	4	7.351	2.332	0.4983 9695	0.799	-12.460
36559-22-5	2,2',3,4'-Tetrachlorobiphenyl	Training	0.572	0.369	-0.203	-0.469	0.012	1	0	12.064	1.47	0.4099 2177	0.472	-8.219
37680-65-2	2,2',5-Trichlorobiphenyl	Training	0.580	0.239	-0.341	-0.788	0.015	1	0	11.910	1.418	0.4257 7608	0.361	-4.155
37680-66-3	2,2',4-Trichlorobiphenyl	Training	0.204	0.171	-0.033	-0.077	0.017	1	0	12.058	1.38	0.4270 8998	0.306	-4.197
37680-73-2	2,2',4,5,5'-Pentachlorobiphenyl	Training	0.783	0.539	-0.244	-0.563	0.012	1	0	11.961	1.603	0.3890 2128	0.583	-5.018
38379-99-6	2,2',3,5',6-Pentachlorobiphenyl	Training	0.734	0.542	-0.192	-0.443	0.012	1	0	11.670	1.603	0.3868 0658	0.556	-5.258
38380-01-7	2,2',4,4',5-Pentachlorobiphenyl	Training	0.868	0.505	-0.363	-0.838	0.011	1	0	12.115	1.565	0.3914 3966	0.583	-5.030
38380-02-8	2,2',3,4,5'-Pentachlorobiphenyl	Prediction	0.760	0.515	-0.244	-0.564	0.011	1	0	11.968	1.56	0.3890 2128	0.583	-5.198
38380-03-9	2,3,3',4',6-Pentachlorobiphenyl	Prediction	0.919	0.514	-0.405	-0.934	0.011	1	0	11.940	1.56	0.3922 3851	0.583	-5.687
38380-04-0	2,2',3,4',5',6-Hexachlorobiphenyl	Training	0.792	0.669	-0.123	-0.285	0.012	1	0	11.757	1.655	0.3737 9456	0.667	-8.553
38380-05-1	2,2',3,3',4,6'-Hexachlorobiphenyl	Prediction	0.743	0.649	-0.094	-0.217	0.012	1	0	11.763	1.612	0.3750 703	0.667	-10.083
38380-07-3	2,2',3,3',4,4'-Hexachlorobiphenyl	Training	0.769	0.812	0.043	0.099	0.032	1	0	12.096	1.569	0.3804 5201	0.694	-62.440
38380-08-4	2,3,3',4,4',5-Hexachlorobiphenyl	Training	0.869	0.555	-0.314	-0.726	0.012	1	0	12.228	1.569	0.3899 899	0.667	-4.434
38411-22-2	2,2',3,3',6,6'-Hexachlorobiphenyl	Training	0.678	0.882	0.204	0.477	0.034	1	0	11.520	1.655	0.3704 563	0.639	-65.119

38411-25-5	2,2',3,3',4,5,6'-Heptachlorobiphenyl	Training	0.830	0.784	-0.047	-0.108	0.017	1	0	11.693	1.664	0.3681 8861	0.833	-5.512
38444-73-4	2,2',6-Trichlorobiphenyl	Training	0.568	0.141	-0.428	-0.992	0.021	1	0	11.754	1.38	0.4237 5172	0.222	-4.450
38444-76-7	2,3',6-Trichlorobiphenyl	Prediction	-0.046	0.268	0.313	0.724	0.014	1	0	11.928	1.38	0.4175 7116	0.417	-4.920
38444-77-8	2,4',6-Trichlorobiphenyl	Training	0.580	0.198	-0.382	-0.884	0.017	1	0	12.022	1.38	0.4122 7233	0.306	-5.303
38444-78-9	2,2',3-Trichlorobiphenyl	Prediction	0.477	0.215	-0.262	-0.605	0.015	1	0	11.918	1.375	0.4257 7608	0.361	-4.326
38444-81-4	2,3',5-Trichlorobiphenyl	Training	0.653	0.257	-0.396	-0.916	0.014	1	0	12.065	1.418	0.4203 9438	0.389	-4.529
38444-84-7	2,3,3'-Trichlorobiphenyl	Training	-0.222	0.233	0.455	1.052	0.014	1	0	12.073	1.375	0.4203 9438	0.389	-4.765
38444-85-8	2,3,4'-Trichlorobiphenyl	Training	0.352	0.226	-0.127	-0.293	0.015	1	0	12.285	1.375	0.4175 5208	0.389	-5.108
38444-86-9	2,3',4'-Trichlorobiphenyl	Training	0.519	0.246	-0.273	-0.630	0.014	1	0	12.218	1.375	0.4291 1435	0.444	-4.005
38444-93-8	2,2',3,3'-Tetrachlorobiphenyl	Training	0.514	0.555	0.041	0.095	0.028	1	0	11.880	1.465	0.4086 0787	0.472	-55.177
3891-98-3	2,6,10-Trimethyl dodecane	Training	-0.002	-0.672	-0.670	-1.576	0.047	0	0	1.000	0.01	0	0.389	-6.604
39227-61-7	1,2,3,4,7-P5CDD	Training	-1.092	-0.545	0.547	1.285	0.046	1	4	7.391	2.309	0.5399 0586	0.653	-6.003
39635-31-9	2,3,3',4,4',5,5'-Heptachlorobiphenyl	Prediction	0.631	0.671	0.040	0.092	0.014	1	0	12.203	1.621	0.3594 6864	0.722	-6.158
40186-70-7	2,2',3,3',4,5',6-Heptachlorobiphenyl	Training	0.778	0.801	0.022	0.052	0.017	1	0	11.765	1.669	0.3561 113	0.833	-5.977

40186-71-8	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	Training	0.803	0.948	0.145	0.338	0.021	1	0	11.587	1.721	0.3357 2586	0.917	-12.645
40186-72-9	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	Training	0.532	0.955	0.423	0.985	0.027	1	0	11.797	1.687	0.3313 1278	1.000	-6.678
40458-98-8	2,7-Diisopropyl naphthalene	Prediction	-1.438	-1.025	0.413	0.968	0.041	0	0	9.992	0.793	0.3972 2647	0.583	-54.871
41411-64-7	2,3,3',4,4',5,6-Heptachlorobiphenyl	Training	0.894	0.648	-0.246	-0.569	0.014	1	0	11.947	1.583	0.3790 0225	0.750	-3.931
41464-39-5	2,2',3,5'-Tetrachlorobiphenyl	Prediction	0.789	0.403	-0.386	-0.891	0.012	1	0	11.873	1.508	0.4086 0787	0.472	-8.059
41464-41-9	2,2',5,6'-Tetrachlorobiphenyl	Training	-0.398	0.397	0.795	1.835	0.012	1	0	11.729	1.513	0.4057 6558	0.444	-7.135
41464-43-1	2,3,3',4'-Tetrachlorobiphenyl	Training	0.668	0.367	-0.300	-0.693	0.012	1	0	12.203	1.465	0.4119 4614	0.500	-6.728
41464-46-4	2,3',4',6-Tetrachlorobiphenyl	Prediction	0.322	0.406	0.084	0.194	0.011	1	0	11.972	1.47	0.4079 8028	0.528	-6.252
41464-47-5	2,2',3,6'-Tetrachlorobiphenyl	Training	-0.398	0.376	0.774	1.787	0.012	1	0	11.736	1.47	0.4065 8351	0.444	-8.388
41464-49-7	2,3,3',5'-Tetrachlorobiphenyl	Training	0.238	0.384	0.146	0.338	0.012	1	0	12.010	1.47	0.4106 3224	0.500	-6.875
41464-51-1	2,2',3',4,5-Pentachlorobiphenyl	Training	0.842	0.493	-0.349	-0.807	0.011	1	0	11.968	1.56	0.4043 1582	0.583	-4.824
4175-54-6	1,2,3,4-Tetrahydro-1,4-Dimethyl naphthalene (1,4-Dimethyl Tetralin)	Training	-0.801	-1.079	-0.277	-0.651	0.042	0	0	3.479	0.601	0.3904 8611	0.125	-41.263

42740-50-1	2,2',3,3',4,4',5,6'-Octachlorobiphenyl	Prediction	0.833	0.915	0.083	0.192	0.023	1	0	11.840	1.678	0.3389 4309	0.944	-10.628
4292-75-5	n-hexyl cyclohexane	Prediction	-1.377	-0.758	0.619	1.451	0.040	0	0	1.000	0.238	0	0.090	-2.103
43121-43-3	Triadimefon	Prediction	-1.921	-2.403	-0.482	-1.218	0.174	1	8	4.411	1.789	0.7449 3308	0.871	-2.373
4316-65-8	3,5,5' Trimethyl hexene	Training	-1.201	-1.433	-0.232	-0.545	0.046	0	0	1.178	0.049	0.3601 3889	0.000	-2.286
438-22-2	5α(H)-androstane	Training	-0.172	-0.271	-0.099	-0.232	0.047	0	0	1.000	0.413	0	0.667	-5.322
475-03-6	1,1,6 Trimethyl Tetralin	Training	-0.484	-1.064	-0.580	-1.356	0.035	0	0	3.480	0.576	0.3596 5278	0.319	-3.409
483-65-8	1-methyl-7-(1methylethyl)-phenanthrene	Training	-1.553	-1.488	0.065	0.151	0.031	0	0	17.081	1.174	0.4270 8546	0.563	-3.852
488-23-3	1,2,3,4 Tetramethyl benzene	Prediction	-1.292	-1.250	0.042	0.099	0.038	0	0	3.537	0.481	0.3809 7222	0.000	-32.642
4920-95-0	3,3',4,4' Tetramethyl 1,1'-biphenyl	Training	-2.046	-1.153	0.893	2.090	0.039	0	0	12.631	0.923	0.4123 2852	0.528	-59.239
496-10-6	Bicyclo[4.3.0] nonane	Prediction	-1.102	-0.646	0.457	1.068	0.035	0	0	1.000	0.349	0	0.000	-31.250
50-29-3	4,4'-DDT	Training	0.752	1.045	0.293	0.689	0.047	1	0	5.938	1.448	0.3675 7154	0.528	-67.420
50-32-8	Benzo[a]pyrene	Training	-1.745	-1.876	-0.131	-0.312	0.067	0	0	27.149	1.845	0.45	0.375	-4.691
50876-32-9	cis 1,1,3,5 Tetramethyl cyclohexane	Training	-0.265	-0.881	-0.616	-1.446	0.045	0	0	1.000	0.12	0	0.000	-2.468
5103-74-2	1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-Hexahydro-4,7-methano-1H-indene	Training	0.326	0.360	0.034	0.082	0.105	0	0	1.401	1.442	0	0.768	-9.294

51655-65-3	2-butyl-1-decene	Prediction	-0.975	-1.237	-0.262	-0.612	0.037	0	0	1.127	0.143	0.3147 1085	0.111	-3.544
51908-16-8	2,2',3,4',5,5'-Hexachlorobiphenyl	Training	0.917	0.697	-0.219	-0.507	0.013	1	0	11.950	1.655	0.3670 9896	0.694	-11.751
52663-58-8	2,3,4',6-Tetrachlorobiphenyl	Prediction	0.806	0.332	-0.474	-1.096	0.013	1	0	11.962	1.47	0.4032 2617	0.417	-3.967
52663-59-9	2,2',3,4-Tetrachlorobiphenyl	Training	0.218	0.319	0.101	0.234	0.012	1	0	11.940	1.427	0.4214 8403	0.472	-3.564
52663-60-2	2,2',3,3',6-Pentachlorobiphenyl	Prediction	0.505	0.498	-0.008	-0.018	0.011	1	0	11.676	1.56	0.4009 7756	0.556	-5.044
52663-61-3	2,2',3,5,5'-Pentachlorobiphenyl	Training	0.744	0.551	-0.194	-0.448	0.012	1	0	11.793	1.603	0.3881 2048	0.583	-5.038
52663-62-4	2,2',3,3',4-Pentachlorobiphenyl	Training	0.738	0.469	-0.269	-0.621	0.011	1	0	11.974	1.517	0.4043 1582	0.583	-4.983
52663-65-7	2,2',3,3',4,6,6'-Heptachlorobiphenyl	Training	0.767	0.742	-0.025	-0.058	0.015	1	0	11.580	1.669	0.3662 4712	0.750	-5.659
52663-66-8	2,2',3,3',4,5'-Hexachlorobiphenyl	Training	0.431	0.651	0.220	0.507	0.012	1	0	11.956	1.612	0.3784 2764	0.694	-10.120
52663-68-0	2,2',3,4',5,5',6-Heptachlorobiphenyl	Training	0.756	0.799	0.043	0.099	0.016	1	0	11.731	1.707	0.3479 0638	0.778	-5.960
52663-69-1	2,2',3,4,4',5',6-Heptachlorobiphenyl	Training	0.790	0.768	-0.022	-0.052	0.016	1	0	11.856	1.669	0.3499 3075	0.778	-6.091
52663-70-4	2,2',3,3',4,5',6'-Heptachlorobiphenyl	Training	0.796	0.747	-0.049	-0.114	0.015	1	0	11.736	1.664	0.3674 3999	0.778	-5.760
52663-71-5	2,2',3,3',4,4',6-Heptachlorobiphenyl	Training	0.848	0.716	-0.133	-0.307	0.015	1	0	11.861	1.626	0.3694 6436	0.778	-5.876

52663-72-6	2,3',4,4',5,5'-Hexachlorobiphenyl	Prediction	0.732	0.663	-0.069	-0.159	0.013	1	0	12.277	1.612	0.3670 9896	0.722	-9.615
52663-74-8	2,2',3,3',4,5,5'-Heptachlorobiphenyl	Training	0.854	0.732	-0.122	-0.283	0.015	1	0	11.865	1.664	0.3594 6864	0.750	-5.806
52663-75-9	2,2',3,3',4,5,5',6'-Octachlorobiphenyl	Training	0.820	0.916	0.096	0.223	0.020	1	0	11.688	1.716	0.3370 3975	0.889	-11.709
52663-77-1	2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	Training	0.728	1.012	0.284	0.661	0.029	1	0	11.531	1.73	0.3314 3381	1.028	-6.465
52663-78-2	2,2',3,3',4,4',5,6-Octachlorobiphenyl	Training	0.641	0.804	0.163	0.377	0.020	1	0	11.799	1.635	0.3618 3404	0.889	-4.784
52663-79-3	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	Prediction	0.799	0.986	0.187	0.435	0.029	1	0	11.644	1.692	0.3300 3704	1.028	-6.416
526-73-8	1,3,5-Trimethylbenzene	Training	-1.602	-1.383	0.219	0.514	0.044	0	0	3.524	0.505	0.4087 5	0.000	-3.688
52712-04-6	2,2',3,4,5,5'-Hexachlorobiphenyl	Training	0.839	0.626	-0.213	-0.491	0.013	1	0	11.852	1.612	0.3847 2923	0.694	-4.190
52712-05-7	2,2',3,4,5,5',6-Heptachlorobiphenyl	Prediction	0.845	0.708	-0.137	-0.316	0.015	1	0	11.624	1.626	0.3791 2328	0.778	-3.730
52744-13-5	2,2',3,3',5,6'-Hexachlorobiphenyl	Training	0.724	0.716	-0.008	-0.019	0.013	1	0	11.642	1.655	0.3724 8067	0.722	-8.942
52886-35-8	3-methyl-1-hexyl cyclohexane	Training	-1.181	-0.740	0.440	1.031	0.039	0	0	1.000	0.199	0	0.146	-2.835
53-19-0	o,p'-DDD	Training	0.380	0.712	0.331	0.770	0.025	1	0	6.040	1.431	0.4019 2854	0.472	-5.118
5325-97-3	1,2,3,4,5,6,7,8-	Training	-0.893	-1.045	-0.152	-0.357	0.039	0	0	3.470	0.781	0.3384 0278	0.125	-3.984

	octahydrophenanthrene													
53-70-3	Dibenzo[a,h]anthracene	Training	-2.155	-1.680	0.475	1.124	0.060	0	0	26.582	1.945	0.45	0.528	-6.205
541-02-6	Decamethylcyclopentasiloxane	Training	0.532	0.847	0.316	0.858	0.287	0	0	1.000	0.452	0	1.944	-74.624
544-76-3	n-Hexadecane	Prediction	-0.314	-0.641	-0.327	-0.765	0.038	0	0	1.000	0.127	0	0.056	-55.784
55215-18-4	2,2',3,3',4,5-Hexachlorobiphenyl	Prediction	0.839	0.582	-0.257	-0.593	0.013	1	0	11.857	1.569	0.39870988	0.694	-4.081
556-67-2	Octamethylcyclotetrasiloxane	Prediction	0.602	0.105	-0.497	-1.181	0.068	0	0	1.000	0.417	0	0.944	-56.561
55702-45-9	2,3,6-Trichlorobiphenyl	Training	0.470	0.149	-0.321	-0.743	0.017	1	0	11.773	1.337	0.43449606	0.306	-2.839
55712-37-3	2,3',4-Trichlorobiphenyl	Prediction	0.556	0.254	-0.303	-0.700	0.014	1	0	12.329	1.38	0.42241875	0.444	-4.609
5617-41-4	n-heptyl cyclohexane	Training	-1.699	-0.757	0.942	2.207	0.040	0	0	1.000	0.238	0	0.090	-2.265
56-49-5	3-methylcholanthene	Training	-1.523	-1.331	0.192	0.449	0.033	0	0	19.474	1.681	0.44094122	0.601	-7.639
56-55-3	Benzo[a]anthracene	Training	-2.301	-1.815	0.487	1.144	0.048	0	0	23.672	1.603	0.45	0.347	-5.702
56558-16-8	2,2',4,6,6'-Pentachlorobiphenyl	Training	0.393	0.358	-0.035	-0.080	0.015	1	0	11.606	1.532	0.40106044	0.361	-4.858
5707-44-8	4-ethyl-1,1'-biphenyl	Prediction	-1.745	-1.489	0.256	0.594	0.024	0	0	12.296	0.995	0.44441358	0.313	-3.010
57465-28-8	3,3',4,4',5-Pentachlorobiphenyl	Training	0.581	0.441	-0.140	-0.323	0.012	1	0	12.527	1.517	0.40097756	0.583	-5.242
581-40-8	2,3-Dimethylnaphthalene	Training	-1.921	-1.397	0.523	1.220	0.030	0	0	10.705	0.871	0.43795352	0.167	-43.252
60145-20-2	2,2',3,3',5-Pentachlorobiphenyl	Training	0.761	0.505	-0.256	-0.592	0.011	1	0	11.799	1.56	0.40300193	0.583	-4.843

60145-23-5	2,2',3,4,4',5,6'-Heptachlorobiphenyl	Training	0.836	0.810	-0.025	-0.059	0.020	1	0	11.858	1.631	0.3548 3556	0.889	-5.555
60233-25-2	2,2',3,4',6'-Pentachlorobiphenyl	Training	0.230	0.467	0.237	0.547	0.011	1	0	11.843	1.527	0.4022 9145	0.556	-5.057
608-93-5	Pentachlorobenzene	Training	-0.387	0.473	0.860	2.019	0.043	1	0	3.548	0.918	0.3436 334	0.000	-38.270
6117-97-1	4-methyl dodecane	Training	-1.114	-0.824	0.290	0.680	0.042	0	0	1.000	0.088	0	0.111	-3.143
62338-09-4	2,2,3-Trimethyl decane	Prediction	-1.181	-0.799	0.382	0.896	0.046	0	0	1.000	0.009	0	0.222	-2.035
629-50-5	n-Tridecane	Training	-0.569	-0.678	-0.110	-0.256	0.035	0	0	1.000	0.127	0	0.056	-45.803
629-59-4	n-Tetradecane	Training	0.029	-0.661	-0.690	-1.614	0.036	0	0	1.000	0.127	0	0.056	-50.461
629-73-2	1-Hexadecene	Training	0.183	-1.133	-1.316	-3.108	0.055	0	0	1.083	0.167	0.3664 1337	0.056	-55.784
66246-88-6	1H-1,2,4-Triazole, 1-[2-(2,4-Dichlorophenyl)pentyl]-	Training	-2.000	-1.541	0.459	1.105	0.092	1	5	4.617	1.307	0.6791 6108	0.569	-16.746
67129-08-2	Metazachlor	Training	-4.494	-3.203	1.291	3.119	0.098	0	7	4.692	2	0.6003 5435	0.715	-4.971
68194-04-7	2,2',4,6'-Tetrachlorobiphenyl	Training	-0.854	0.296	1.150	2.661	0.015	1	0	11.814	1.475	0.4066 6638	0.333	-7.174
68194-05-8	2,2',3,4',6-Pentachlorobiphenyl	Training	0.303	0.476	0.173	0.399	0.012	1	0	11.801	1.565	0.3876 2451	0.500	-5.282
68194-14-9	2,2',3,4,5',6-Hexachlorobiphenyl	Training	0.799	0.620	-0.180	-0.415	0.013	1	0	11.739	1.617	0.3834 1533	0.667	-4.254
68194-15-0	2,2',3,4,5,6'-Hexachlorobiphenyl	Training	-0.523	0.652	1.175	2.717	0.015	1	0	11.659	1.574	0.3980 8228	0.778	-3.961
68194-16-1	2,2',3,3',4,5,6-Heptachlorobiphenyl	Prediction	0.009	0.667	0.659	1.524	0.015	1	0	11.629	1.583	0.3910 7956	0.778	-3.653
6975-98-0	2-methyl decane	Training	-1.444	-0.824	0.620	1.455	0.042	0	0	1.000	0.088	0	0.111	-3.142

7012-37-5	2,4,4'-Trichlorobiphenyl	Prediction	0.290	0.220	-0.071	-0.163	0.015	1	0	12.452	1.38	0.41623819	0.389	-4.923
702-79-4	1,3-Dimethyladamantane	Training	-1.174	-0.599	0.575	1.344	0.036	0	0	1.000	0.341	0	0.000	-44.862
70356-09-1	1-(4-tert-butylphenyl)-3-(4-methoxyphenyl)propane-1,3-Dione	Training	-0.914	-1.736	-0.821	-1.970	0.084	0	4	4.621	1.979	0.56084205	1.056	-5.420
70362-45-7	2,2',3,6-Tetrachlorobiphenyl	Training	0.568	0.310	-0.259	-0.598	0.014	1	0	11.664	1.47	0.41814577	0.389	-3.566
70362-46-8	2,2',3,5-Tetrachlorobiphenyl	Prediction	0.829	0.389	-0.440	-1.017	0.012	1	0	11.804	1.47	0.42017014	0.528	-3.482
70424-68-9	2,3,3',4',5-Pentachlorobiphenyl	Training	1.033	0.478	-0.555	-1.282	0.011	1	0	12.140	1.56	0.39559585	0.556	-5.400
70424-70-3	2,3',4',5,5'-Pentachlorobiphenyl	Prediction	0.380	0.523	0.143	0.330	0.012	1	0	12.087	1.56	0.39033517	0.611	-4.903
7045-71-8	2-methyl undecane	Training	-1.292	-0.822	0.470	1.103	0.042	0	0	1.000	0.088	0	0.111	-3.532
7116-96-3	4-pentyl-1,1'-Biphenyl	Training	-1.174	-1.370	-0.196	-0.456	0.026	0	0	10.753	0.995	0.43913206	0.340	-3.036
71608-00-9	1-octylpyrene	Training	-1.108	-1.568	-0.460	-1.074	0.033	0	0	20.215	1.479	0.43283919	0.486	-3.439
717-74-8	Benzene, 1,3,5-Tris(1-methylethyl)-	Prediction	-0.398	-0.433	-0.035	-0.085	0.103	0	0	3.407	0.388	0.30805556	1.042	-53.426
71888-89-6	Diisoheptyl phthalate	Training	-2.509	-2.726	-0.217	-0.528	0.107	0	6	3.096	1.313	0.56966446	0.694	-94.461
72-43-5	Methoxy chlor	Training	-0.969	-1.961	-0.992	-2.332	0.047	0	4	5.764	1.504	0.47595165	0.653	-73.385
72-54-8	p,p'-DDD	Training	0.602	0.956	0.354	0.829	0.042	1	0	6.173	1.431	0.37520186	0.472	-62.499

73575-52-7	2,3',4,5'-Tetrachlorobiphenyl	Prediction	0.218	0.460	0.242	0.559	0.012	1	0	12.296	1.475	0.40040295	0.611	-7.708
74472-33-6	2,3,3',6-Tetrachlorobiphenyl	Training	0.720	0.364	-0.356	-0.822	0.012	1	0	11.817	1.47	0.41196521	0.472	-3.798
74472-34-7	2,3,4',5-Tetrachlorobiphenyl	Training	0.857	0.368	-0.490	-1.131	0.012	1	0	12.189	1.47	0.40658351	0.500	-3.861
74472-36-9	2,3,3',5,6-Pentachlorobiphenyl	Training	0.477	0.444	-0.034	-0.077	0.012	1	0	11.685	1.522	0.40635927	0.528	-3.299
74472-37-0	2,3,4,4',5-Pentachlorobiphenyl	Training	0.829	0.450	-0.379	-0.876	0.012	1	0	12.215	1.479	0.40097756	0.611	-3.463
74472-38-1	2,3,4,4',6-Pentachlorobiphenyl	Prediction	0.857	0.416	-0.441	-1.019	0.012	1	0	12.010	1.484	0.39762022	0.528	-3.498
74472-42-7	2,3,3',4,4',6-Hexachlorobiphenyl	Training	0.826	0.592	-0.234	-0.542	0.013	1	0	12.047	1.574	0.38663257	0.694	-4.509
74472-44-9	2,3,3',4',5,6-Hexachlorobiphenyl	Training	0.929	0.590	-0.340	-0.785	0.012	1	0	11.875	1.612	0.3846082	0.639	-4.415
74472-48-3	2,2',3,4,4',6,6'-Heptachlorobiphenyl	Training	0.928	0.701	-0.227	-0.525	0.014	1	0	11.669	1.636	0.35281119	0.694	-5.714
74472-53-0	2,3,3',4,4',5,5',6-Octachlorobiphenyl	Training	0.806	0.795	-0.011	-0.026	0.019	1	0	11.962	1.635	0.34848099	0.861	-5.041
74487-85-7	2,2',3,4',5,6,6'-Heptachlorobiphenyl	Prediction	0.884	0.799	-0.085	-0.196	0.017	1	0	11.621	1.674	0.3514973	0.806	-5.618
779-02-2	9-Methylanthracene	Prediction	-2.398	-1.759	0.639	1.489	0.030	0	0	18.248	1.237	0.44305556	0.236	-4.039
781-17-9	4,5,9,10-Tetrahydropyrene	Training	-1.553	-1.039	0.514	1.210	0.050	0	0	9.124	1.223	0.39875	0.111	-56.126

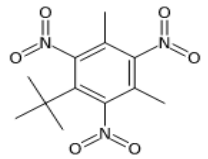
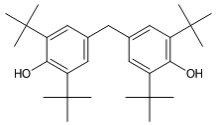
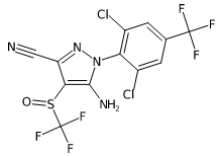
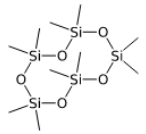
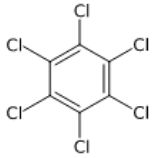
789-02-6	1-Chloro-2-(2,2,2-Trichloro-1-(4-chlorophenyl) ethyl)benzene (o,p'-DDT)	Training	0.839	0.805	-0.033	-0.078	0.025	1	0	5.819	1.448	0.3963 2259	0.569	-4.992
81-15-2	Musk-xylene	Prediction	-0.210	-0.799	-0.589	-1.525	0.213	0	3	4.638	0.882	0	1.618	-6.160
81777-89-1	Clomazone	Prediction	-3.699	-0.893	2.806	6.662	0.065	1	4	3.099	1.238	0.4566 1226	0.476	-3.035
821-95-4	1-undecene	Training	-1.409	-1.201	0.208	0.489	0.049	0	0	1.152	0.167	0.3729 9195	0.056	-41.173
83164-33-4	Diflufenican	Training	-2.991	-3.083	-0.092	-0.226	0.126	0	7	6.296	2.563	0.8111 6504	0.972	-12.309
832-69-9	1-Methylphenanthrene	Training	-1.721	-1.711	0.011	0.025	0.029	0	0	18.216	1.237	0.4460 9375	0.299	-6.643
84-15-1	o-Terphenyl	Prediction	-0.499	-1.346	-0.847	-1.990	0.046	0	0	18.180	1.461	0.45	0.333	-65.396
84632-59-7	3,6-Bis-(4-tert-butyl-phenyl)-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione	Training	-1.413	-1.530	-0.116	-0.291	0.161	0	6	7.163	2.449	0.4752 2555	1.654	-107.949
85-01-8	Phenanthrene	Training	-1.122	-1.847	-0.725	-1.693	0.035	0	0	18.554	1.261	0.45	0.125	-3.984
872-05-9	1-decene	Training	-0.991	-1.230	-0.239	-0.561	0.047	0	0	1.164	0.167	0.3750 5807	0.056	-34.385
88671-89-0	Myclobutanil	Training	-2.097	-1.561	0.536	1.282	0.079	1	6	4.618	1.975	0.7026 1728	0.684	-7.169
91-17-8	t-decalin	Training	-0.068	-0.633	-0.566	-1.322	0.035	0	0	1.000	0.349	0	0.000	-34.486
91-20-3	Naphthalene	Prediction	-2.301	-1.530	0.771	1.800	0.034	0	0	10.721	0.919	0.45	0.000	-34.486
91-57-6	2-Methylnaphthalene	Training	-2.000	-1.600	0.400	0.932	0.028	0	0	10.744	0.895	0.4448 9796	0.083	-3.391
92-06-8	m-terphenyl	Training	-1.347	-1.306	0.040	0.095	0.047	0	0	19.290	1.461	0.45	0.500	-64.879
92-51-3	Bicyclohexyl	Training	-0.770	-0.503	0.266	0.620	0.030	0	0	1.000	0.349	0	0.139	-44.916
933-12-0	3,5,5 Trimethyl cyclohexene	Training	-1.137	-1.205	-0.068	-0.159	0.031	0	0	1.416	0.259	0.2694 4444	0.000	-2.054

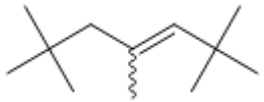
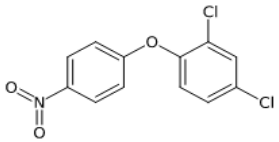
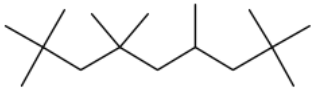
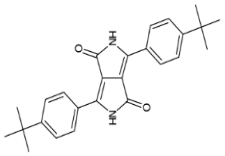
93-46-9	N,N′-Di-2-naphthyl-p-phenyleneDiamine	Training	-1.096	-1.787	-0.692	-1.835	0.252	0	4	11.419	3.309	0.4934 0278	0.361	0.000
94361-06-5	Cyproconazole	Training	-1.959	-1.686	0.273	0.660	0.102	1	6	4.021	1.566	0.6952 7817	0.771	-7.107
98-51-1	1-tert butyl-4-methyl benzene	Training	-1.018	-1.133	-0.115	-0.270	0.040	0	0	3.323	0.45	0.3765 9722	0.354	-1.549

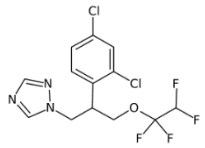
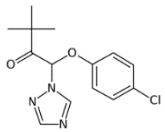
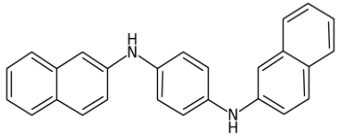
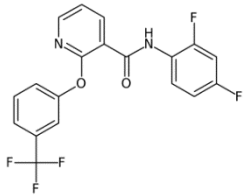
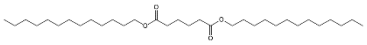
Table S4 – List of the excluded molecules.

CAS	Chemical Name	SMILES	Log_BMF$_L$ Low Quality	Outliers info
60207-90-1	Propiconazole	CCCC1COC(O1)(Cn1cncn1)c1ccc(cc1Cl)Cl	-2.222	out AD of Equation 1
70362-49-1	3,3',4,5-Tetrachlorobiphenyl	Clc1cccc(c1)c1cc(Cl)c(c(c1)Cl)Cl	-2.523	out AD of Equation 1
10605-21-7	Carbendazim	COC(=O)Nc1nc2c([nH]1)cccc2	-3.745	out AD of Equation 2
120068-36-2	Fipronil sulfone	N#Cc1nn(c(c1S(=O)(=O)C(F)(F)F)N)c1c(Cl)cc(cc1Cl)C(F)(F)F	0.777	out AD of Equation 2
131860-33-8	Azoxystrobin	COC=C(c1ccccc1Oc1ncnc(c1)Oc1ccccc1C#N)C(=O)OC	-3.347	out AD of Equation 2
208465-21-8	Mesosulfuron-methyl	COC(=O)c1ccc(cc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(n1)OC)CNS(=O)(=O)C	-5.699	out AD of Equation 2
2385-85-5	Mirex	ClC12C(Cl)(Cl)C3(C4(C1(Cl)C1(C2(Cl)C3(C4(C1(Cl)Cl)Cl)Cl)Cl)Cl)Cl	0.371	out AD of Equation 2
2471-09-2	OctacosamethylTridecasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)C	-1.699	out AD of Equation 2
2471-10-5	Triacontamethyltetradecasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)C	-1.699	out AD of Equation 2
2652-13-3	Eicosamethylnonasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)C	-1.097	out AD of Equation 2
34123-59-6	Isoproturon	O=C(N(C)C)Nc1ccc(cc1)C(C)C	-3.211	out AD of Equation 2
36734-19-7	Iprodione	CC(NC(=O)N1CC(=O)N(C1=O)c1cc(Cl)cc(c1)Cl)C	-2.673	out AD of Equation 2
50563-36-5	Dimethachlor	COCCN(c1c(C)cccc1C)C(=O)CCl	-4.462	out AD of Equation 2
541-01-5	Hexadecamethylheptasiloxane	C[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)C	-1.398	out AD of Equation 2
556-69-4	Octadecamethyloctasiloxane	C[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)C	-0.796	out AD of Equation 2
556-70-7	Docosamethyldecasiloxane	C[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)(O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(C)C)(C)C)C	-1.222	out AD of Equation 2
79277-27-3	Thifensulfuron-methyl	COc1nc(nc(n1)C)NC(=O)NS(=O)(=O)c1ccsc1C(=O)OC	-4.297	out AD of Equation 2

Table S5 – List of the molecules outside the Applicability Domain (AD) of equations 1 and 3. CAS numbers, SMILES, Structures, chemicals common names, and information on the AD.

CAS	SMILES	Structure	Common Name	out AD Eq.1	out AD Eq.3
81-15-2	O=N(=O)c1c(C)c(N(=O)=O)c(c(c1C(C)(C)C)N(=O)=O)C		Musk-xylene	**x**	**x**
118-82-1	CC(c1cc(Cc2cc(c(c(c2)C(C)(C)C)O)C(C)(C)C)cc(c1O)C(C)(C)C)(C)C		Binox M	**x**	**x**
120068-37-3	N#Cc1nn(c(c1S(=O)C(F)(F)F)N)c1c(Cl)cc(cc1Cl)C(F)(F)F		Fipronil	**x**	**x**
541-02-6	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](O[Si](O1)(C)C)(C)C		Decamethylcyclopentasiloxane	**x**	**x**
118-74-1	Clc1c(Cl)c(Cl)c(c(c1Cl)Cl)Cl		Hexachlorobenzene	**x**	

123-48-8	CC(=CC(C)(C)C)CC(C)(C)C		2,2,4,4,6,6 pentamethyl-3-heptene	**x**	
1836-75-5	Clc1ccc(c(c1)Cl)Oc1ccc(cc1)N(=O)=O		2,4-Dichloro-1-(4-nitrophenoxy) benzene	**x**	
4390-04-9	CC(CC(CC(C)(C)C)(C)C)CC(C)(C)C		2,2,4,4,6,8,8-heptamethyl nonane	**x**	
84632-59-7	CC(c1ccc(cc1)c1[nH]c(=O)c2c1c(=O)[nH]c2c1ccc(cc1)C(C)(C)C)(C)C		3,6-Bis-(4-tert-butyl-phenyl)-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione		**x**

112281-77-3	Clc1ccc(c(c1)Cl)C(Cn1cncn1)C)F)(F)F		Tetraconazole		**x**
43121-43-3	O=C(C(C)(C)C)C(n1ncnc1)Oc1ccc(cc1)Cl		Triadimefon		**x**
93-46-9	c1ccc2c(c1)cc(cc2)Nc1ccc(cc1)Nc1ccc2c(c1)cccc2		N,N′-Di-2-naphthyl-p-phenyleneDiamine		**x**
83164-33-4	Fc1ccc(c(c1)F)NC(=O)c1cccnc1Oc1cccc(c1)C(F)(F)F		Diflufenican		**x**
16958-92-2	CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCC		Diisotridecyl adipate		**x**