Supporting Information

SUPPLEMENTARY MATERIAL

Nonequivalent effects of diverse Log*P* algorithms in three QSAR studies.

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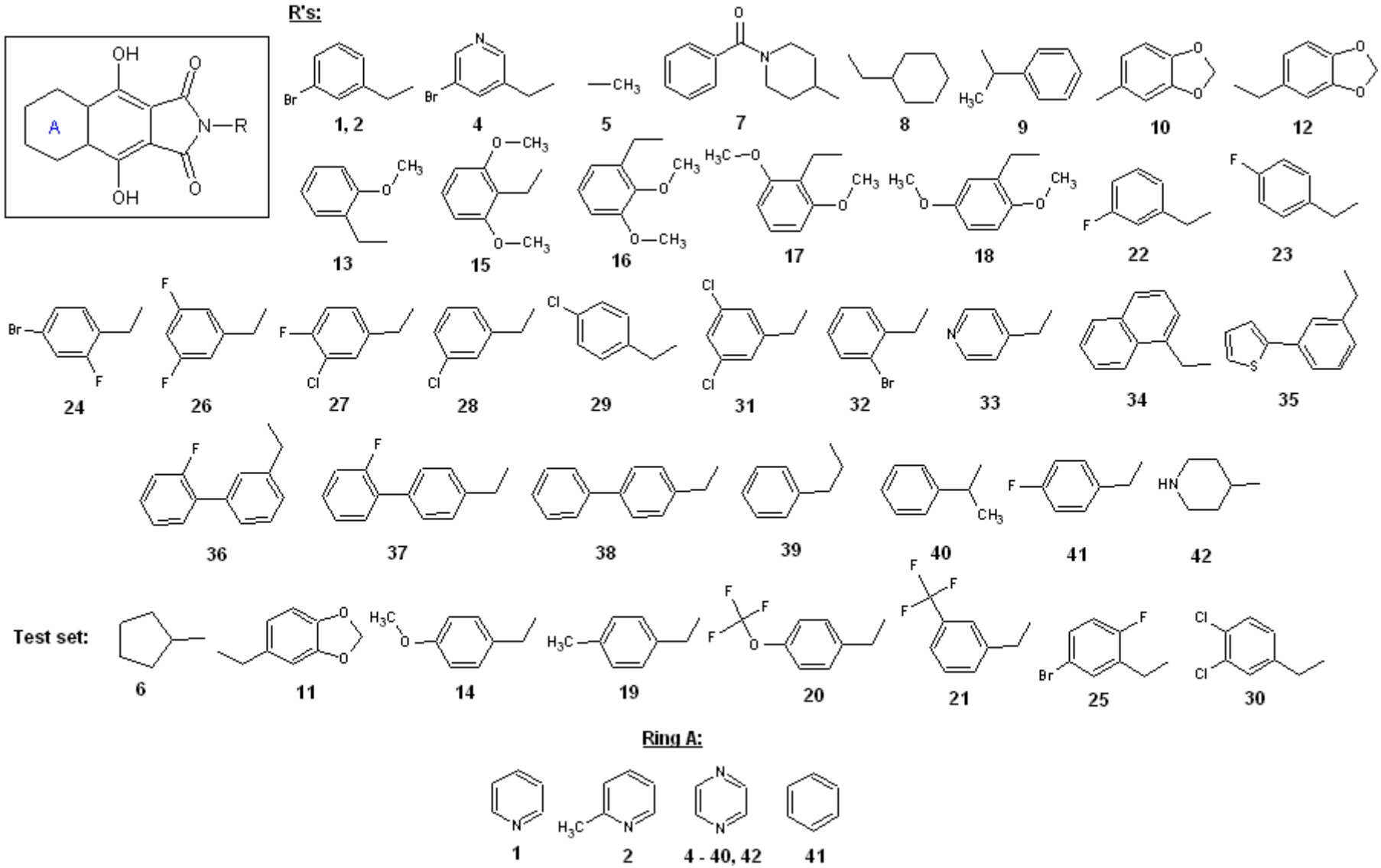
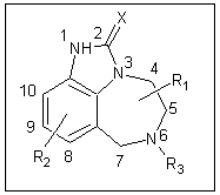


Figure S1. Training set 1



	R_1	X	R_2	R_3
1	H	S	8-Cl	DMA
2	H	S	9-Cl	DMA
3	5-CH_2CH_3	O	H	2-MA
4	5-$CH(CH_3)_2$	O	H	2-MA
5	5-$CH(CH_3)_2$	O	H	DMA
6	5,5-di-CH_3	O	H	2-MA
7	4-CH_3	O	H	2-MA
8	4-CH_3(S)	S	9-Cl	2-MA
9	4-CH_3	S	9-Cl	$CH_2CH(CH_2)_2$
10	4-$CH(CH_3)_2$	O	H	$CH_2CH_2CH_3$
11	4-$CH(CH_3)_2$	O	H	2-MA
12	4-$CH_2CH_2CH_3$	O	H	$CH_2CH_2CH_3$
13	4-$CH_2CH_2CH_3$	O	H	2-MA
14	7-CH_3	O	H	$CH_2CH_2CH_3$
15	7-CH_3	O	H	DMA
16	7-CH_3	O	8-Cl	DMA
17	7-CH_3	O	9-Cl	DMA
18	7-CH_3	S	H	$CH_2CH_2CH_3$
19	7-CH_3	S	H	DMA
20	7-CH_3	S	8-Cl	DMA
21	7-CH_3	S	9-Cl	DMA
22	4,5-di-CH_3(cis)	O	H	DMA
23	4.5-di-CH_3(cis)	S	H	DMA
24	4,5-di-CH3(trans)	S	H	$CH_2CH(CH_2)_2$
25	4,5-di-CH3(trans)	S	H	DMA
26	4-keto-5-CH3	S	9-Cl	$CH_2CH_2CH_3$
27	4,5-benzo	S	H	$CH_2CH(CH_2)_2$
28	5,7-di-CH3(trans)	S	H	DMA
29	5,7-di-CH3(cis)	S	H	DMA
30	5,7-di-CH3(R,R; trans)	O	9-Cl	DMA
32	5,7-di-CH3 (S,S; trans)	O	9-Cl	DMA
33	4,7-di-CH3(trans)	S	H	DMA
36	5-CH3(S)	S	8-Cl	DMA
37	5-CH3(S)	O	9-Cl	DMA
38	5-CH3(S)	S	9-Cl	DMA
39	5-CH3(S)	S	9-Cl	$CH_2CH(CH_2)_2$
41	5-CH3	O	H	$CH_2CH_2CH_3$
42	5-CH3	S	H	$CH_2CH_2CH_3$
43	5-CH3	O	H	2-MA
44	5-CH3	S	H	DMA
45	5-CH3(S)	O	H	DMA

Test set

	R_1	X	R_2	R_3
T1	H	O	H	DMA
T2	H	O	H	2-MA
T3	H	O	H	$CH_2CH_2CH_3$
T4	H	O	H	$CH_2C(C_2H_5)=CH_2$
T5	5-CH_3	S	H	DMA
T6	5-CH_3	O	H	$CH_2CH=CH_2$
T7	5-CH_3	O	H	$CH_2CH_2CH_2CH_3$
T8	5-CH_3	S	8-F	DMA
T9	5-CH_3	O	8-Br	DMA
T10	5-CH_3	S	8-Br	DMA
T11	5-CH_3	S	8-CH_3	DMA
T12	5-CH_3	S	8-O-CH_3	DMA
T13	5-CH_3	S	9,10-di Cl	DMA
T14	5-CH_3	O	8-CN	DMA
T15	5-CH_3	S	8-CN	DMA
T16	5-CH_3	O	8-CH_3	DMA
T17	5-CH_3	S	10-OCH_3	DMA
T18	5-CH_3	O	10-OCH_3	DMA
T19	5-CH_3	S	10-Br	DMA
T20	5-CH_3	S	8-CHO	DMA
T22	5-CH_3	O	8-I	DMA
T22	5-CH_3	S	8-I	DMA
T23	5-CH_3	O	8-C≡CH	DMA
T24	5-CH_3	S	8-C≡CH	DMA

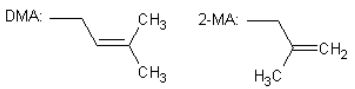


Figure S2. Training set 2

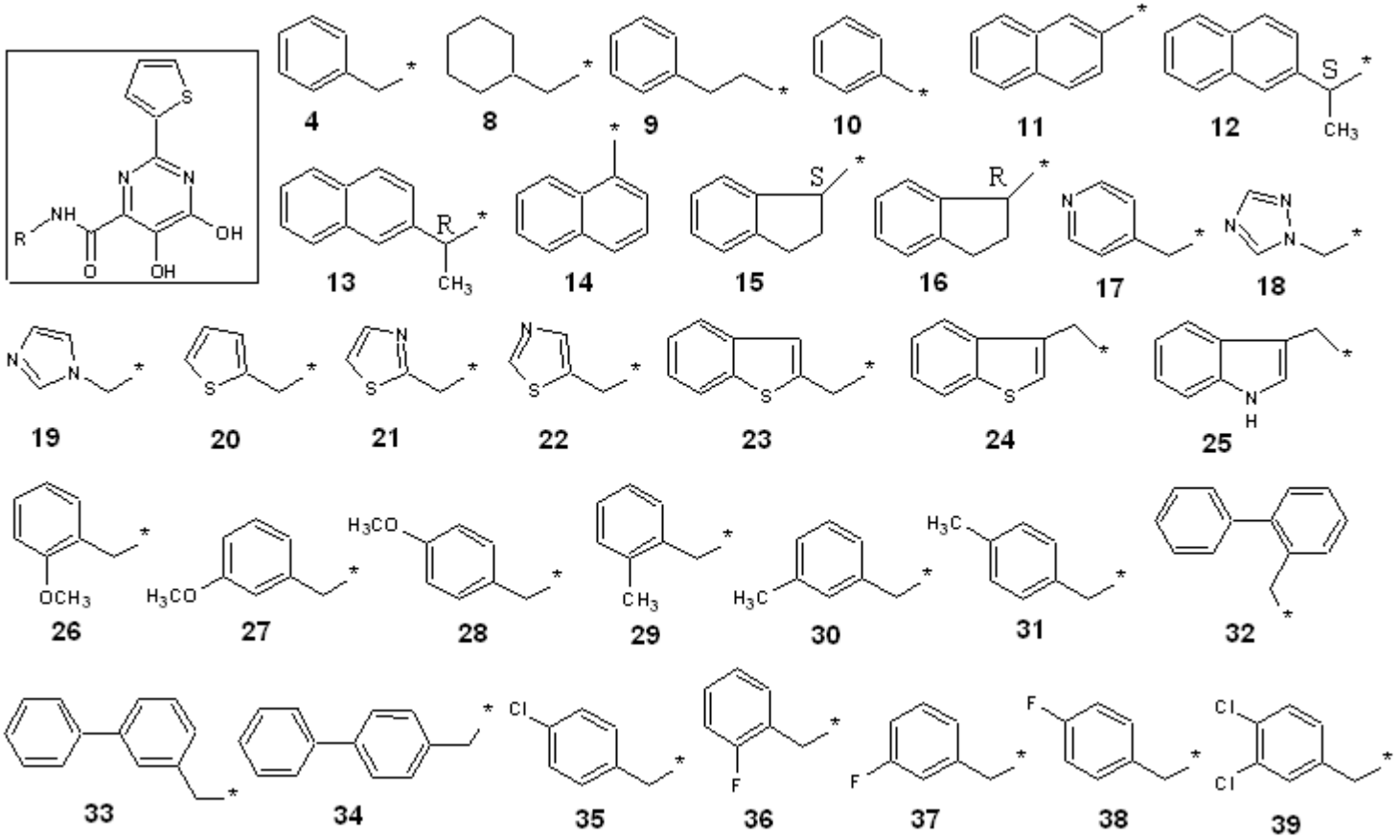


Figure S3. Training set 3.

Table S1. Values of another descriptors and biological activity from TS1 [Source: ref. 20].

	RBF	nPhX	Jhete	pIC_{50}
1	0.100	2.087	1.000	6.420
2	0.120	2.096	1.000	6.590
4	0.110	2.097	1.000	6.680
5	0.110	2.919	0.000	4.310
7	0.060	1.605	0.000	5.620
8	0.090	2.012	0.000	5.660
9	0.120	2.171	0.000	5.980
10	0.050	1.986	0.000	5.000
12	0.110	1.650	0.000	5.850
13	0.140	2.102	0.000	6.090
15	0.170	2.114	0.000	5.700
16	0.170	2.081	0.000	6.370
17	0.170	2.047	0.000	6.370
18	0.170	2.077	0.000	6.110
22	0.110	2.103	1.000	6.250
23	0.110	2.081	1.000	6.389
24	0.110	2.086	2.000	6.360
26	0.110	2.090	2.000	6.430
27	0.110	2.067	2.000	6.750
28	0.110	2.099	1.000	6.660
29	0.110	2.077	1.000	6.380
31	0.110	2.083	2.000	6.730
32	0.110	2.120	1.000	6.200

33	0.110	2.134	0.000	5.170
34	0.090	1.847	0.000	5.850
35	0.090	1.747	0.000	6.170
36	0.080	1.750	1.000	6.300
37	0.080	1.677	1.000	6.000
38	0.080	1.679	0.000	5.840
39	0.120	1.963	0.000	5.690
Test set				
6	0.050	2.257	0.000	4.980
11	0.100	1.799	0.000	6.250
14	0.140	2.023	0.000	6.250
19	0.120	2.071	0.000	5.800
20	0.140	1.907	0.000	5.690
21	0.120	2.005	0.000	6.370
25	0.110	2.106	2.000	6.450
30	0.110	2.064	2.000	6.950

Table S2. Values of another descriptors and biological activity from TS2 [ref. 21].

	C2	C4	C8	C9	Log(1/C)
Training set					
1	0.660	0.874	0.804	1.929	7.340
2	0.660	0.890	2.039	0.733	6.790
3	-0.122	0.718	2.101	1.986	4.300
4	-0.125	0.706	2.105	1.989	5.000
5	-0.114	0.723	2.123	2.003	5.000
6	-0.141	0.659	2.090	1.978	4.640
7	-0.132	0.139	2.087	1.976	4.490
8	0.647	0.300	2.028	0.719	6.170
9	0.685	0.369	2.078	0.758	5.660
10	-0.093	0.211	2.130	2.008	4.130
11	-0.117	0.158	2.105	1.989	4.900
12	-0.079	0.257	2.136	2.013	3.740
13	-0.104	0.204	2.111	1.994	4.320
14	-0.108	0.747	2.124	2.000	4.080
15	-0.122	0.716	2.117	1.995	4.920
16	-0.176	0.656	0.709	1.844	6.840
17	-0.176	0.672	1.965	0.637	6.790
18	0.725	0.955	2.216	2.093	5.610
19	0.712	0.924	2.209	2.088	7.110
20	0.657	0.865	0.801	1.937	7.920
21	0.657	0.880	2.058	0.730	7.640
22	-0.124	0.122	2.111	1.994	4.250
23	0.709	0.330	2.204	2.087	5.650

24	0.736	0.384	2.236	2.111	4.870
25	0.709	0.330	2.204	2.087	4.840
26	0.318	-0.007	1.908	0.630	4.300
27	0.681	0.091	2.255	2.125	5.000
28	0.709	0.910	2.216	2.093	7.380
29	0.709	0.910	2.216	2.093	5.940
30	-0.179	0.658	1.972	0.635	6.640
32	-0.179	0.658	1.972	0.635	5.300
33	0.710	0.346	2.216	2.093	4.590
36	0.657	0.860	0.801	1.931	8.300
37	-0.177	0.667	1.953	0.638	6.740
38	0.657	0.876	2.046	0.730	7.370
39	0.684	0.927	2.078	0.758	7.470
41	-0.109	0.742	2.112	1.995	4.220
42	0.725	0.951	2.204	2.087	5.780
43	-0.133	0.694	2.087	1.976	4.660
44	0.711	0.920	2.197	2.082	7.010
45	-0.122	0.711	2.105	1.990	5.480
Test set					
T1	-0.119	0.725	2.098	1.985	4.900
T2	-0.130	0.708	2.080	1.971	4.330
T3	-0.106	0.756	2.105	1.990	4.050
T4	-0.126	0.712	2.090	1.979	4.430
T5	0.711	0.920	2.197	2.082	7.360
T6	-0.118	0.711	1.236	2.073	4.150

T7	-0.105	0.746	2.122	2.002	4.000
T8	0.549	0.752	-0.171	1.499	8.240
T9	-0.139	0.690	1.049	1.990	7.320
T10	0.695	0.898	1.141	2.082	8.520
T11	0.716	0.919	1.329	2.166	7.870
T12	0.667	0.867	0.917	1.999	7.470
T13	0.580	0.816	1.951	0.542	7.590
T14	-0.220	0.605	0.630	1.767	5.940
T15	0.613	0.813	0.722	1.860	7.250
T16	-0.118	0.711	1.236	2.073	6.000
T17	0.650	0.867	2.141	1.999	5.330
T18	-0.184	0.659	2.048	1.906	5.180
T19	0.689	0.898	2.187	2.082	5.970
T20	0.607	0.807	0.736	1.835	6.730
T21	-0.121	0.707	1.206	2.060	7.060
T22	0.712	0.916	1.299	2.152	7.320
T23	-0.145	0.680	1.088	2.010	6.360
T24	0.688	0.888	1.181	2.103	7.530
T25	-0.119	0.725	2.098	1.985	4.900

Table S3. Algoritms used for Log*P* obtention.

Algorithm	Source	Approch	Further information
AB/Log*P*	www.vcclab.org/lab/alogps	Fragmental	www.ap-algorithms.com
ACD/Log*P*	ACD/Log*P* freeware 10	Fragmental	www.acdlabs.com
ACLog*P*	www.vcclab.org/lab/alogps	Atom-based	www.actelion.com
ALog*P*	www.vcclab.org/lab/edragon	Atom-based	V.N. Viswanadhan, A.K. Ghose, G.R. Revankar, R.K. Robins, *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 163-172.
ALOG*P*s	www.vcclab.org/lab/alogps	Whole-molecule	Same URL
ChemOffLog*P*	Chem3D Ultra 5.0	Atom-based	ChemOffice manual
CLogP	Chem3D Ultra 5.0	Fragmental	www.biobyte.com
COSMOfrag	www.vcclab.org/lab/alogps	Whole-molecule	www.cosmologic.de/LifeScience/cosmofrag.html
CSLog*P*	www.chemsilico.com/CS_prLogP/LPhome.html	Whole-molecule	Same URL
IALog*P*	www.logp.com	Whole-molecule	Unavailable
KOWWIN	www.vcclab.org/lab/alogps	Fragmental/atom-based	www.syrres.com/esc/kowwin.htm
miLog*P*	www.vcclab.org/lab/alogps	Fragmental	www.molinspiration.com
MLog*P*	www.vcclab.org/lab/edragon	Whole-molecule	I. Moriguchi, S. Hirono, Q. Liu, I. Nakagome, Y. Matsushita, *Chem. Pharm. Bull.* **1992**, *40*, 127-130.
molLog*P*	www.molsoft.com/mprop	Fragmental	www.molsoft.com
XLog*P*2	www.vcclab.org/lab/alogps	Atom-based	http://cheminfo.pku.edu.cn/calculator/xlogp/manual
XLog*P*3	www.vcclab.org/lab/alogps	Atom-based	www.sioc-ccbg.ac.cn/software/xlogp3

Table S4. All Log*P* values for all samples of TS1[(a)].

	AB/Log*P*	ACD/Log*P*	AcLogP	ALog*P*	ALOG*P*s	ChemOffLog*P*	CLog*P*	COSMOfrag	CSLog*P*	KOWWIN	miLog*P*	MLog*P*	molLog*P*	XLog*P*2	XLog*P*3
1	3.540	3.020	3.080	2.846	2.970	2.854	5.101	3.460	2.930	4.850	2.950	1.710	4.030	2.510	3.750
2	3.950	3.480	3.490	3.128	3.450	3.558	5.620	4.610	3.880	5.400	3.010	1.945	4.350	2.830	4.150
4	3.690	2.850	2.210	2.124	2.410	1.940	6.221	3.830	1.890	3.820	2.440	0.731	3.290	1.830	2.760
5	1.230	0.300	0.140	-0.208	0.390	-0.621	3.590	1.380	-0.590	1.230	0.060	-0.969	3.460	-0.680	0.580
7	4.000	3.010	2.440	2.609	2.130	1.742	5.789	4.060	1.890	4.260	2.510	0.329	2.070	1.940	3.190
8	3.560	2.890	1.800	1.981	1.900	1.355	6.240	3.840	1.570	3.990	2.350	0.597	3.210	1.770	2.950
9	3.160	2.420	1.970	1.753	1.960	1.430	5.667	3.430	1.230	3.350	2.020	0.614	2.560	1.560	2.470
10	2.580	1.010	1.500	1.137	0.760	0.821	4.996	2.060	1.000	2.090	1.440	-0.705	1.790	0.650	1.950
12	3.370	2.350	1.950	1.465	1.020	1.170	6.214	3.050	1.250	3.490	1.760	-0.235	2.220	0.950	2.350
13	2.870	1.990	1.400	1.359	1.360	0.985	6.015	3.100	0.870	3.010	1.670	-0.134	2.340	0.950	2.040
15	2.820	1.790	1.300	1.343	0.980	0.858	6.672	3.730	0.770	3.100	1.680	-0.641	2.070	0.860	2.010
16	2.600	1.810	1.300	1.343	1.000	0.858	6.672	3.640	0.790	2.580	1.480	-0.641	2.120	0.600	2.010
17	2.820	1.790	1.300	1.343	1.060	0.858	6.672	3.440	1.050	3.100	1.700	-0.641	2.470	0.860	2.010
18	2.870	1.960	1.300	1.343	1.070	0.858	6.672	3.310	1.030	3.100	1.700	-0.641	2.430	0.860	2.010
22	2.950	2.130	1.570	1.581	1.700	1.269	5.501	3.260	0.750	3.130	1.800	0.496	2.480	1.200	2.170
23	2.950	2.130	1.570	1.581	1.680	1.269	5.501	3.250	0.770	3.130	1.820	0.496	2.520	1.200	2.170

24	3.800	2.890	2.270	2.329	2.290	2.098	6.364	3.800	1.680	4.020	2.560	0.847	3.570	1.990	2.860
26	3.100	2.220	1.630	1.786	1.690	1.427	5.644	3.260	0.640	3.330	1.910	0.614	2.430	1.360	2.270
27	3.480	2.830	2.180	2.245	2.130	1.827	4.212	3.700	1.370	3.780	2.430	0.731	3.240	1.820	2.800
28	3.470	2.670	2.120	2.040	2.340	1.669	4.069	3.590	1.570	3.580	2.310	0.614	3.100	1.660	2.700
29	3.470	2.670	2.120	2.040	2.340	1.669	4.069	3.620	1.600	3.580	2.340	0.614	3.090	1.660	2.700
31	4.040	3.280	2.730	2.704	2.840	2.228	4.782	3.890	2.320	4.220	2.940	0.847	3.790	2.280	3.330
32	3.690	2.850	2.210	2.124	2.400	1.940	4.219	3.690	1.550	3.820	2.420	0.731	3.030	1.830	2.760
33	1.530	0.580	0.430	0.225	0.140	-0.225	1.859	1.880	-0.660	1.750	0.370	-0.615	1.250	-0.220	1.000
34	4.160	3.310	2.690	2.284	2.770	2.108	4.530	3.880	1.400	4.110	2.820	1.515	3.780	2.300	3.320
35	4.250	3.640	3.310	2.847	2.930	2.768	5.100	4.490	1.950	4.520	3.210	1.157	4.050	2.000	3.410
36	4.640	4.340	3.250	3.099	2.990	2.944	7.389	4.900	2.270	4.900	3.550	1.595	4.070	3.130	3.800
37	4.640	4.340	3.250	3.099	3.070	2.944	7.389	4.850	2.330	4.900	3.570	1.595	4.130	3.130	3.800
38	4.590	3.830	3.190	2.894	3.020	2.786	7.246	4.580	2.560	4.700	3.450	1.489	4.380	2.970	3.700
39	3.290	2.490	1.850	1.696	1.860	1.391	5.687	3.490	1.210	3.420	1.870	0.164	2.350	1.190	2.530
Test set															
6	2.680	1.800	1.410	1.190	0.970	0.509	4.972	2.880	0.480	3.000	1.460	0.104	1.050	0.580	1.850
11	2.980	1.940	1.610	1.140	0.870	0.891	5.885	2.610	0.930	3.000	1.550	-0.467	2.260	0.790	1.890

14	2.870	1.990	1.400	1.360	1.400	0.985	6.015	2.860	1.210	3.010	1.720	-0.134	2.450	0.950	2.040
19	3.320	2.540	1.820	1.860	1.770	1.598	5.857	3.630	1.850	3.480	2.110	0.614	2.860	1.470	2.440
20	3.960	3.030	2.340	3.490	2.480	2.638	6.574	3.930	1.040	3.980	2.630	0.213	3.590	2.20	3.250
21	3.860	2.650	2.270	2.320	2.620	2.032	7.708	3.400	1.060	3.900	2.550	0.961	3.250	1.960	2.960
25	3.660	2.840	2.270	2.330	2.320	2.098	6.364	3.990	1.690	4.020	2.560	0.847	3.590	1.990	2.860
30	4.000	3.140	2.730	2.700	2.900	2.228	6.664	4.070	2.180	4.220	2.940	0.847	3.800	2.280	3.330

[(a)] The values of MLog P is the same presented in the ref. [20].

Table S5. All Log P values for all samples of TS2[(a)].

	AB/Log*P*	ACD/Log*P*	AcLog*P*	ALog*P*	ALOG*P*s	ChemOffLog*P*	CLog*P*[(a)]	COSMOfrag	CSLog*P*	KOWWIN	miLog*P*	MLog*P*	molLog*P*	XLog*P*2	XLog*P*3
Training set															
1	2.700	3.610	3.570	3.820	2.890	3.905	4.159	4.400	2.270	3.470	3.410	2.820	3.870	2.220	3.080
2	2.700	3.910	3.570	3.820	2.880	3.905	4.159	4.400	2.620	3.470	3.410	2.820	4.280	2.220	3.080
3	1.730	2.780	2.630	2.760	1.980	2.086	4.165	3.430	2.540	2.970	2.820	2.760	2.990	1.430	2.580
4	2.010	3.130	2.900	3.010	2.390	2.627	4.564	4.170	2.530	3.260	2.840	2.390	3.670	2.400	2.800
5	2.500	3.650	3.380	3.480	2.460	2.852	5.093	4.530	2.560	3.800	3.540	2.630	4.120	2.460	3.250
6	1.590	2.790	2.510	2.440	1.900	1.817	3.955	3.310	2.430	2.490	2.760	2.150	2.650	1.490	2.240
7	1.250	2.250	2.170	2.270	1.520	1.599	3.636	3.020	2.160	2.480	2.310	1.900	3.020	1.070	2.060
8	2.580	3.880	3.450	3.800	2.730	3.856	4.349	4.420	3.560	3.480	3.230	2.820	4.340	1.940	3.280
9	2.760	3.460	3.080	3.550	3.140	3.713	4.149	4.400	2.940	3.370	2.960	2.900	3.140	2.210	2.760
10	1.990	2.860	2.790	2.880	2.670	2.440	4.249	3.920	3.040	2.980	2.750	2.230	2.870	2.040	2.650
11	1.990	3.130	2.970	3.080	2.130	2.484	4.564	3.940	2.790	3.390	3.060	2.390	3.430	1.720	3.020
12	2.220	3.050	2.920	3.020	3.280	2.459	4.579	3.990	3.180	3.050	3.060	2.230	3.260	2.310	2.570
13	2.220	3.310	3.100	3.210	2.210	2.503	4.694	4.010	2.910	3.470	3.380	2.390	3.830	2.000	2.940

14	1.250	1.990	2.500	2.040	2.820	1.556	3.321	2.910	2.460	2.070	2.200	1.730	1.190	1.450	1.650
15	1.760	2.770	3.080	2.630	1.950	1.967	4.165	3.490	2.040	2.900	2.990	2.150	2.170	1.870	2.260
16	2.900	3.630	3.700	3.300	2.920	2.525	4.878	4.220	2.410	3.540	3.620	2.660	2.760	2.490	2.880
17	2.900	3.630	3.700	3.300	2.900	2.525	4.878	4.180	2.630	3.540	3.620	2.660	2.920	2.490	2.880
18	1.400	2.410	3.110	2.790	2.300	3.086	3.321	3.580	2.650	2.350	2.330	2.130	1.800	1.800	2.160
19	2.140	3.380	3.760	3.530	2.670	3.666	4.165	4.360	2.250	3.250	3.340	2.550	2.780	2.120	2.860
20	3.090	4.100	4.370	4.200	3.310	4.224	4.878	5.100	2.740	3.890	3.970	3.060	3.380	2.740	3.480
21	3.090	4.410	4.370	4.200	3.280	4.224	4.878	5.030	3.140	3.890	3.970	3.060	3.530	2.740	3.480
22	2.140	3.260	2.860	3.010	2.220	2.285	4.684	4.340	2.280	3.310	3.130	2.390	3.010	2.260	2.720
23	2.530	3.870	3.530	3.910	3.020	3.984	4.684	5.120	2.620	3.660	3.470	2.790	3.380	2.510	3.320
24	2.200	2.920	2.750	3.270	2.900	3.473	3.955	4.370	2.580	3.150	2.660	2.630	2.010	2.050	2.570
25	2.530	3.870	3.530	3.910	3.020	3.984	4.684	5.120	2.620	3.660	3.470	2.790	3.380	2.510	3.320
26	3.530	2.830	2.660	3.470	2.840	2.662	3.475	3.880	2.790	1.710	2.820	2.160	1.730	1.860	2.690
27	6.040	6.490	5.420	6.400	5.500	6.573	5.983	7.240	4.790	6.220	5.760	4.850	5.060	5.380	5.390
28	2.530	3.870	4.040	3.910	3.050	3.984	4.684	4.950	2.650	3.660	3.670	2.790	3.440	2.580	3.290
29	2.530	3.870	4.040	3.910	3.050	3.984	4.684	4.950	2.650	3.660	3.670	2.790	3.440	2.580	3.290
30	3.480	4.900	4.650	4.570	3.690	4.542	5.397	5.420	3.520	4.310	4.300	3.300	3.580	3.200	3.920

32	3.480	4.900	4.650	4.570	3.690	4.542	5.397	5.420	3.520	4.310	4.300	3.300	3.580	3.200	3.920
33	2.530	3.870	4.040	3.910	3.040	3.984	4.684	4.970	2.600	3.660	3.700	2.790	3.030	2.580	3.290
36	3.090	4.100	3.860	4.200	3.230	4.224	4.878	5.110	2.740	3.890	3.740	3.060	3.800	2.680	3.520
37	2.900	3.630	3.180	3.300	2.670	2.525	4.878	4.050	2.620	3.540	3.390	2.660	3.590	2.430	2.920
38	3.090	4.410	3.860	4.200	3.220	4.224	4.878	5.140	3.100	3.890	3.740	3.060	4.200	2.680	3.520
39	2.760	3.460	3.080	3.550	3.160	3.713	4.149	4.600	3.000	3.370	2.930	2.900	2.840	2.210	2.760
41	1.250	1.990	1.990	2.040	2.280	1.556	3.321	2.940	2.450	2.070	1.970	1.730	1.780	1.380	1.680
42	1.630	2.590	2.660	2.940	2.440	3.254	3.321	3.880	2.390	2.420	2.310	2.130	2.390	1.640	2.280
43	1.250	2.250	2.170	2.230	1.490	1.599	3.636	2.980	2.140	2.480	2.280	1.900	2.320	1.070	2.060
44	2.140	3.380	3.240	3.530	2.570	3.666	4.165	4.510	2.210	3.250	3.110	2.550	3.380	2.060	2.890
45	1.760	2.770	2.570	2.630	2.060	1.967	4.165	3.590	2.030	2.900	2.760	2.150	2.760	1.800	2.290
Test set															
T1	1.370	2.280	2.290	2.260	1.540	1.650	3.446	2.820	1.750	2.480	2.430	1.900	2.460	1.340	1.850
T2	0.860	1.760	1.890	1.850	0.800	1.280	2.917	2.270	1.790	2.070	1.950	1.640	2.160	0.610	1.620
T3	0.860	1.460	1.710	1.660	1.980	1.240	2.802	2.240	2.160	1.650	1.640	1.460	1.600	0.920	1.250
T4	1.340	2.290	2.350	2.310	1.410	1.698	3.446	2.960	2.410	2.560	2.220	1.900	2.010	1.070	2.050
T5	2.140	3.380	3.240	3.530	2.570	3.660	4.165	4.510	2.210	3.250	3.110	2.550	3.380	2.060	2.890

T6	1.010	1.700	1.700	1.780	2.050	1.420	4.664	2.840	1.830	1.940	1.730	1.640	1.870	1.220	1.430
T7	1.730	2.520	2.450	2.500	2.960	1.970	3.850	3.600	2.890	2.560	2.530	1.980	2.240	1.950	2.040
T8	2.510	3.560	3.300	3.740	2.790	4.160	4.308	4.730	2.510	3.450	3.220	2.940	3.110	2.220	2.990
T9	3.050	3.670	3.270	3.380	2.990	3.130	5.028	4.450	2.610	3.790	3.530	2.780	3.320	2.600	2.980
T10	3.250	4.280	3.940	4.280	3.360	4.830	5.028	5.260	2.480	4.140	3.870	3.180	3.930	2.850	3.580
T11	2.550	3.840	3.560	4.020	2.800	4.490	4.664	5.130	2.450	3.790	3.510	2.790	3.700	2.490	3.250
T12	2.310	3.450	3.140	3.520	2.550	3.870	4.084	5.130	2.260	3.330	3.120	2.250	3.290	1.970	2.860
T13	3.910	4.790	4.470	4.860	3.890	5.120	5.471	5.360	3.720	4.540	4.340	3.570	4.480	3.300	4.140
T14	2.340	2.580	2.380	2.510	1.570	2.340	3.598	2.890	1.660	2.440	2.470	1.790	2.410	1.530	2.010
T15	2.450	3.180	3.050	3.410	2.220	4.030	3.598	3.840	2.350	2.790	2.810	2.170	3.030	1.780	2.610
T16	2.170	3.230	2.890	3.120	2.190	2.790	4.664	4.210	2.360	3.440	3.160	2.390	3.090	2.240	2.650
T17	2.120	3.270	3.140	3.520	2.560	3.870	3.884	5.370	2.640	3.330	3.120	2.250	2.910	1.970	2.860
T18	1.490	2.670	2.470	2.620	1.960	2.180	3.884	4.320	2.360	2.980	2.770	1.870	2.290	1.720	2.260
T19	3.230	4.060	3.940	4.280	3.370	4.830	5.028	5.320	2.480	4.140	3.870	3.180	3.810	2.850	3.580
T20	2.270	2.970	2.930	3.290	2.420	3.750	3.518	3.810	1.970	2.960	2.850	2.170	2.820	1.750	2.350
T21	3.460	3.930	3.500	3.210	3.510	3.660	5.288	4.600	2.680	4.060	3.800	2.890	3.460	2.870	2.940
T22	3.510	4.540	4.170	4.110	3.590	5.360	5.288	5.510	2.480	4.410	4.140	3.300	4.070	3.120	3.540

T23	2.420	3.250	3.170	3.190	2.280	2.940	4.889	4.430	2.480	3.800	3.390	2.540	2.830	2.740	3.060
T24	2.800	3.860	3.840	4.090	2.950	4.640	4.889	5.350	3.300	4.150	3.730	2.950	3.440	2.990	3.660

[(a)] The values of CLog*P* is the same presented in the ref. [21].

Table S6. All Log*P* values from TS3.

	AB/Log*P*	ACD/Log*P*	AcLog*P*	ALog*P*	ALOG*P*s	ChemOffLog*P*	CLog*P*	COSMOfrag	CSLog*P*	IALog*P*	KOWWIN	miLog*P*	MLog*P*	MolLog*P*	XLog*P*2	XLog*P*3
4	4.440	2.850	2.930	2.710	2.859	3.883	5.500	3.680	2.080	3.270	3.650	2.574	2.804	2.760	2.550	2.860
8	5.030	3.350	3.220	3.380	3.454	4.127	6.182	4.010	2.330	2.760	4.710	3.464	3.037	3.800	3.280	3.740
9	4.870	2.780	3.280	2.920	3.170	4.163	5.296	3.730	2.270	3.620	4.140	2.979	3.047	3.130	2.700	3.320
11	5.230	4.060	4.330	4.210	3.751	4.811	5.965	3.990	1.530	4.160	4.920	4.032	3.371	4.640	3.670	4.170
13	5.950	4.430	4.570	4.260	4.135	5.199	6.453	4.970	1.640	2.030	5.250	4.316	3.821	4.750	4.340	4.510
14	5.10	4.060	4.330	4.070	3.957	4.811	9.96	4.700	2.010	3.950	4.740	4.277	3.598	4.630	3.810	4.360
15	4.970	2.990	3.590	3.160	3.409	4.259	5.914	3.940	2.090	3.590	4.510	3.020	3.285	4.180	2.850	3.290
18	2.110	-0.180	1.080	0.60	0.862	2.105	3.172	0.410	-0.430	0.690	0.900	0.310	2.434	0.140	0.500	1.170
19	2.740	0.480	1.080	0.830	0.990	1.753	3.224	0.930	2.120	0.060	1.720	0.844	1.821	0.920	1.030	1.180
20	4.10	2.530	2.780	2.830	2.803	3.865	5.146	3.290	1.520	1.630	3.470	2.473	2.374	2.510	1.610	2.580
21	2.610	1.790	1.570	2.040	1.711	3.272	3.844	1.680	0.510	1.450	2.650	1.236	1.351	1.800	0.750	1.930
22	2.820	1.070	1.710	1.840	1.596	2.677	3.844	1.760	0.460	1.450	2.650	1.744	1.351	1.340	0.750	1.930
23	5.350	5.010	3.950	4.150	4.002	4.918	6.53	4.100	2.120	1.880	4.650	3.780	3.211	3.620	2.950	3.910
24	5.350	5.010	3.810	4.150	3.711	4.862	6.53	3.900	2.120	1.850	4.650	3.469	3.211	3.100	3.240	3.880
27	4.400	2.760	2.830	2.910	2.833	3.757	4.889	2.330	1.970	3.540	3.730	2.606	2.288	2.820	2.460	2.830

28	4.400	2.760	2.830	2.950	2.833	3.757	4.889	3.560	1.960	3.580	3.730	2.630	2.288	2.810	2.460	2.830
29	4.850	3.310	3.250	3.180	3.335	4.370	5.419	3.890	2.080	3.700	4.200	2.974	3.047	3.260	2.980	3.220
30	4.850	3.310	3.250	3.200	3.335	4.370	5.419	4.130	2.140	3.820	4.200	2.998	3.047	3.240	2.980	3.220
31	4.850	3.310	3.250	3.240	3.335	4.370	5.419	3.930	2.160	3.880	4.200	3.022	3.047	3.220	2.980	3.220
32	6.130	4.610	4.610	4.500	4.368	5.558	7.088	4.050	1.610	1.900	5.420	4.321	3.969	4.430	4.490	3.490
33	6.130	4.610	4.610	4.540	4.368	5.558	7.388	3.720	1.500	1.950	5.420	4.345	3.969	4.610	4.490	2.960
34	6.130	4.610	4.610	4.550	4.368	5.558	7.388	3.580	1.530	1.980	5.420	4.369	3.969	4.740	4.490	2.960
36	4.490	2.900	2.990	2.810	3.055	4.041	5.643	4.500	2.050	1.990	3.850	2.690	2.926	2.990	2.710	4.120
37	4.490	2.900	2.990	2.820	3.055	4.041	5.643	5.190	2.010	2.410	3.850	2.714	2.926	2.840	2.710	4.490
38	4.490	2.900	2.990	2.880	3.055	4.041	5.643	5.180	1.970	2.950	3.850	2.738	2.926	2.880	2.710	4.490
39	5.540	3.910	4.160	4.250	4.178	4.999	6.806	5.130	2.920	3.890	4.940	3.858	3.285	4.150	3.790	4.490
Test set																
12	5.950	4.430	4.570	4.260	4.135	5.199	6.453	4.970	2.120	2.030	5.250	4.316	3.821	4.750	4.340	4.510
10	3.980	2.830	3.140	3.110	2.842	3.814	5.321	2.940	1.920	3.400	3.740	2.872	2.555	3.320	2.400	2.920
16	4.970	2.990	3.590	3.160	3.409	4.259	5.914	3.940	2.090	3.590	4.510	3.020	3.285	4.180	2.850	3.290
17	3.070	1.360	1.860	1.800	1.699	2.546	4.003	1.820	0.940	2.540	2.460	1.285	1.795	1.610	1.290	1.790
25	4.520	2.770	3.000	3.060	3.143	3.424	5.49	3.100	1.680	1.450	3.710	2.724	2.452	3.030	2.620	2.990

26	4.400	2.760	2.830	2.860	2.833	3.757	4.889	2.330	1.970	3.470	3.730	2.582	2.288	2.670	2.460	2.830
35	5.010	3.440	3.550	3.400	3.514	4.441	6.213	3.670	1.610	3.000	4.300	3.252	3.047	3.440	3.170	2.960

Table S7. Softwares utilized for obtain another descriptors for TS3, quantities and classifications.

Software	Quantities of descriptors	Classifications
ACD/ChemSketch 10.0	9	Sterics, solubility
E-Dragon 1.0[(a)]	34	Conectivity indices
ETState[(a)]	30	Atom and bond-types E-state indices, and number of determined atoms and bonds
Gaussian 03[(b)]	20	Thermodinamics, electronics
HyperChem 7.1	4	Sterics
Marvin 4.1.8[(c)]	63	Topologicals, solubility, sterics and constitucionals
MolSoft[(d)]	1	Solubility (Log*S*)

(a) By the PClient interface - http://www.vcclab.org/lab/pclient;
(b) Obtained from most stable geometries calculated at B3LYP/6-31G(d,p) theory level. The three-dimensional structures are built from DOTRUZ file obtained in Cambridge Structural Database version 5.29 (November 2007) + 1 update;
(c) Freeware version obtained in http://www.chemaxon.com;
(d) www.molsoft.com/mprop.

Table S8. Evaluated statiscal parameters and the corresponding equations[(a)].

Parameter	Symbol	Equation
Correlation coefficient of calibration	R^2	$1 - [\Sigma_i(y_{obsi} - y_{ci})^2] / \Sigma_i(y_{obsi} - \bar{y}_{obsi})^2]$
Standard error of calibration	*SEC*	$[\Sigma_i(y_{obsi} - y_{ci})^2/n\text{-}k\text{-}1]^{½}$
Predictive Residual Sum of Squares of Calibration	$PRESS_{cal}$	$\Sigma_i(y_{obsi} - y_{ci})^2$
F-test (with 95% confidence interval)	*F*	$[\Sigma_i(y_{obsi} - y_{ci})^2/k] / [\Sigma_i(y_{obsi} - \bar{y}_{obs})^2/n\text{-}k\text{-}1]$
Correlation coefficient of cross-validation	Q^2_{LNO}	$1 - [\Sigma_i(y_{obsi} - y_{vi})^2] / \Sigma_i(y_{obsi} - \bar{y}_{obs})^2]$
Standard error of cross-validation	*SEV*	$[\Sigma_i(y_{obsi} - y_{vi})^2]/n]^{½}$
Predictive Residual Sum of Squares of Calibration of Validation	$PRESS_{val}$	$\Sigma_i(y_{obsi} - y_{vi})^2$
Correlation coefficient of prediction	R^2_{pred}	$1 - [\Sigma_i(y_{evi} - y_{testi})^2] / \Sigma_i(y_{obsi} - \bar{y}_{obs})^2]$
Average relative error of prediction	ARE_{pred}	$[\Sigma_i(\lvert y_{obsi} - y_{evi}\rvert) / y_{obsi}]*100/n$
Standard error of prediction	*SEP*	$[\Sigma_i(y_{obsi} - y_{evi})^2/n]^{½}$

(a) Legends. y: biological activity; $\bar{y}$: average observed biological activity; obs: experimental values; c: estimated activity in the regression model; v: estimated activity in the cross-validation; ev: estimated activity in the external validation; n: number of samples of training set; k: number of latent variables; $\bar{y}_{obs}$: average observed activity for the complete training set; test: test-set

Table S9. Obtained models for TS1.

	MLog*P*	RBF	nPhX	Jhete	Independent term
AB/Log*P*	0.276	10.581	0.454	-0.547	4.795
ACD/Log*P*	0.204	10.285	0.459	-0.670	5.478
ACLog*P*	0.263	11.171	0.458	-0.669	5.361
ALog*P*	0.307	10.589	0.409	-0.551	5.163
ALOG*P*s	0.255	11.280	0.425	-0.834	5.744
ChemOffLog*P*	0.231	10.574	0.432	-0.705	5.679
CLog*P*	-0.013	10.036	0.564	-1.253	7.215
COSMOFrag	0.221	8.644	0.482	-0.661	5.363
CSLog*P*	0.196	10.189	0.479	-0.834	6.051
KOWWIN	0.200	9.971	0.459	-0.705	5.385
miLog*P*	0.274	10.540	0.437	-0.595	5.231
MLog*P*	0.240	11.690	0.440	-0.920	6.240
molLog*P*	0.128	10.754	0.514	-1.188	6.580
XLog*P*2	0.226	10.835	0.440	-0.710	5.679
XLog*P*3	0.262	10.802	0.457	-0.665	5.240

Table S10. Obtained models for TS2.

	Log*P*	C2	C4	C8	C9	Independent term
AB/Log*P*	0.250	0.996	2.174	-1.073	-0.556	6.537
ACD/Log*P*	0.333	0.928	2.094	-1.091	-0.542	6.079
ACLog*P*	0.352	0.943	1.933	-1.080	-0.595	6.217
ALog*P*	0.336	0.822	2.135	-1.089	-0.571	6.125
ALOG*P*s	0.119	1.101	1.979	-1.184	-0.666	7.308
ChemOffLog*P*	0.250	0.720	2.026	-1.144	-0.600	6.729
CLog*P*	0.524	1.172	2.121	-1.053	-0.595	4.850
COSMOFrag	0.349	0.800	2.138	-1.119	-0.609	5.896
CSLog*P*	0.114	1.157	1.993	-1.219	-0.667	7.378
KOWWIN	0.395	0.982	2.085	-1.100	-0.626	6.062
miLog*P*	0.399	1.005	2.094	-1.056	-0.594	5.931
MLog*P*	0.432	0.939	2.068	-1.114	-0.597	6.249
molLog*P*	0.361	1.018	2.086	-1.106	-0.600	6.201
XLog*P*2	0.285	1.030	2.058	-1.146	-0.642	6.857
XLog*P*3	0.425	0.908	2.179	-1.086	-0.587	6.006

Table S11. Results of y-randomization test of TS1.

AB/Log*P*		**ACD/Log*P***		**ACLog*P***		**ALog*P***		**ALOG*P*s**	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.179	-0.214	0.061	-0.537	0.176	-0.579	0.092	-0.289	0.153	-0.303
0.014	-0.387	0.037	-0.803	0.274	-0.022	0.062	-0.376	0.035	-0.540
0.146	-0.411	0.048	-0.391	0.129	-0.253	0.386	-0.217	0.312	-0.047
0.205	-0.660	0.206	-0.190	0.033	-0.282	0.086	-0.524	0.024	-0.356
0.070	-0.268	0.227	-0.089	0.265	-0.204	0.412	0.143	0.289	-0.068
0.053	-0.674	0.336	0.035	0.056	-0.238	0.040	-0.338	0.113	-0.283
0.052	-0.248	0.069	-0.583	0.088	-0.410	0.501	0.242	0.123	-0.314
0.167	-0.311	0.142	-0.304	0.271	-0.065	0.040	-0.334	0.245	-0.100
0.050	-0.291	0.036	-0.340	0.271	-0.179	0.218	-0.226	0.106	-0.255
0.082	-0.225	0.197	-0.299	0.130	-0.234	0.244	-0.793	0.126	-0.304

CLog*P*		**CSLog*P***		**KOWWIN**		**miLog*P***		**MLog*P***	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.057	-0.765	0.112	-0.427	0.033	-0.686	0.024	-0.407	0.014	-0.524
0.295	-0.019	0.121	-0.230	0.017	-0.324	0.071	-0.348	0.089	-0.402
0.190	-0.083	0.121	-0.834	0.052	-0.368	0.319	-0.014	0.085	-0.202
0.192	-0.350	0.073	-0.392	0.058	-0.374	0.040	-0.655	0.046	-0.342
0.035	-0.373	0.112	-0.283	0.063	-0.354	0.065	-0.246	0.212	-0.270
0.107	-0.298	0.062	-0.300	0.085	-0.262	0.164	-0.623	0.116	-0.280
0.118	-0.312	0.234	-0.129	0.180	-0.369	0.161	-0.511	0.214	-0.113
0.116	-0.206	0.111	-0.140	0.145	-0.278	0.097	-0.247	0.148	-0.399
0.272	-0.637	0.003	-0.366	0.067	-0.261	0.088	-0.388	0.096	-0.369
0.305	-0.276	0.108	-0.601	0.362	-0.124	0.023	-0.396	0.079	-0.455

XLog*P*3		**COSMOfrag**		**molLog*P***		**ChemOffLog*P***		**XLog*P*2**	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.131	-0.274	0.030	-0.600	0.055	-0.324	0.137	-0.277	0.032	-0.384
0.258	-0.053	0.055	-0.406	0.056	-0.368	0.142	-0.238	0.078	-0.153

0.253	-0.028	0.071	-0.268	0.117	-0.252	0.299	-0.082	0.309	-0.497
0.184	-0.035	0.057	-0.265	0.132	-0.187	0.146	-0.728	0.215	-0.138
0.074	-0.451	0.040	-0.299	0.019	-0.311	0.154	-0.325	0.012	-0.386
0.168	-0.100	0.324	-0.250	0.030	-0.716	0.117	-0.395	0.151	-0.701
0.023	-0.396	0.069	-0.333	0.069	-0.237	0.105	-0.332	0.048	-0.278
0.118	-0.178	0.186	-0.160	0.137	-0.269	0.399	-0.237	0.178	-0.433
0.167	-0.261	0.130	-0.218	0.078	-0.231	0.140	-0.101	0.040	-0.231
0.072	-0.381	0.138	-0.397	0.102	-0.379	0.231	-0.201	0.088	-0.604

Table S12. Results of LNO validation of TS1.

AB/Log*P*					**ACD/Log*P***					**CLog*P***				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.572	0.572	0.572	0.572	0.000	0.544	0.544	0.544	0.544	0.000	0.503	0.503	0.503	0.503	0.000
0.568	0.557	0.550	0.558	0.008	0.588	0.562	0.534	0.561	0.027	0.541	0.507	0.526	0.524	0.017
0.579	0.605	0.530	0.571	0.037	0.525	0.619	0.577	0.574	0.047	0.512	0.497	0.473	0.494	0.020
0.519	0.548	0.472	0.513	0.038	0.564	0.581	0.478	0.541	0.055	0.519	0.530	0.520	0.523	0.006
0.549	0.538	0.530	0.539	0.009	0.576	0.585	0.539	0.567	0.024	0.615	0.397	0.544	0.518	0.111
0.453	0.653	0.670	0.592	0.120	0.640	0.519	0.598	0.585	0.062	0.476	0.383	0.525	0.461	0.072
0.586	0.579	0.492	0.552	0.052	0.591	0.621	0.550	0.587	0.036	0.439	0.517	0.205	0.387	0.162
0.582	0.531	0.467	0.527	0.057	0.390	0.518	0.641	0.516	0.126	0.539	0.485	0.522	0.515	0.028
0.480	0.546	0.507	0.511	0.033	0.203	0.545	0.527	0.425	0.192	0.367	0.485	0.488	0.447	0.069
0.562	0.583	0.623	0.589	0.030	0.602	0.476	0.328	0.469	0.137	-0.132	0.153	0.468	0.163	0.300
	Average Q^2_{LNO}		0.553			Average Q^2_{LNO}		0.537			Average Q^2_{LNO}		0.454	
CSLog*P*					**XLog*P*3**					**COSMOfrag**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.657	0.657	0.657	0.657	0.000	0.653	0.653	0.653	0.653	0.000	0.571	0.571	0.571	0.571	0.000
0.657	0.662	0.665	0.661	0.004	0.668	0.654	0.644	0.655	0.012	0.564	0.571	0.590	0.575	0.014
0.600	0.687	0.673	0.654	0.047	0.649	0.610	0.629	0.629	0.019	0.589	0.581	0.568	0.579	0.010
0.655	0.653	0.674	0.661	0.011	0.689	0.387	0.644	0.573	0.163	0.564	0.647	0.540	0.584	0.056
0.704	0.677	0.676	0.686	0.016	0.706	0.651	0.644	0.667	0.034	0.527	0.566	0.597	0.563	0.035
0.700	0.657	0.703	0.687	0.026	0.610	0.670	0.704	0.662	0.048	0.490	0.588	0.516	0.531	0.051
0.644	0.692	0.696	0.677	0.029	0.654	0.654	0.634	0.647	0.012	0.592	0.649	0.575	0.605	0.038
0.599	0.696	0.555	0.617	0.072	0.677	0.557	0.617	0.617	0.060	0.422	0.488	0.646	0.519	0.115
0.625	0.495	0.622	0.581	0.074	0.616	0.641	0.627	0.628	0.013	0.542	0.561	0.557	0.554	0.010
0.712	0.641	0.664	0.672	0.036	0.607	0.601	0.583	0.597	0.012	0.617	0.443	0.231	0.430	0.193
	Average Q^2_{LNO}		0.655			Average Q^2_{LNO}		0.633			Average Q^2_{LNO}		0.551	
ACLog*P*					**ALog*P***					**KOWWIN**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.626	0.626	0.626	0.626	0.000	0.652	0.652	0.652	0.652	0.000	0.607	0.607	0.607	0.607	0.000
0.626	0.622	0.629	0.626	0.004	0.646	0.611	0.638	0.632	0.018	0.591	0.599	0.614	0.601	0.012
0.591	0.634	0.617	0.614	0.022	0.698	0.633	0.669	0.667	0.033	0.599	0.611	0.607	0.606	0.006

0.654	0.661	0.599	0.638	0.034	0.660	0.623	0.597	0.627	0.031	0.563	0.585	0.584	0.577	0.012
0.628	0.542	0.554	0.575	0.047	0.672	0.647	0.650	0.656	0.014	0.569	0.527	0.657	0.584	0.067
0.613	0.557	0.690	0.620	0.067	0.695	0.591	0.642	0.643	0.052	0.566	0.544	0.587	0.566	0.022
0.691	0.650	0.610	0.650	0.041	0.628	0.515	0.544	0.562	0.059	0.564	0.593	0.684	0.613	0.062
0.517	0.570	0.617	0.568	0.050	0.641	0.582	0.619	0.614	0.030	0.563	0.634	0.626	0.608	0.039
0.601	0.443	0.636	0.560	0.103	0.577	0.629	0.651	0.619	0.038	0.553	0.624	0.595	0.591	0.036
0.609	0.551	0.451	0.537	0.080	0.421	0.432	0.565	0.472	0.080	0.456	0.584	0.574	0.538	0.072
	Average Q^2_{LNO}		0.601			Average Q^2_{LNO}		0.614			Average Q^2_{LNO}		0.589	
miLog*P*					**molLog*P***					**ALOGPs**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.622	0.622	0.622	0.622	0.000	0.445	0.445	0.445	0.445	0.000	0.669	0.669	0.669	0.669	0.000
0.578	0.611	0.608	0.599	0.018	0.435	0.426	0.472	0.444	0.024	0.671	0.713	0.669	0.685	0.025
0.624	0.581	0.664	0.623	0.042	0.449	0.458	0.421	0.443	0.019	0.624	0.663	0.618	0.635	0.025
0.596	0.719	0.696	0.670	0.065	0.291	0.421	0.362	0.358	0.065	0.717	0.732	0.688	0.712	0.022
0.667	0.646	0.609	0.641	0.030	0.245	0.484	0.500	0.409	0.143	0.700	0.666	0.638	0.668	0.031
0.647	0.635	0.566	0.616	0.044	0.444	0.406	0.500	0.450	0.047	0.714	0.728	0.615	0.686	0.062
0.709	0.519	0.570	0.600	0.098	0.498	0.494	0.428	0.473	0.039	0.667	0.757	0.687	0.704	0.047
0.531	0.621	0.602	0.585	0.048	0.415	0.215	0.363	0.331	0.104	0.666	0.608	0.630	0.634	0.029
0.663	0.593	0.655	0.637	0.038	0.527	0.407	0.301	0.412	0.113	0.662	0.604	0.681	0.649	0.040
0.618	0.509	0.594	0.574	0.058	0.433	0.142	0.575	0.383	0.221	0.609	0.482	0.721	0.604	0.120
	Average Q^2_{LNO}		0.617			Average Q^2_{LNO}		0.415			Average Q^2_{LNO}		0.664	
ChemOffLog*P*					**MLog*P***					**XLog*P*2**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.652	0.652	0.652	0.652	0.000	0.665	0.665	0.665	0.665	0.000	0.631	0.631	0.631	0.631	0.000
0.652	0.680	0.651	0.661	0.016	0.579	0.645	0.717	0.647	0.069	0.634	0.645	0.648	0.642	0.008
0.700	0.662	0.653	0.672	0.025	0.693	0.671	0.673	0.679	0.012	0.637	0.626	0.640	0.634	0.008
0.665	0.661	0.663	0.663	0.002	0.641	0.671	0.646	0.653	0.016	0.589	0.635	0.671	0.632	0.041
0.633	0.678	0.553	0.621	0.064	0.678	0.630	0.605	0.638	0.037	0.599	0.621	0.643	0.621	0.022
0.614	0.622	0.546	0.594	0.042	0.651	0.722	0.637	0.670	0.045	0.656	0.480	0.683	0.606	0.110
0.440	0.625	0.609	0.558	0.103	0.596	0.708	0.604	0.636	0.063	0.639	0.623	0.636	0.633	0.009
0.570	0.570	0.699	0.613	0.075	0.749	0.420	0.689	0.619	0.175	0.591	0.674	0.603	0.623	0.045
0.597	0.664	0.676	0.646	0.043	0.574	0.674	0.690	0.646	0.063	0.734	0.677	0.585	0.666	0.075
0.516	0.624	0.541	0.560	0.057	0.545	0.780	0.717	0.680	0.122	0.673	0.689	0.449	0.604	0.134
	Average Q^2_{LNO}		0.624			Average Q^2_{LNO}		0.653			Average Q^2_{LNO}		0.629	

Table S13. Results of y-randomization test of TS2.

AB/Log*P*		**ACD/Log*P***		**ACLog*P***		**ALog*P***		**ALOG*P*s**	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.111	-0.247	0.206	-0.286	0.082	-0.278	0.166	-0.098	0.059	-0.417
0.176	-0.182	0.065	-0.327	0.146	-0.179	0.083	-0.198	0.023	-0.302
0.117	-0.164	0.028	-0.301	0.113	-0.167	0.135	-0.167	0.127	-0.161
0.142	-0.162	0.081	-0.280	0.099	-0.250	0.026	-0.387	0.113	-0.172
0.125	-0.432	0.154	-0.146	0.026	-0.439	0.085	-0.196	0.101	-0.221
0.112	-0.179	0.074	-0.332	0.246	0.022	0.151	-0.127	0.112	-0.221
0.054	-0.569	0.061	-0.290	0.012	-0.320	0.049	-0.377	0.064	-0.216
0.063	-0.529	0.157	-0.101	0.135	-0.194	0.054	-0.372	0.109	-0.241
0.242	-0.034	0.263	-0.046	0.064	-0.297	0.331	0.106	0.251	-0.001
0.079	-0.268	0.159	-0.138	0.145	-0.204	0.139	-0.114	0.106	-0.266

CLog*P*		**CSLog*P***		**KOWWIN**		**miLog*P***		**MLog*P***	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.108	-0.217	0.194	-0.199	0.045	-0.336	0.144	-0.215	0.053	-0.419
0.099	-0.256	0.088	-0.254	0.147	-0.236	0.085	-0.214	0.164	-0.119
0.111	-0.196	0.118	-0.192	0.086	-0.251	0.436	0.218	0.112	-0.324
0.220	-0.024	0.156	-0.176	0.079	-0.278	0.192	-0.103	0.032	-0.285
0.102	-0.198	0.298	-0.133	0.107	-0.202	0.105	-0.214	0.061	-0.227
0.128	-0.227	0.188	-0.139	0.175	-0.141	0.068	-0.310	0.180	-0.221
0.116	-0.230	0.105	-0.197	0.275	-0.023	0.045	-0.267	0.109	-0.178
0.097	-0.296	0.286	-0.172	0.250	0.021	0.054	-0.281	0.248	-0.024
0.139	-0.161	0.056	-0.459	0.030	-0.386	0.023	-0.317	0.151	-0.157
0.039	-0.344	0.121	-0.114	0.109	-0.359	0.287	0.036	0.223	-0.033

XLog*P*3		**COSMOfrag**		**molLog*P***		**ChemOffLog*P***		**XLog*P*2**	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.148	-0.140	0.178	-0.097	0.126	-0.209	0.090	-0.248	0.075	-0.207
0.050	-0.337	0.077	-0.233	0.113	-0.253	0.048	-0.309	0.016	-0.392
0.068	-0.332	0.218	-0.118	0.140	-0.137	0.090	-0.291	0.078	-0.315

0.138	-0.254	0.211	-0.115	0.230	-0.116	0.190	-0.185	0.133	-0.197
0.110	-0.223	0.089	-0.277	0.048	-0.308	0.046	-0.392	0.046	-0.315
0.155	-0.153	0.118	-0.197	0.075	-0.242	0.185	-0.121	0.282	-0.012
0.163	-0.215	0.074	-0.261	0.090	-0.224	0.109	-0.222	0.174	-0.112
0.160	-0.148	0.066	-0.249	0.099	-0.208	0.085	-0.372	0.108	-0.344
0.081	-0.268	0.041	-0.374	0.088	-0.216	0.225	-0.060	0.135	-0.121
0.105	-0.231	0.082	-0.196	0.036	-0.379	0.011	-0.456	0.095	-0.216

Table S14 Results of LNO cross-validation of TS2.

AB/Log*P*					**ACD/Log*P***					**CLog*P***				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.726	0.726	0.726	0.726	0.000	0.761	0.761	0.761	0.761	0.000	0.799	0.799	0.799	0.799	0.000
0.738	0.702	0.729	0.723	0.019	0.759	0.745	0.765	0.756	0.010	0.797	0.804	0.799	0.800	0.003
0.683	0.732	0.715	0.710	0.025	0.738	0.785	0.740	0.754	0.026	0.788	0.796	0.796	0.793	0.004
0.723	0.716	0.729	0.723	0.006	0.781	0.788	0.754	0.774	0.018	0.800	0.797	0.806	0.801	0.005
0.710	0.703	0.724	0.712	0.011	0.717	0.762	0.753	0.744	0.024	0.796	0.779	0.812	0.796	0.016
0.715	0.755	0.728	0.733	0.021	0.755	0.784	0.760	0.766	0.016	0.807	0.768	0.819	0.798	0.027
0.749	0.692	0.726	0.722	0.028	0.772	0.753	0.740	0.755	0.016	0.798	0.791	0.778	0.789	0.010
0.657	0.676	0.711	0.681	0.027	0.772	0.769	0.766	0.769	0.003	0.782	0.790	0.816	0.796	0.017
0.706	0.750	0.760	0.738	0.029	0.766	0.729	0.757	0.751	0.019	0.779	0.809	0.764	0.784	0.023
0.743	0.715	0.675	0.711	0.034	0.736	0.751	0.790	0.759	0.028	0.743	0.819	0.778	0.780	0.038
	Average Q^2_{LNO}		0.718			Average Q^2_{LNO}		0.759			Average Q^2_{LNO}		0.794	
CSLog*P*					**XLog*P*3**					**COSMOfrag**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.717	0.717	0.717	0.717	0.000	0.762	0.762	0.762	0.762	0.000	0.761	0.761	0.761	0.761	0.000
0.700	0.728	0.709	0.712	0.014	0.767	0.755	0.763	0.762	0.006	0.761	0.755	0.765	0.760	0.005
0.710	0.713	0.712	0.712	0.002	0.748	0.760	0.753	0.754	0.006	0.735	0.747	0.761	0.748	0.013
0.682	0.708	0.727	0.706	0.022	0.769	0.754	0.754	0.759	0.009	0.772	0.730	0.730	0.744	0.025
0.739	0.741	0.724	0.735	0.010	0.785	0.759	0.745	0.763	0.020	0.758	0.755	0.778	0.764	0.013
0.732	0.706	0.717	0.718	0.013	0.775	0.755	0.776	0.769	0.012	0.754	0.766	0.753	0.758	0.007
0.717	0.697	0.700	0.705	0.011	0.749	0.757	0.766	0.757	0.008	0.791	0.757	0.768	0.772	0.017
0.727	0.718	0.664	0.703	0.034	0.756	0.720	0.760	0.745	0.022	0.771	0.771	0.686	0.743	0.050
0.632	0.675	0.679	0.662	0.026	0.743	0.729	0.773	0.748	0.022	0.747	0.715	0.775	0.746	0.030
0.713	0.688	0.687	0.696	0.015	0.786	0.756	0.743	0.762	0.022	0.729	0.731	0.714	0.725	0.009
	Average Q^2_{LNO}		0.707			Average Q^2_{LNO}		0.758			Average Q^2_{LNO}		0.752	
ACLog*P*					**ALog*P***					**KOWWIN**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.758	0.758	0.758	0.758	0.000	0.748	0.748	0.748	0.748	0.000	0.778	0.778	0.778	0.778	0.000
0.763	0.755	0.744	0.754	0.010	0.754	0.740	0.728	0.741	0.013	0.776	0.782	0.778	0.779	0.003
0.757	0.765	0.777	0.766	0.010	0.760	0.745	0.749	0.751	0.008	0.774	0.780	0.774	0.776	0.003
0.749	0.767	0.760	0.759	0.009	0.750	0.757	0.717	0.742	0.022	0.782	0.757	0.750	0.763	0.017

0.758	0.756	0.771	0.762	0.008	0.754	0.730	0.749	0.744	0.013	0.768	0.779	0.760	0.769	0.010
0.740	0.765	0.725	0.743	0.020	0.766	0.754	0.707	0.742	0.031	0.750	0.761	0.789	0.767	0.020
0.758	0.771	0.771	0.767	0.008	0.741	0.775	0.705	0.740	0.035	0.781	0.787	0.728	0.765	0.033
0.754	0.664	0.755	0.724	0.052	0.732	0.754	0.751	0.746	0.012	0.766	0.713	0.774	0.751	0.033
0.754	0.740	0.737	0.743	0.009	0.679	0.723	0.762	0.721	0.042	0.786	0.753	0.786	0.775	0.019
0.729	0.761	0.778	0.756	0.024	0.744	0.758	0.771	0.758	0.014	0.747	0.807	0.771	0.775	0.030
	Average Q^2_{LNO}		0.753			Average Q^2_{LNO}		0.743			Average Q^2_{LNO}		0.770	
miLog*P*					**ALOG*P*s**					**ChemOffLog*P***				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.765	0.765	0.765	0.765	0.000	0.723	0.723	0.723	0.723	0.000	0.738	0.738	0.738	0.738	0.000
0.773	0.761	0.755	0.763	0.009	0.719	0.731	0.715	0.722	0.009	0.742	0.744	0.740	0.742	0.002
0.752	0.757	0.769	0.759	0.008	0.721	0.729	0.723	0.724	0.004	0.713	0.705	0.704	0.707	0.005
0.760	0.775	0.747	0.761	0.014	0.726	0.723	0.728	0.726	0.002	0.736	0.738	0.724	0.733	0.008
0.754	0.752	0.773	0.759	0.012	0.749	0.688	0.725	0.721	0.031	0.713	0.728	0.724	0.722	0.008
0.742	0.762	0.775	0.760	0.017	0.722	0.735	0.723	0.727	0.007	0.679	0.637	0.738	0.685	0.051
0.779	0.764	0.778	0.774	0.008	0.740	0.723	0.739	0.734	0.010	0.755	0.731	0.730	0.739	0.014
0.764	0.753	0.764	0.761	0.007	0.676	0.742	0.745	0.721	0.039	0.737	0.709	0.757	0.734	0.024
0.774	0.759	0.757	0.763	0.009	0.729	0.745	0.741	0.738	0.008	0.753	0.702	0.730	0.728	0.026
0.740	0.774	0.714	0.743	0.030	0.709	0.737	0.693	0.713	0.022	0.688	0.703	0.715	0.702	0.013
	Average Q^2_{LNO}		0.761			Average Q^2_{LNO}		0.725			Average Q^2_{LNO}		0.723	
MLog*P*					**molLog*P***					**XLog*P*2**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.738	0.738	0.738	0.738	0.000	0.783	0.783	0.783	0.783	0.000	0.741	0.741	0.741	0.741	0.000
0.742	0.741	0.746	0.743	0.003	0.787	0.773	0.780	0.780	0.007	0.736	0.745	0.749	0.743	0.006
0.755	0.723	0.752	0.744	0.018	0.784	0.780	0.783	0.782	0.002	0.757	0.752	0.749	0.753	0.004
0.754	0.769	0.728	0.750	0.021	0.789	0.775	0.762	0.776	0.014	0.738	0.744	0.717	0.733	0.014
0.700	0.686	0.772	0.719	0.046	0.766	0.779	0.801	0.782	0.018	0.753	0.741	0.750	0.748	0.006
0.750	0.703	0.744	0.733	0.026	0.788	0.779	0.781	0.783	0.005	0.731	0.737	0.723	0.730	0.007
0.742	0.735	0.699	0.725	0.023	0.792	0.802	0.797	0.797	0.005	0.703	0.716	0.753	0.724	0.026
0.725	0.748	0.746	0.740	0.013	0.778	0.797	0.780	0.785	0.010	0.733	0.734	0.770	0.746	0.021
0.762	0.697	0.744	0.734	0.034	0.802	0.762	0.699	0.754	0.052	0.754	0.735	0.741	0.743	0.010
0.754	0.727	0.785	0.755	0.029	0.766	0.779	0.790	0.778	0.012	0.776	0.729	0.758	0.755	0.024
	Average Q^2_{LNO}		0.738			Average Q^2_{LNO}		0.780			Average Q^2_{LNO}		0.742	

Table S15. Values for another selected descriptors for TS3 (including outliers)

	LUMO	X0sol	SeaC2C2aa
4	-0.062	16.587	12.465
8	-0.06	16.587	14.306
9	-0.062	17.294	10.451
10	-0.071	15.88	10.451
11	-0.072	18.449	7.604
12	-0.061	20.027	3.940
13	-0.062	20.027	5.626
14	-0.062	19.319	8.111
15	-0.061	17.742	5.781
16	-0.061	17.742	3.972
17	-0.068	16.587	10.300
18	-0.076	15.880	10.301
19	-0.074	15.880	10.149
20	-0.063	16.234	9.817
21	-0.059	16.234	7.868
22	-0.066	16.234	7.866
23	-0.063	18.803	10.123
24	-0.065	18.803	8.095
25	-0.059	18.449	8.143
26	-0.056	18.165	7.896
27	-0.061	18.165	9.366
28	-0.061	18.165	7.532
29	-0.061	17.458	7.441

30	-0.061	17.458	5.911
31	-0.061	17.458	18.471
32	-0.061	17.958	16.427
33	-0.062	16.587	16.505
34	-0.062	16.587	12.465
35	-0.066	16.587	14.306
36	-0.06	19.328	10.451
37	-0.065	20.571	10.451
38	-0.064	20.571	7.604
39	-0.007	20.571	3.940

Table S16. Obtained models for TS3.

	LV1(%)[a]	LV2(%)[a]	LUMO	X0sol	SeaC2C2aa	Log P	Independent term
AB/Log*P*	47.964	16.973	0.255	116.145	0.082	0.005	11.512
ACD/Log*P*	35.414	19.891	-0.085	152.432	0.183	0.033	13.176
ACLog*P*	39.165	17.151	-0.042	153.631	0.163	0.021	13.583
ALog*P*	36.125	19.030	-0.027	149.833	0.169	0.024	13.144
ALOG*P*s	38.626	18.404	-0.068	155.677	0.163	0.023	13.762
ChemOffLog*P*	37.511	17.375	-0.180	162.071	0.185	0.026	14.281
CLog*P*	33.807	17.558	-0.244	165.643	0.195	0.035	14.863
COSMOFrag	51.737	23.791	0.249	111.924	0.043	0.030	11.959
CSLog*P*	35.836	34.027	0.033	147.031	0.157	0.031	12.948
IALog*P*	39.214	31.107	0.064	144.655	0.139	0.036	12.954
KOWWIN	37.511	17.375	-0.180	162.071	0.185	0.026	14.281
miLog*P*	39.153	16.868	0.002	149.341	0.161	0.016	13.242
MLog*P*	38.381	24.917	-0.0005	151.987	0.148	0.025	13.564
molLog*P*	39.888	18.764	-0.056	157.771	0.154	0.022	14.025

XLog*P*2	46.480	16.644	0.128	137.023	0.096	0.008	13.356
XLog*P*3	51.383	25.738	0.297	122.707	0.039	0.036	12.598

[(a)] information available in the latent variable

Table S17. Results of y-randomization test of TS3.

AB/Log*P*		**ACD/Log*P***		**ACLog*P***		**ALog*P***		**ALOG*P*s**	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.096	-0.572	0.454	0.133	0.296	-0.381	0.300	-0.298	0.353	-0.101
0.105	-0.238	0.220	-0.285	0.102	-0.429	0.192	-0.316	0.735	0.560
0.084	-0.460	0.136	-0.527	0.302	-0.023	0.257	-0.353	0.236	-0.256
0.121	-0.217	0.188	-0.414	0.020	-0.471	0.048	-0.542	0.218	-0.396
0.062	-0.733	0.254	-0.301	0.181	-0.285	0.214	-0.583	0.151	-0.261
0.104	-0.322	0.151	-0.260	0.261	-0.223	0.236	-0.243	0.111	-0.821
0.151	-0.554	0.011	-0.367	0.330	-0.058	0.309	0.041	0.069	-0.470
0.341	-0.211	0.222	-0.405	0.126	-0.876	0.098	-0.554	0.257	-0.482
0.204	-0.360	0.210	-0.650	0.428	-0.010	0.141	-0.991	0.222	-0.226
0.178	-0.233	0.226	-0.438	0.080	-0.764	0.228	-0.515	0.136	-0.436

CLog*P*		**CSLog*P***		**KOWWIN**		**miLog*P***		**MLog*P***	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.442	0.107	0.082	-0.583	0.124	-0.391	0.167	-0.730	0.350	-0.226
0.425	-0.168	0.126	-0.716	0.060	-0.575	0.042	-0.441	0.449	0.060
0.067	-0.417	0.238	-0.880	0.085	-0.586	0.238	-0.441	0.037	-0.433
0.218	-0.247	0.137	-0.484	0.078	-0.332	0.108	-0.446	0.132	-0.591
0.045	-0.518	0.013	-0.388	0.296	-0.697	0.074	-0.739	0.122	-0.584
0.268	-0.269	0.288	-0.499	0.338	-0.097	0.138	-0.400	0.202	-0.277
0.151	-0.282	0.324	-0.067	0.264	-0.464	0.246	-0.239	0.253	-0.351
0.290	-0.238	0.219	-0.205	0.431	0.023	0.152	-0.531	0.241	-0.522
0.208	-0.314	0.067	-0.788	0.452	-0.315	0.228	-0.190	0.024	-0.410
0.206	-0.387	0.143	-0.373	0.111	-0.273	0.485	0.122	0.130	-0.515

XLog*P*3		**COSMOfrag**		**molLog*P***		**ChemOffLog*P***		**XLog*P*2**	
R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2	R^2	Q^2
0.050	-0.371	0.025	-0.638	0.323	-0.100	0.307	-0.174	0.035	-0.403
0.036	-0.397	0.073	-0.284	0.193	-0.505	0.156	-0.228	0.075	-0.343
0.225	-0.349	0.017	-0.435	0.275	-0.178	0.189	-0.743	0.081	-0.564
0.049	-0.615	0.047	-0.722	0.125	-0.228	0.146	-0.366	0.037	-0.312
0.258	-0.016	0.234	-0.123	0.177	-0.303	0.170	-0.372	0.374	-0.153

0.244	-0.277	0.293	-0.143	0.027	-0.316	0.353	-0.222	0.046	-0.590
0.137	-0.308	0.114	-0.372	0.095	-0.232	0.140	-0.323	0.329	-0.125
0.033	-0.440	0.057	-0.264	0.160	-0.166	0.205	-0.149	0.032	-0.505
0.181	-0.548	0.266	-0.342	0.064	-0.688	0.190	-0.314	0.209	-0.554
0.110	-0.662	0.050	-0.496	0.114	-0.182	0.345	-0.346	0.385	0.067

Table S18. Results of LNO cross-validation of TS3.

AB/Log*P*					**ACD/Log*P***					**CLog*P***				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.424	0.424	0.424	0.424	0.000	0.397	0.397	0.397	0.397	0.000	0.473	0.473	0.473	0.473	0.000
0.468	0.372	0.308	0.383	0.081	0.369	0.437	0.380	0.395	0.036	0.465	0.495	0.085	0.348	0.228
0.394	0.399	0.464	0.419	0.039	0.400	0.415	0.412	0.409	0.008	0.530	0.477	0.434	0.481	0.048
0.549	0.270	0.460	0.426	0.142	0.321	0.402	0.392	0.372	0.044	0.415	0.484	0.386	0.428	0.051
0.400	0.419	0.399	0.406	0.011	0.490	0.460	-0.278	0.224	0.435	0.488	0.373	0.548	0.470	0.089
0.424	0.522	0.347	0.431	0.088	0.472	0.366	0.314	0.384	0.080	0.210	0.305	0.581	0.365	0.193
	Average Q^2_{LNO}		0.415			Average Q^2_{LNO}		0.363			Average Q^2_{LNO}		0.427	
CSLog*P*					**XLog*P*3**					**COSMOfrag**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.444	0.444	0.444	0.444	0.000	0.500	0.500	0.500	0.500	0.000	0.516	0.516	0.516	0.516	0.000
0.435	0.390	0.441	0.422	0.028	0.487	0.467	0.503	0.486	0.018	0.560	0.479	0.513	0.517	0.041
0.495	0.345	0.410	0.416	0.075	0.424	0.439	0.544	0.469	0.065	0.450	0.460	0.528	0.479	0.042
0.506	0.414	0.416	0.445	0.052	0.445	0.507	0.498	0.483	0.034	0.548	0.501	0.561	0.536	0.032
0.466	0.518	0.336	0.440	0.094	0.489	0.516	0.465	0.490	0.026	0.549	0.463	0.546	0.519	0.048
0.498	0.217	0.166	0.293	0.179	0.531	0.564	0.489	0.528	0.038	0.501	0.513	0.480	0.498	0.016
	Average Q^2_{LNO}		0.410			Average Q^2_{LNO}		0.493			Average Q^2_{LNO}		0.511	
ACLog*P*					**ALog*P***					**KOWWIN**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.369	0.369	0.369	0.369	0.000	0.372	0.372	0.372	0.372	0.000	0.413	0.413	0.413	0.413	0.000
0.331	0.379	0.357	0.356	0.024	0.378	0.404	0.322	0.368	0.042	0.350	0.477	0.435	0.421	0.065
0.407	0.241	0.387	0.345	0.091	0.410	0.413	0.111	0.311	0.173	0.377	0.383	0.489	0.416	0.063
0.323	-0.061	0.372	0.211	0.237	0.405	0.410	0.463	0.426	0.032	0.403	0.316	0.460	0.393	0.073
0.258	0.147	0.394	0.266	0.124	0.400	0.194	0.441	0.345	0.133	0.498	0.084	0.476	0.353	0.233
0.488	0.444	0.297	0.410	0.100	0.516	0.405	0.386	0.436	0.070	-2.087	0.398	0.362	-0.442	1.425
	Average Q^2_{LNO}		0.326			Average Q^2_{LNO}		0.376			Average Q^2_{LNO}		0.259	
miLog*P*					**ALOG*P*s**					**ChemOffLog*P***				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.353	0.353	0.353	0.353	0.000	0.378	0.378	0.378	0.378	0.000	0.413	0.413	0.413	0.413	0.000
0.349	0.383	0.358	0.364	0.018	0.352	0.468	0.328	0.383	0.075	0.411	0.431	0.392	0.411	0.019
0.305	0.329	0.167	0.267	0.087	0.380	0.397	0.245	0.341	0.083	0.382	0.354	0.268	0.335	0.059
0.023	0.323	-2.164	-0.606	1.358	-0.224	0.356	0.284	0.139	0.316	0.455	0.361	0.433	0.416	0.049

0.496	0.377	-0.191	0.227	0.368	-0.116	0.378	0.376	0.213	0.284	0.536	0.473	0.355	0.455	0.092
0.230	0.447	0.302	0.326	0.111	0.295	0.133	0.388	0.272	0.129	0.333	0.391	0.369	0.364	0.029
	Average Q^2_{LNO}		0.155			Average Q^2_{LNO}		0.288			Average Q^2_{LNO}		0.399	
MLog*P*					**molLog*P***					**XLog*P*2**				
$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD	$Q^2$1	$Q^2$2	$Q^2$3	Average	SD
0.410	0.410	0.410	0.410	0.000	0.378	0.378	0.378	0.378	0.000	0.367	0.367	0.367	0.367	0.000
0.390	0.333	0.414	0.379	0.042	0.318	0.416	0.380	0.371	0.049	0.367	0.383	0.375	0.375	0.008
0.320	0.397	-0.145	0.191	0.293	0.339	0.412	0.252	0.334	0.080	0.342	0.046	-0.079	0.103	0.216
0.451	0.344	0.012	0.269	0.229	0.211	0.321	0.418	0.317	0.103	0.414	0.327	0.329	0.357	0.050
0.200	-0.134	0.432	0.166	0.284	0.452	0.397	0.311	0.386	0.071	0.023	0.513	0.297	0.278	0.246
0.498	0.135	-0.238	0.132	0.368	0.313	0.267	0.177	0.252	0.069	0.388	0.378	-0.056	0.237	0.254
	Average Q^2_{LNO}		0.258			Average Q^2_{LNO}		0.340			Average Q^2_{LNO}		0.286	