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Supplementary Information

QSPR Modeling Using Catalan Solvent and Solute Parameters

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Table S1. List of parameters used in this study

Parameter	Definition	Parameter	Definition
A	Abraham' hydrogen bonding acidity parameter for the solute	SPP	Catalan polarity/polarizability parameter for the solvent
B	Abraham' hydrogen bonding basicity parameter for the solute	SP (cp)	Catalan polarizability parameter for the solvent
S	Abraham' polarity/polarizability parameter for the solute	SdP (cd)	Catalan dipolarity parameter for the solvent
E	Excess molar refraction of the solute	SB (cb)	Catalan basicity parameter for the solvent
V	One percent of McGowan volume of the solute	SA (ca)	Catalan acidity parameter for the solvent
c	Abraham' constant value for the solvent	i_{Solute}	Catalan constant value for the solute*
a	Abraham' interaction term of the solvent with acidity of the solute (solvent basicity)	CP	Catalan polarizability parameter for the solute*
b	Abraham' interaction term of the solvent with basicity of the solute (solvent acidity)	CD	Catalan dipolarity parameter for the solute*
s	Abraham' interaction term of the solvent with polarity/polarizability of the solute	CB	Catalan basicity parameter for the solute*
e	Abraham' interaction term of the solvent with molar refraction of the solute	CA	Catalan acidity parameter for the solute*
v	Abraham' interaction term of the solvent with molar volume of the solute	i_W	Intercept of the aqueous solubility prediction equation*

*These parameters were resulted from this study.

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Table S2. Abraham solvent parameters (c, e, s, a, b, and v) for available solvents and their related Catalan solvent parameters (cp, cd, cb, and ca)

No.	Solvent	c	e	s	a	b	v	cp	cd	ca	cb
1	1,2-Dichloroethane	0.227	0.278	–0.167	–2.816	–4.324	4.205	0.771	0.742	0.030	0.126
2	1,4-Dioxane	0.098	0.350	–0.083	–0.556	–4.826	4.172	0.737	0.312	0.000	0.444
3	Butan-1-ol	0.152	0.437	–1.175	0.098	–3.914	4.119	0.674	0.655	0.341	0.809
4	Decan-1-ol	–0.062	0.754	–1.461	0.063	–4.053	4.293	0.722	0.383	0.259	0.912
5	Heptan-1-ol	–0.026	0.491	–1.258	0.035	–4.155	4.415	0.706	0.499	0.302	0.912
6	Hexan-1-ol	0.044	0.470	–1.153	0.083	–4.057	4.249	0.698	0.552	0.315	0.879
7	Octan-1-ol	–0.034	0.490	–1.048	–0.028	–4.229	4.219	0.713	0.454	0.299	0.923
8	Pentan-1-ol	0.080	0.521	–1.294	0.208	–3.908	4.208	0.687	0.587	0.319	0.860
9	Propan-1-ol	0.148	0.436	–1.098	0.389	–3.893	4.036	0.658	0.748	0.367	0.782
10	Butan-2-ol	0.106	0.272	–0.988	0.196	–3.805	4.110	0.656	0.706	0.221	0.888
11	2-Methyl propan-1-ol	0.177	0.335	–1.099	0.069	–3.570	3.990	0.657	0.684	0.311	0.828
12	2-Methyl propan-2-ol	0.197	0.136	–0.916	0.318	–4.031	4.113	0.632	0.732	0.145	0.928
13	Propan-2-ol	0.063	0.320	–1.024	0.445	–3.824	4.067	0.633	0.808	0.283	0.830
14	Propan-2-one	0.335	0.349	–0.231	–0.411	–4.793	3.963	0.651	0.907	0.000	0.475
15	Acetonitrile	0.413	0.077	0.326	–1.566	–4.391	3.364	0.645	0.974	0.044	0.286
16	Benzene	0.142	0.464	–0.588	–3.099	–4.625	4.491	0.793	0.270	0.000	0.124
17	Carbon disulfide	0.047	0.686	–0.943	–3.603	–5.818	4.921	1.000	0.000	0.000	0.104
18	Carbone tetrachloride	0.260	0.573	–1.254	–3.558	–4.558	4.589	0.768	0.000	0.000	0.044
19	Chlorobenzene	0.040	0.246	–0.462	–3.038	–4.769	4.640	0.833	0.537	0.000	0.182
20	Chloroform	0.327	0.157	–0.391	–3.191	–3.437	4.191	0.783	0.614	0.047	0.071
21	Cyclohexane	0.159	0.784	–1.678	–3.740	–4.929	4.577	0.683	0.000	0.000	0.073
22	Dibutyl ether	0.203	0.369	–0.954	–1.488	–5.426	4.508	0.672	0.175	0.000	0.637
23	Dichloromethane	0.314	0.001	0.022	–3.238	–4.137	4.259	0.761	0.769	0.040	0.178
24	Diethyl ether	0.308	0.377	–0.813	–0.468	–5.012	4.379	0.617	0.385	0.000	0.562
25	Dimethylformamide	–0.438	–0.099	0.670	0.878	–4.970	4.552	0.759	0.977	0.031	0.613
26	Dodecane	0.114	0.668	–1.644	–3.545	–5.006	4.459	0.683	0.000	0.000	0.086
27	Ethanol	0.208	0.409	–0.959	0.186	–3.645	3.928	0.633	0.783	0.400	0.658
28	Ethyl acetate	0.358	0.362	–0.449	–0.668	–5.016	4.155	0.656	0.603	0.000	0.542
29	Ethylene glycol	0.243	0.695	–0.670	0.726	–2.399	2.670	0.777	0.910	0.717	0.534
30	Heptane	0.325	0.670	–2.061	–3.317	–4.733	4.543	0.635	0.000	0.000	0.083
31	Hexadecane	0.087	0.667	–1.617	–3.587	–4.869	4.433	0.704	0.000	0.000	0.086
32	Hexane	0.361	0.579	–1.723	–3.599	–4.764	4.344	0.616	0.000	0.000	0.056
33	Isooctane	0.288	0.382	–1.668	–3.639	–5.000	4.461	0.618	0.000	0.000	0.044
34	Methanol	0.329	0.299	–0.671	0.080	–3.389	3.512	0.608	0.904	0.605	0.545
35	Methylcyclohexane	0.246	0.782	–1.982	–3.517	–4.293	4.528	0.675	0.000	0.000	0.069
36	Methy-*tert*-butyl ether	0.376	0.264	–0.788	–1.078	–5.030	4.410	0.622	0.422	0.000	0.567
37	Nonane	0.240	0.619	–1.713	–3.532	–4.921	4.482	0.660	0.000	0.000	0.053
38	Octane	0.223	0.642	–1.647	–3.480	–5.067	4.526	0.650	0.000	0.000	0.079
39	Tetrahydrofuran	0.207	0.372	–0.392	–0.236	–4.934	4.447	0.714	0.634	0.000	0.591
40	Toluene	0.143	0.527	–0.720	–3.010	–4.824	4.545	0.782	0.284	0.000	0.128
41	Undecane	0.058	0.603	–1.661	–3.421	–5.120	4.619	0.678	0.000	0.000	0.080

Table S3. Melting point (mp), boiling point (bp), flash point (fp), refractive index (*n*), surface tension (γ), viscosity (η), density (ρ), and solubility parameter (SP) data of 54 common solvents[a]

No.	Solvent	mp (K)	bp (K)	fp (K)	*n*	γ (dyn cm^{-1})	η (cP)	ρ (g cm^{-3})	SP
1	1,1,1-Tricloroethane	243	347		1.438	30	0.65	1.338	7.7
2	1,2-Dichloroethane	237	356.5	286	1.444	32.2	0.9	1.253	9.8
3	1,2-Propanediol	213	460	372	1.431	72	54	1.0362	
4	1,4-Dioxane	285	374	285	1.42	40	1.3	1.034	10
5	2,2,4-Trimethyl pentane	166	372	261	1.389	18.33	0.477	0.692	7.4
6	Acetic Acid	290	391	313	1.37	27.4	1.13	1.051	10.1
7	Acetone	178	329	255	1.357	23.3	0.33	0.79	10
8	Acetonitrile	229	354.6	279	1.342	29.1	0.38	0.782	11.9
9	Acetophenone	292.6	475	355	1.532	12	1.74	1.024	
10	Aniline	267	457	349	1.583	45.5	4.4	1.022	10.3
11	Benzene	278.5	353	262	1.498	28.9	0.65	0.879	9.2
12	Carbon disulphide	162	319	243	1.628	32	0.36	1.26	10
13	Carbon tetrachloride	250	349		1.459	27	0.97	1.58	8.6
14	Chloroform	250	334		1.444	27.16	0.57	1.48	9.3
15	Cyclohexane	279.5	354	256	1.424	24.98	0.98	0.778	8.2
16	Cyclohexanone	241	429	316	1.448	34.5	2.2	0.948	9.9
17	Dibutyl ether	178	415	298	1.397	22.4[a]	0.63	0.769	7.2
18	Diethyl ether	157	307.5	228	1.352	17	0.24	0.715	7.4
19	Diisopropyl ether	187	341	245	1.367	18	0.33	0.724	6.9
20	Dimethylacetamide	253	439	343	1.436	34	0.92	0.945	11
21	Dimethylformamide	212	426	335	1.427	35	0.82	0.945	12.1
22	Dimethylsulphoxide	291.5	462	368	1.476	43.7	2	1.101	13
23	Ethanediol	260	471	384	1.429	46.5	20	1.115	14.6
24	Ethanol	159	351	286	1.359	22.3	1.08	0.789	13.4
25	Ethyl acetate	189	350	269	1.37	24	0.46	0.895	9.1
26	Ethylbenzene	179	409	288	1.493	29.2	0.72	0.867	8.9
27	*i*-Butanol	165	381	298	1.394	22.8	3.96	0.802	10.7
28	*i*-Propanol	185	355	285	1.375	21.7	2	0.786	11.5
29	Methanol	175	337	288	1.326	22.6	0.6	0.792	14.5
30	Methyl acetate	175	330	263	1.36	24	0.37	0.927	9.6
31	Methyl ethyl ketone	186	353	267	1.377	24.6	0.41	0.805	9.3
32	Methy-*tert*-butyl ether	164	328	239	1.369	18.3	0.35	0.741	7.4
33	Methylene chloride	178	313		1.4211	28.1	0.44	1.326	9.7
34	Monochlorobenzene	227	405	302	1.523	33	0.8	1.106	9.5
35	*n*-Amyl alcohol	195	411	321	1.408	25.6	4	0.815	
36	*n*-Butanol	193	391	308	1.397	24.6	3	0.81	11.4
37	*n*-Butyl acetate	200	399	295	1.392	25.1	0.73	0.876	8.6
38	*n*-Decane	243	447	317	1.408			0.73	6.7
39	*n*-Heptane	182	371	269	1.385	19.3	0.41	0.664	7.5
40	*n*-Hexane	178	342	251	1.372	18.4	0.31	0.659	6.9
41	Nitrobenzene	279	484	361	1.55	43.9	1.8	1.204	10
42	*n*-Methyl-2-pyrrolidone	249	475	368	1.468	40.7	1.8	1.03	11
43	*n*-Nonane	220	424	304	1.403	22.9	0.67	0.718	
44	*n*-Octane	216	399	286.3	1.395	21.7	0.5	0.703	
45	*n*-Octanol	257	467	354	1.427	27.5	7.5	0.827	10.4
46	*n*-Pentane	144	309	233	1.358	16	0.235	0.626	7
47	*n*-Propanol	146	370	298	1.383	23.7	1.72	0.804	11.9
48	Pyridine	231	388	293	1.507	36.6	0.88	0.983	10.7
49	2-Butanol	158	372.5	294	1.395	23	3.7	0.807	10.8
50	Sulfolane	300.4	558	450	1.471	35.5	10.3	1.26	
51	Tetrahydrofuran	164	339	258	1.404	28	0.55	0.888	9.1
52	Toluene	178	383.6	277	1.494	28.5	0.59	0.867	8.9
53	Water	273	373		1.332	72.75	0.89	0.998	23.4
54	Xylenes (mixed isomers)		409	296	1.496	28.6	0.7	0.87	8.9

[a] http://www.springerlink.com/content/r364t1631p53p436/, accessed in September 2009.