Supporting Information

On the Solubility of Ferrocene in Non-Aqueous Solvents

Saeed Yousefinejad [*a], Fatemeh Honarasa [b], Aida Solhjoo [c]

[a] School of Health, Shiraz University of Medical Science, Shiraz, Iran
[b] Department of Chemistry, Shiraz Branch, Islamic Azad University, Shiraz, Iran
[c] Department of Chemistry, Yasouj University, Yasouj, Iran

* Corresponding author, Tel.: +98 917 704 2635

E-mail address: yousefinejad.s@gmail.com (S. Yousefinejad)

Table S1. The MLR-coefficient of model #1 and their t- and p-values.

	Unstandardized Coefficients	Standardized Coefficients	t-value	p-value
Intercept	5.812 (±0.407)	---	14.292	0.000
Mv	5.897(±0.378)	0.935(±0.060)	15.612	0.000
MATS4v	-0.214(±0.059)	-0.160(±0.044)	-3.630	0.001
MATS1e	2.502(±0.303)	0.634(±0.077)	8.247	0.000
BEHm1	-0.875(±0.136)	-0.606(±0.094)	-6.411	0.000

Table S2 Various statistical parameter of the developed solvent's structure-ferrocene solubility QSPR model (model 1) using three random-selected training-test sets with different composition from which are shown in Table 1 (main manuscript)

	R^2_{train} [a]	$RMSE_{train}$ [b]	R^2_{LOO} [c]	R^2_{L3O} [c]	$RMSE_{LOO}$ [d]	R^2_{test} [e]	$RMSE_{test}$ [f]	Q^2_{MP} [g]
Train-Test 2 †	0.96	0.20	0.94	0.95	0.24	0.97	0.16	0.11
Train- Test 3 ‡	0.96	0.21	0.94	0.93	0.25	0.92	0.30	0.09
Train- Test 4 §	0.96	0.19	0.95	0.94	0.22	0.89	0.33	0.08

[a] Squared correlation coefficient of training
[b] Root mean square error of training
[c] Squared correlation coefficients of Leave-one-out and leave-3-out cross-validation
[d] Root-mean-square error of leave-one-out cross-validation
[e] Squared correlation coefficient of the test set
[f] Root mean square error of test set
[g] Maximum cross-validation correlation coefficient for Y-randomization test

† Number of test solvents : Comps 5, 10, 17, 21, 22, 25, 27
‡ Number of test solvents: Comps 7, 8, 13, 16, 17, 30, 31
§ Number of test solvents: Comps 3, 6, 11, 16, 22, 32, 34

Table S3. Numerical values of structural descriptors involved in model #1

No.	solvent name	Mv	MATS4v	MATS1e	BEHm1
S 1	hexane	0.51	-0.021	-0.123	3.457
S 2 [a]	octane	0.51	-0.01	-0.09	3.51
S 3	nonane	0.52	-0.008	-0.079	3.526
S 4	decane	0.52	-0.006	-0.071	3.54
S 5	cyclohexane	0.53	0	0	3.592
S 6 [a]	methylcyclohexane	0.53	-0.056	0	3.639
S 7	2,2,4-trimethylpentane	0.51	0.276	-0.09	3.613
S 8	1,2-dichloroethane	0.66	0	-0.012	3.784
S 9	benzene	0.65	0	0	3.702
S 10	toluene	0.63	-0.129	0	3.746
S 11 [a]	m-xylene	0.61	-0.063	0	3.783
S 12	p-xylene	0.61	-0.175	0	3.782
S 13	ethylbenzene	0.61	-0.295	0	3.761
S 14	methanol	0.45	0	-0.247	2.909
S 15	ethanol	0.48	0.393	-0.161	3.175
S 16	1-propanol	0.49	0.176	-0.126	3.311
S 17	2-propanol	0.49	0.417	-0.126	3.342
S 18	1-butanol	0.5	-0.059	-0.107	3.391
S 19 [a]	2-butanol	0.5	-0.064	-0.107	3.423
S 20	2-methyl-1-propanol	0.5	0.24	-0.107	3.432
S 21	2-methyl-2-butanol	0.51	-0.022	-0.095	3.527
S 22 [a]	3-methyl-1-butanol	0.51	-0.014	-0.095	3.481
S 23	1-pentanol	0.51	-0.032	-0.095	3.442
S 24	4-methyl-2-pentanol	0.51	0.12	-0.087	3.531
S 25	1-hexanol	0.51	-0.02	-0.087	3.477
S 26	2-ethyl-1-hexanol	0.51	-0.103	-0.076	3.573
S 27 [a]	1-heptanol	0.51	-0.014	-0.081	3.502
S 28	1-octanol	0.51	-0.01	-0.076	3.52
S 29	dibutyl ether	0.51	-0.012	0.054	3.489
S 30	methyl t-buthyl ether	0.51	-0.158	0.045	3.514
S 31	methyl acetate	0.53	-0.793	-0.051	3.396
S 32 [a]	ethyl acetate	0.53	-0.576	-0.024	3.438
S 33	butyl acetate	0.53	-0.111	0.001	3.492
S 34	dimethyl sulfoxide	0.54	0.539	0.202	4.197
S35	acetonitrile	0.60	0	0	3.246

[a] Compounds in the test set of model #1

Table S4. MLR-coefficients of model #2 and their t- and p-values.

	Unstandardized Coefficients	Standardized Coefficients	t-value	p-value
Intercept	8.609(±0.574)	---	14.997	0.000
SVB	2.945(±0.251)	0.681(±0.058)	14.752	0.000
ΔH^0_{BF3}	-0.005(±0.001)	-0.417(±0.061)	-6.891	0.000
$\log\gamma K_c$	-0.280(±0.058)	-0.257(±0.053)	-4.817	0.000

Table S5 Various statistical parameter of the developed solvent's structure-ferrocene solubility LSER model (model 2) using two random-selected training-test sets with different composition from which are shown in Table 1 (main manuscript)

	R^2_{train} [a]	$RMSE_{train}$ [b]	R^2_{LOO} [c]	R^2_{L4O} [c]	$RMSE_{LOO}$ [d]	R^2_{test} [e]	$RMSE_{test}$ [f]	Q^2_{MP} [g]
Train-Test 2 †	0.95	0.22	0.93	0.93	0.26	0.89	0.46	0.11
Train- Test 3 ‡	0.95	0.22	0.92	0.92	0.28	0.95	0.23	0.14

[a] Squared correlation coefficient of training

[b] Root mean square error of training

[c] Squared correlation coefficients of Leave-one-out and leave-4-out cross-validation

[d] Root-mean-square error of leave-one-out cross-validation

[e] Squared correlation coefficient of the test set

[f] Root mean square error of test set

[g] Maximum cross-validation correlation coefficient for Y-randomization test

† Number of test solvents : Comps 6,14,19,25,29,30

‡ Number of test solvents: Comps 6,8,9,14,29,30

Table S6. Numerical values of solvent empirical parameters involved in model #2 (LSER)

	solvent name	*SVB*	ΔH^0_{BF3}	*logKc*
S 1	hexane	0.074	116.104	9.22981
S 2	octane	0.042339	116.101	9.08936
S 3	nonane	0.068	116.234	9.02134
S 4	decane	0.017266	116.1	8.95353
S 5 [b]	cyclohexane	0.06026	115.386	8.95
S 6	methylcyclohexane	0.041621	115.652	8.89771
S 7	2,2,4-trimethylpentane	-0.022	115.706	8.73264
S 8	1,2-dichloroethane	0.155	14.5266	9.73351
S 9	benzene	0.230255	107.227	9.1
S 10 [b]	toluene	0.228061	111.351	9.03826
S 11	m-xylene	0.217855	111.271	8.94932
S 12 [b]	p-xylene	0.223667	110.888	8.95532
S 13	ethylbenzene	0.223292	111.973	8.98723
S 14	methanol	0	124.739	9.82
S 15	ethanol	0.017	125.122	9.64
S 16	1-propanol	0.014	123.936	9.48032
S 17	2-propanol	-0.017	134.333	9.45
S 18 [b]	1-butanol	0.03	125.302	9.37833
S 19	2-butanol	0.01	135.588	9.28779
S 20	2-methyl-1-propanol	-0.018	129.829	9.29034
S 21	2-methyl-2-butanol	0.012972	132.48	9.0542
S 22 [b]	3-methyl-1-butanol	-0.01111	134.11	9.18573
S 23	1-pentanol	0.022829	124.104	9.29075
S24	4-methyl-2-pentanol	---	---	---
S 25	1-hexanol	0.017729	125.365	9.21138
S 26	2-ethyl-1-hexanol	0.023855	137.932	9.04103
S 27	1-heptanol	0.010761	124.834	9.13507
S 28	1-octanol	0.002098	125.402	9.06132
S 29	dibutyl ether	0.076637	78.57	9.07
S 30	methyl t-buthyl ether	0.08191	72.79	9.47872
S 31 [b]	methyl acetate	0.055858	86.2905	9.06912
S 32	ethyl acetate	0.112161	75.55	9.3
S 33	butyl acetate	0.097652	65.6006	9.14327
S 34	dimethyl sulfoxide	0.089	105.34	9.57142
S35	acetonitrile	0.065	60.4	9.83

[b] Compounds in the test set of model #2