Supplementary Materials

Application of COSMO-RS-DARE as a tool for testing consistency of solubility data: case of coumarin in neat alcohols

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Table S1. The solubility values of coumarin (CAS: 91-64-5) expressed as molar fractions ($\times 10^3$) along with the standard deviation values (n = 3).

Solvent	Temperature [°C]			
	25	**30**	**35**	**40**
methanol, MeOH (CAS: 67-56-1)	77.01 ± 4.68	127.52 ± 5.07	196.63 ± 7.30	286.50 ± 6.20
ethanol, EtOH (CAS: 64-17-5)	49.43 ± 2.59	90.16 ± 5.57	142.45 ± 5.12	210.96 ± 6.24
1-propanol, 1PrOH (CAS: 71-23-8)	41.02 ± 0.72	74.27 ± 2.42	121.65 ± 5.97	181.10 ± 4.99
2-propanol, 2PrOH (CAS: 67-63-0)	30.17 ± 0.60	60.35 ± 1.81	101.22 ± 4.59	154.88 ± 5.76
1-butanol, 1BuOH (CAS: 71-36-3)	16.95 ± 1.09	34.87 ± 1.34	60.64 ± 0.77	94.59 ± 2.12
1-pentanol, 1PeOH (CAS: 71-41-0)	19.66 ± 0.28	42.95 ± 1.59	77.44 ± 0.55	126.01 ± 7.64
1-octanol, 1OcOH (CAS: 111-87-5)	19.18 ± 0.67	37.37 ± 1.24	67.23 ± 2.91	104.05 ± 0.71

Table S2. Statistical characteristics of linear regressions exemplified in Figure 8 and used for back-computations of solubility using COSMO-RS-DARE approach.

T[°C]	a±SD	b±SD	P	R^2_{adj}	F
SpMin2_Bhm					
25	-2.67±0.24	-1.18±0.31	<0.001	0.952	119.37
30	-2.44±0.20	-0.87±0.26	<0.001	0.960	143.82
35	-2.25±0.21	-0.66±0.26	<0.001	0.952	120.39
40	-2.12±0.21	-0.48±0.27	=0.001	0.941	97.395
R_a					
25	0.55±0.06	-12.47±0.90	<0.001	0.931	81.683
30	0.51±0.06	-11.20±0.82	<0.001	0.932	83.039
35	0.47±0.05	-10.17±0.80	<0.001	0.923	73.298
40	0.44±0.06	-9.42±0.83	=0.001	0.908	60.016

Table S3. Collection of molecular descriptors used for determination of linear regression. The Hansen solubility space distance, R_a, was calculated according to eq. 3 based on the Hansen solubility parameters (δ_d, δ_p ,δ_{HB}). The last column compiles the values of SpMin2_Bhm of considered alcohols.

Compound	δ_d	δ_p	δ_{HB}	R_a	SpMin2_Bhm
methanol	15.1	12.3	22.3	18.42	0.42
ethanol	15.8	8.8	19.4	15.67	0.91
1-propanol	16.0	6.8	17.4	14.53	1.21
2-propanol	15.8	6.1	16.4	14.34	1.25
1-butanol	16.0	5.7	15.8	13.89	1.41
1-pentanol	15.9	5.9	13.9	12.75	1.54
1-octanol	16.0	5.0	11.9	12.14	1.74
coumarin	20.0	12.5	6.7	-	-