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Prediction of solubility of two-component molecular crystals

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Table S1. Calculated, X_{Cal}^{CC}, and experimental, X_{Exp}^{CC}, solubility values of two-component molecular crystals with stoichiometry 1:1 in the solvents at different temperatures

CF1	CF2	T [°C]	Solvent	pH	$\ln X_{id}^{CF1}$	$\ln X_{id}^{CF2}$	$\ln X_{id}^{CC}$	Unit[d]	X^{CF1} [Unit]	X^{CF2} [Unit]	γ(CF1)	γ(CF2)	X_{cal}^{CC} [mol fr]	$X_{\exp}^{CC}$ [mol fr]	Ref
Carbamazepine	Nicotinamide	25.0	Buffer	6.0	-2.94	-2.15	-2.87	mol/L	4.60E-04	7.50E+00	6.35E+03	1.89E-01	8.17E-04	1.27E-03	[1]
Carbamazepine	Saccharin	25.0	Buffer	2.0	-2.94	-4.01	-3.03	mol/L	4.60E-04	1.80E-02	6.35E+03	5.56E+01	4.06E-05	2.13E-05	[1]
Carbamazepine	Salicylic Acid	25.0	Buffer	2.9	-2.94	-2.82	-2.55	mol/L	4.60E-04	1.40E-02	6.35E+03	2.36E+02	3.18E-05	1.63E-05	[1]
Benzamide	dibenzyl sulfoxide	37.0	Water		-1.72	-2.46	-1.97	mol/L	1.08E-01	1.43E-03	9.08E+01	3.32E+03	1.27E-04	9.59E-05	[2]
Paracetamol	Theophylline	37.0	Water		-2.73	-3.77	-1.76	mol/L	1.39E-01	6.09E-02	2.55E+01	2.08E+01	3.73E-03	3.51E-03	[3]
Drug_1	Benzoic Acid	25.0	67THF-33H[b]		-4.85	-1.48	-2.71	mol/L	1.67E-02	2.18E+00	4.71E+00	9.40E-01	1.59E-02	3.55E-02	[4]
Diflunisal	Theophylline	25.0	Buffer	7.4	-4.34	-3.94	-3.47	mol/L	1.50E-02	3.10E-02	4.80E+01	3.48E+01	3.80E-04	6.34E-04	[5]
Diclofenac	Theophylline	25.0	Buffer	7.4	-4.54	-3.94	-4.00	mol/L	5.00E-03	3.10E-02	1.18E+02	3.48E+01	1.42E-04	1.44E-04	[5]
Theophylline	Salicylic acid	25.0	Buffer	2.6	-3.95	-2.80	-2.64	mol/L	3.10E-02	1.40E-02	3.45E+01	2.41E+02	3.91E-04	2.28E-04	[6]
Indomethacin	Saccharine	25.0	MeOH		-4.00	-3.34	-4.36	mol/L	5.15E-02	2.77E-01	8.64E+00	2.99E+00	1.25E-03	2.38E-03	[7]
Bicalutamide	Benzamide	25.0	Chloroform		-5.88	-1.99	-3.34	mol/L	6.70E-03	2.10E-01	5.17E+00	8.09E+00	2.74E-03	1.52E-03	[8]
Bicalutamide	Salicylamide	25.0	Chloroform		-5.88	-2.77	-3.73	mol/L	6.70E-03	4.90E-02	5.17E+00	1.58E+01	1.32E-03	9.43E-04	[8]
Vanillin isoniazid	Saccharin	25.0	Water		-6.20	-3.77	-4.20	mol/L	6.90E-05	1.70E-02	1.63E+03	7.51E+01	2.14E-05	1.51E-05	[9]
Salinazid	Saccharin	25.0	Water		-5.49	-3.77	-3.78	mol/L	5.70E-05	1.70E-02	4.04E+03	7.51E+01	2.08E-05	2.03E-05	[9]
TDZ[a]	Vanillic Acid	25.0	Buffer	2.0	-2.80	-4.10	-3.34	mol/L	3.70E-04	9.02E-03	9.13E+03	1.02E+02	1.84E-05	1.13E-05	[10]
Caffeine	Gallic Acid	30.0	Water		-2.17	-8.34	-5.99	mol fr	2.54E-03	1.76E-03	4.49E+01	1.35E-01	5.06E-04	1.90E-04	[11]
Sulfathiazole	Theophylline	25.0	Water		-3.23	-3.95	-4.57	mol/L	1.80E-03	2.50E-02	1.22E+03	4.25E+01	2.27E-05	3.24E-05	[12]
Flurbiprofen	Benzamide	25.0	Buffer	2.0	-2.26	-1.99	-1.97	mol/L	4.53E-05	1.02E-01	1.28E+05	7.37E+01	2.26E-05	1.69E-05	[13]
Flurbiprofen	Picolinamide	25.0	Buffer	2.0	-2.26	-1.50	-1.42	mol/L	4.53E-05	6.10E-01	1.28E+05	1.90E+01	7.80E-05	5.76E-05	[13]
Flurbiprofen	Salicylamide	25.0	Buffer	2.0	-2.26	-2.77	-2.39	mol/L	4.53E-05	1.88E-02	1.28E+05	1.84E+02	9.47E-06	7.92E-06	[13]
Diclofenac	L-proline	25.0	Buffer	6.8	-4.54	-1.65	-2.58	mol/L	1.17E-03	6.98E-01	5.06E+02	1.43E+01	4.46E-04	5.23E-04	[14]
Niflumic Acid	L-proline	25.0	Buffer	6.8	-4.32	-1.65	-3.22	mol/L	5.45E-03	5.37E+00	1.36E+02	9.49E-01	1.77E-03	8.99E-04	[14]
Clonixin	L-proline	25.0	Buffer	6.8	-4.38	-1.65	-3.14	mol/L	2.40E-03	5.37E+00	2.89E+02	9.49E-01	1.31E-03	8.99E-04	[14]
Paracetamol	Maleic Acid	25.0	Acetonitrile		-3.04	-2.54	-2.59	mol/L	1.50E-01	4.40E-01	5.90E+00	3.25E+00	8.53E-03	2.56E-02	[15]
Fluconazole	4-OH-Benzoic acd	25.0	MeOH		-3.32	-3.67	-2.97	mol/L	3.10E-01	2.05E+00	2.54E+00	2.24E-01	3.41E-02	1.93E-02	[16]
Fluconazole	Vanillic acid	25.0	MeOH		-3.32	-4.12	-3.26	mol/L	3.10E-01	2.23E+00	2.54E+00	1.11E-01	3.63E-02	1.76E-02	[16]
Sulfadimidine	3-Me-Salicylic acid	30.0	Acetonitrile		-4.06	-2.58	-3.02	mol fr	3.18E-03	2.04E-02	5.45E+00	3.70E+00	4.89E-02	8.72E-02	[17]
Flurbiprofen	Benzamide	25.0	Buffer	6.8	-2.26	-1.99	-1.97	mol/L	7.89E-03	1.02E-01	7.31E+02	7.37E+01	2.99E-04	2.53E-04	[13]
Flurbiprofen	Picolinamide	25.0	Buffer	6.8	-2.26	-1.50	-1.42	mol/L	7.90E-03	6.10E-01	7.30E+02	1.90E+01	1.03E-03	5.61E-04	[13]
Flurbiprofen	Salicylamide	25.0	Buffer	6.8	-2.26	-2.77	-2.39	mol/L	7.90E-03	1.88E-02	7.31E+02	1.84E+02	1.25E-04	1.19E-04	[13]
Arbidol	Benzoic Acid	20.0	EtOAc		-4.12	-1.70	-2.87	mol/L	4.40E-03	1.44E+00	3.77E+01	1.22E+00	4.16E-03	4.34E-03	[18]
Arbidol	Saicylic Acid	20.0	EtOH		-4.12	-2.93	-3.39	mol/L	3.30E-03	1.91E+00	8.42E+01	3.73E-01	3.00E-03	8.80E-04	[18]
Fluconazole	Vanillic acid	25.0	Water		-3.32	-4.12	-3.26	mol/L	1.60E-02	9.10E-03	1.25E+02	9.87E+01	1.73E-04	1.20E-04	[16]
Indomethacin	Saccharine	25.0	EtOH		-4.00	-3.34	-4.36	mol/L	6.18E-02	1.79E-01	5.08E+00	3.35E+00	1.54E-03	2.31E-03	[7]
Indomethacin	Saccharine	25.0	Water		-4.00	-3.34	-4.36	mol/L	8.38E-06	1.88E-02	1.22E+05	1.04E+02	1.79E-06	9.32E-07	[7]
Theophylline	Salicylic acid	30.0	Acetonitrile		-3.84	-2.67	-2.54	mol fr	5.40E-04	3.44E-02	3.99E+01	2.00E+00	4.40E-03	5.77E-03	[6]
Carbamazepine	Glutaric acid	25.0	Isopropyl		-2.94	-1.46	-2.04	mol/L	5.00E-02	3.60E+00	1.36E+01	5.62E-01	2.36E-02	2.46E-02	[1]
Carbamazepine	Glutaric acid	25.0	EtOH		-2.94	-1.46	-2.04	mol/L	1.40E-01	2.80E+00	6.22E+00	9.83E-01	2.63E-02	1.89E-02	[1]
Carbamazepine	Glutaric acid	25.0	EtOAc		-2.94	-1.46	-2.04	mol/L	4.90E-02	1.00E+00	1.09E+01	2.25E+00	1.31E-02	9.31E-03	[1]
Carbamazepine	Nicotinamide	25.0	Isopropyl		-2.94	-2.15	-2.87	mol/L	5.00E-02	6.30E-01	1.36E+01	2.30E+00	5.07E-03	4.70E-03	[1]
Carbamazepine	Nicotinamide	25.0	EtOH		-2.94	-2.15	-2.87	mol/L	2.45E-02	8.21E-02	6.22E+00	1.62E+00	8.91E-03	8.88E-03	[1]
Carbamazepine	Nicotinamide	25.0	EtOAc		-2.94	-2.15	-2.87	mol/L	4.90E-02	1.10E-01	1.09E+01	1.08E+01	2.54E-03	2.54E-03	[1]

Carbamazepine	Saccharin	25.0	Isopropyl		-2.94	-4.01	-3.03	mol/L	5.00E-02	1.60E-02	1.36E+01	1.47E+01	1.70E-03	1.52E-03	[1]
Carbamazepine	Saccharin	25.0	EtOH		-2.94	-4.01	-3.03	mol/L	1.40E-01	2.40E-01	6.22E+00	1.24E+00	8.69E-03	3.83E-03	[1]
Carbamazepine	Saccharin	25.0	EtOAc		-2.94	-4.01	-3.03	mol/L	4.90E-02	1.80E-01	1.09E+01	1.01E+00	7.27E-03	4.92E-03	[1]
Drug_1	Benzoic Acid	25.0	25THF-75H[c]		-4.85	-1.48	-2.71	mol/L	5.30E-04	7.28E-01	1.16E+02	2.39E+00	2.00E-03	3.73E-03	[4]
Caffeine	Gallic Acid	35.0	Water		-2.10	-8.10	-5.81	mol fr	3.14E-03	2.03E-03	3.89E+01	1.50E-01	6.23E-04	2.50E-04	[11]
Caffeine	Gallic Acid	40.0	Water		-2.04	-7.86	-5.62	mol fr	4.14E-03	2.48E-03	3.15E+01	1.55E-01	8.15E-04	3.80E-04	[11]
Caffeine	Gallic Acid	45.0	Water		-1.97	-7.63	-5.45	mol fr	5.19E-03	3.11E-03	2.69E+01	1.56E-01	1.05E-03	5.80E-04	[11]
Caffeine	Gallic Acid	50.0	Water		-1.91	-7.40	-5.27	mol fr	7.93E-03	4.33E-03	1.88E+01	1.41E-01	1.58E-03	7.70E-04	[11]
Caffeine	Gallic Acid	55.0	Water		-1.84	-7.17	-5.09	mol fr	9.57E-03	5.57E-03	1.66E+01	1.38E-01	2.03E-03	9.90E-04	[11]
Sulfathiazole	Theophylline	15.0	Water		-3.47	-4.18	-4.87	mol/L	1.00E-03	1.70E-02	1.73E+03	5.01E+01	1.30E-05	1.80E-05	[12]
Sulfathiazole	Theophylline	40.0	Water		-2.89	-3.63	-4.14	mol/L	2.50E-03	4.00E-02	1.23E+03	3.64E+01	3.76E-05	4.14E-05	[12]
Sulfathiazole	Theophylline	60.0	Water		-2.46	-3.23	-3.59	mol/L	9.00E-03	1.30E-01	5.25E+02	1.65E+01	1.48E-04	1.26E-04	[12]
Sulfadimidine	3-Me-Salicylic acid	30.0	MeOH		-4.06	-2.58	-3.02	mol fr	2.68E-03	1.86E-01	6.45E+00	4.06E-01	6.83E-02	1.45E-01	[17]
Bicalutamide	Benzamide	18.0	Chloroform		-6.19	-2.15	-3.60	mol/L	5.60E-03	1.60E-01	4.53E+00	9.05E+00	2.14E-03	1.12E-03	[8]
Bicalutamide	Benzamide	22.0	Chloroform		-6.01	-2.06	-3.45	mol/L	6.20E-03	1.90E-01	4.89E+00	8.35E+00	2.49E-03	1.34E-03	[8]
Bicalutamide	Benzamide	30.0	Chloroform		-5.66	-1.88	-3.16	mol/L	7.70E-03	2.40E-01	5.60E+00	7.91E+00	3.19E-03	1.86E-03	[8]
Bicalutamide	Salicylamide	18.0	Chloroform		-6.19	-2.97	-3.98	mol/L	5.60E-03	3.80E-02	4.53E+00	1.67E+01	1.08E-03	7.09E-04	[8]
Bicalutamide	Salicylamide	22.0	Chloroform		-6.01	-2.86	-3.84	mol/L	6.20E-03	4.40E-02	4.89E+00	1.62E+01	1.21E-03	8.70E-04	[8]
Bicalutamide	Salicylamide	30.0	Chloroform		-5.66	-2.63	-3.56	mol/L	7.70E-03	6.00E-02	5.60E+00	1.49E+01	1.55E-03	1.15E-03	[8]
Arbidol	Benzoic Acid	25.0	EtOAc		-3.89	-1.61	-2.71	mol/L	5.50E-03	1.70E+00	3.79E+01	1.13E+00	5.14E-03	5.54E-03	[8]
Arbidol	Benzoic Acid	30.0	EtOAc		-3.67	-1.51	-2.55	mol/L	6.80E-03	1.97E+00	3.83E+01	1.06E+00	6.12E-03	7.05E-03	[18]
Arbidol	Benzoic Acid	35.0	EtOAc		-3.45	-1.42	-2.40	mol/L	8.60E-03	2.26E+00	3.77E+01	1.00E+00	7.42E-03	9.29E-03	[18]
Arbidol	Saicylic Acid	25.0	EtOH		-3.89	-2.80	-3.23	mol/L	4.50E-03	2.08E+00	7.75E+01	3.80E-01	3.63E-03	1.12E-03	[18]
Arbidol	Saicylic Acid	30.0	EtOH		-3.67	-2.67	-3.08	mol/L	5.60E-03	2.24E+00	7.79E+01	3.90E-01	4.17E-03	1.41E-03	[18]
Arbidol	Saicylic Acid	35.0	EtOH		-3.45	-2.55	-2.93	mol/L	7.60E-03	2.42E+00	7.15E+01	3.97E-01	5.03E-03	1.77E-03	[18]
Et-Paraben	Nicotinamide	25.0	EtOH		-2.17	-2.15	-1.80	mol/L	1.91E+00	8.21E-02	7.50E-01	2.47E+01	1.92E-02	3.81E-02	[19]

[a]TDZ - (1-[5-(3-Chloro-phenylamino)-1,2,4-thiadiazol-3-yl]-propan-2-ol)
[b]67THF-33H - 67%(V/V) THF +33% Heptane
[c]25THF-75H - 25%(V/V) THF +75% Heptane
[d] Unit corresponds to next two columns X^{CF1} and X^{CF2}

Table S2. Coefficients of the correlation equation $\ln(X_{id}(CC)) = C + D \cdot \ln(X_{id}(CF1))$ for the clusters including the considered compound as one of the components of the two-component crystal

CF1	CF1:CF2	C	D (slope)	R[a]	σ[b]	n[c]	$T_m(CF1)$ [°C]	$H_{fus}^{Tm}(CF1)$ [kJ/mol]
Benzoic Acid	1:1	0.016 ± 0.331	0.508 ± 0.057	0.9424	0.546	12	122.4	18.6
Caffeine	1:1	-0.930 ± 0.256	0.429 ± 0.027	0.9810	0.662	12	236.0	19.3
Carbamazepine	1:1	-2.109 ± 0.322	0.327 ± 0.089	0.8315	0.297	8	192.1	25.6
Fumaric Acid	1:2	2.193 ± 0.430	1.209 ± 0.093	0.9855	0.262	7	287.0	31.8
Isoniazid	1:1	0.102 ± 0.331	0.774 ± 0.061	0.9818	0.496	8	170.5	28.30
Isonicotinamide	1:1	-1.449 ± 0.334	0.368 ± 0.083	0.8433	0.565	10	156.0	24.5
Nicotinamide	1:1	-0.602 ± 0.301	0.519 ± 0.066	0.8851	0.634	19	128.5	24.1
Oxalic Acid	1:2	1.162 ± 1.638	1.135 ± 0.459	0.7418	0.584	7	189.0	59.7
4-NH_2-Benzoic Acid	1:1	-1.596 ± 0.418	0.503 ± 0.115	0.8899	0.572	7	188.5	25.0
Saccharin	1:1	-2.226 ± 0.181	0.374 ± 0.033	0.9768	0.163	8	227.9	26.8
Salicylic Acid	1:1	-0.557 ± 0.313	0.513 ± 0.080	0.9052	0.319	11	160.9	27.1
Succinic acid	1:2	2.622 ± 0.641	1.228 ± 0.133	0.9559	0.816	10	192.3	32.4
Succinic acid	1:1	1.526 ± 0.835	1.085 ± 0.138	0.9692	0.865	6	192.3	32.4
Sulfadimidine	1:1	-3.267 ± 0.362	0.289 ± 0.091	0.7449	0.304	10	198.0	36.3
Theophylline	1:1	-0.526 ± 0.584	0.781 ± 0.153	0.9163	0.665	7	273.0	29.6
4-OH-Benzoic Acid	1:1	-1.556 ± 0.360	0.537 ± 0.087	0.9291	0.357	8	214.5	30.3
Benzamide	1:1	-0.699 ± 0.257	0.475 ± 0.060	0.9553	0.375	8	127.7	22.4
2-OH-Benzamide	1:1	-1.350 ± 0.390	0.374 ± 0.089	0.8838	0.434	7	140.8	29.1
4-NH_2-Benzamide	1:1	-1.596 ± 0.418	0.503 ± 0.115	0.8899	0.572	7	181.6	32.7
4,4'-bipyridine	1:2	-1.024 ± 0.215	0.430 ± 0.047	0.9346	0.429	14	111.8	24.7
Pyrazinamide	1:1	-0.245 ± 0.191	0.341 ± 0.030	0.9885	0.220	5	190.0	28.1
Maleic Acid	1:1	0.102 ± 0.380	0.733 ± 0.072	0.9811	0.482	6	135.0	26.9
Adipic acid	1:1	-0.465 ± 0.658	0.693 ± 0.109	0.9650	0.804	5	153.0	38.6
Meloxicam	1:1	-0.539 ± 0.289	0.594 ± 0.100	0.9032	0.395	10	254.0	49.9
L-proline	1:1	-1.102 ± 0.359	0.466 ± 0.087	0.8975	0.425	9	221.5	13.4
Sertraline	1:1	-0.176 ± 0.181	0.166 ± 0.044	0.8832	0.159	6	not	not
Curcumin	1:1	0.013 ± 0.735	1.027 ± 0.155	0.9286	1.04	9	183.2	50.0
Etodolac	1:1	-2.739 ± 0.197	0.291 ± 0.091	0.9148	0.381	4	147.8	39.7
4-OH-Benzamide	2:1	-1.441 ± 0.928	0.142 ± 0.135	0.5979	0.417	4	159.9	25.2
Diethylstilbestrol	1:2	-0.738 ± 0.934	1.028 ± 0.412	0.8701	0.512	4	182.1	31.8
Tefagur	1:1	0.093 ± 0.934	0.881 ± 0.276	0.9143	0.483	4	171.7	20.3
Gababentin lactam	1:1	-0.231 ± 0.536	0.458 ± 0.141	0.9167	0.309	4	92.0	19.0
Flurbiprofen	1:1	-0.276 ± 0.501	0.749 ± 0.201	0.9347	0.227	4	109.3	28.9

[a] Pair correlation coefficient;

[b] Standard deviation;

[c] Number of points in the cluster;

Table S3. Calculated, $X_{id}^{CC}(Cal)$ [mol fr], and experimental, $X_{id}^{CC}(Exp)$ [mol fr], values of the ideal intrinsic solubility of two-component molecular crystals with stoichiometry 1:1 and calculated, X_{Cal}^{CC} [mol fr], and experimental, X_{Exp}^{CC} [mol fr], values of co-crystals/salts solubility in the solvents at different temperatures

CF1	CF2	Solvent	pH	T [°C]	CF1 / CF2[a]	C[b]	D(slope)[b]	$\ln X_{id}^{CC}(Cal)$ [c]	$\ln X_{id}^{CC}(Exp)$ [c]	X_{cal}^{CC} [d]	$X_{\exp}^{CC}$	Ref
Theophylline	Nicotinamide	Buffer	5.8	25.0	Nicotinamide	-0.602	0.519	-3.42	-1.97	1.60E-02	8.61E-03	[1]
Carbamazepine	Nicotinamide	Buffer	6.0	25.0	Nicotinamide	-0.602	0.519	-2.53	-3.48	1.35E-03	1.27E-03	[1]
Carbamazepine	Saccharin	Buffer	2.0	25.0	Saccharin	-2.226	0.374	-3.71	-3.75	6.23E-05	2.13E-05	[1]
Carbamazepine	Salicylic Acid	Buffer	2.9	25.0	Carbamazepine	-2.109	0.327	-3.23	-3.09	3.21E-05	1.63E-05	[1]
Benzamide	dibenzyl sulfoxide	Water		37.0	Benzamide	-0.699	0.475	-2.27	-2.65	1.93E-04	9.59E-05	[2]
Paracetamol	Theophylline	Water		37.0	Theophylline	-0.526	0.781	-3.44	-2.40	2.78E-03	3.51E-03	[3]
Drug_1	Benzoic Acid	67THF-33H[e]		25.0	Benzoic Acid	0.016	0.508	-3.02	-3.22	2.89E-03	3.73E-03	[4]
Gabapentin lactam	4-NH_2-Benzoic Acid	Buffer	1.2	25.0	4-NH_2-Benzioc Acid	-1.596	0.503	-2.31	-1.81	9.70E-04	5.22E-04	[20]
Diflunisal	Theophylline	Buffer	7.4	25.0	Theophylline	-0.526	0.781	-4.89	-4.34	3.56E-04	6.34E-04	[5]
Diclofenac	Theophylline	Buffer	7.4	25.0	Theophylline	-0.526	0.781	-4.93	-5.01	2.03E-04	1.44E-04	[5]
Theophylline	Salicylic Acid	Buffer	2.6	25.0	Salicylic Acid	-0.557	0.513	-3.34	-3.31	5.47E-04	2.28E-04	[19]
Indomethacin	Saccharin	MeOH		25.0	Saccharin	-2.226	0.374	-4.85	-5.45	4.46E-03	2.38E-03	[7]
Bicalutamide	Benzamide	Chloroform		25.0	Benzamide	-0.699	0.475	-4.22	-3.91	2.88E-03	1.52E-03	[8]
Bicalutamide	Salicylamide	Chloroform		25.0	Salicylamide	-1.350	0.374	-4.12	-4.51	2.48E-03	9.43E-04	[8]
Vanillin isoniazid	Saccharin	Water		25.0	Saccharin	-2.226	0.374	-5.29	-5.36	3.49E-05	1.51E-05	[9]
Salinazid	Saccharin	Water		25.0	Saccharin	-2.226	0.374	-4.98	-4.78	2.86E-05	2.03E-05	[9]
Flurbiprofen	Benzamide	Buffer	2.0	25.0	Benzamide	-0.699	0.475	-1.92	-2.23	3.29E-05	1.69E-05	[13]
Flurbiprofen	Picolinamide	Buffer	2.0	25.0	Flurbiprofen	-0.276	0.749	-1.55	-1.55	8.78E-05	5.76E-05	[13]
Flurbiprofen	Salicylamide	Buffer	2.0	25.0	Salicylamide	-1.350	0.374	-2.31	-2.75	1.54E-05	7.92E-06	[13]
Flurbiprofen	Salicylamide	Buffer	6.8	25.0	Salicylamide	-1.350	0.374	-2.31	-2.75	2.03E-04	1.19E-04	[13]
Diclofenac	L-proline	Buffer	6.8	25.0	L-Proline	-1.102	0.466	-3.73	-3.10	3.14E-04	5.23E-04	[14]
Niflumic Acid	L-proline	Buffer	6.8	25.0	L-Proline	-1.102	0.466	-3.67	-4.11	2.62E-03	8.99E-04	[14]
Clonixin	L-proline	Buffer	6.8	25.0	L-Proline	-1.102	0.466	-3.81	-4.01	1.75E-03	8.98E-04	[14]
Fluconazole	4-OH-Benzoic Acid	MeOH		25.0	4-OH-Benzoic Acid	-1.556	0.537	-3.66	-3.57	3.91E-02	1.93E-02	[16]
Flurbiprofen	Benzamide	Buffer	6.8	25.0	Benzamide	-0.699	0.475	-1.92	-2.23	4.35E-04	2.53E-04	[13]
Flurbiprofen	Picolinamide	Buffer	6.8	25.0	Flurbiprofen	-0.276	0.749	-1.55	-1.55	1.16E-03	5.61E-04	[13]
Arbidol	Benzoic Acid	EtOAc		20.0	Benzoic Acid	0.016	0.508	-2.43	-3.13	1.06E-02	4.35E-03	[18]
Indomethacin	Saccharin	EtOH		25.0	Saccharin	-2.226	0.374	-4.04	-5.45	5.50E-03	2.31E-03	[7]
Theophylline	Salicylic Acid	Acetonitrile		30.0	Salicylic Acid	-0.557	0.513	-3.34	-3.31	6.27E-03	5.77E-03	[19]
Carbamazepine	Glutaric Acid	Isopropyl		25.0	Carbamazepine	-2.109	0.327	-2.65	-2.37	2.05E-02	2.46E-02	[1]
Carbamazepine	Glutaric Acid	EtOH		25.0	Carbamazepine	-2.109	0.327	-2.65	-2.37	2.30E-02	1.89E-02	[1]
Carbamazepine	Glutaric Acid	EtOAc		25.0	Carbamazepine	-2.109	0.327	-2.65	-2.37	1.14E-02	9.31E-03	[1]
Theophylline	Nicotinamide	Isopropyl		25.0	Nicotinamide	-0.602	0.519	-3.42	-1.97	2.94E-03	3.69E-03	[1]
Theophylline	Nicotinamide	EtOH		25.0	Nicotinamide	-0.602	0.519	-3.42	-1.97	7.50E-03	4.49E-03	[1]
Carbamazepine	Nicotinamide	Isopropyl		25.0	Carbamazepine	-2.109	0.327	-2.93	-3.48	8.38E-03	4.70E-03	[1]
Carbamazepine	Nicotinamide	EtOH		25.0	Carbamazepine	-2.109	0.327	-2.93	-3.48	1.47E-02	8.88E-03	[1]
Carbamazepine	Nicotinamide	EtOAc		25.0	Carbamazepine	-2.109	0.327	-2.93	-3.48	4.31E-03	2.54E-03	[1]
Carbamazepine	Saccharin	Isopropyl		25.0	Saccharin	-2.226	0.374	-3.61	-3.75	2.62E-03	1.52E-03	[1]

Carbamazepine	Saccharin	EtOAc		25.0	Saccharin	-2.226	0.374	-3.61	-3.75	1.12E-02	4.92E-03	[1]
Drug_1	Benzoic Acid	25THF-75H[f]		25.0	Benzoic Acid	0.016	0.508	-3.02	-3.22	2.29E-02	3.55E-02	[4]
Bicalutamide	Benzamide	Chloroform		18.0	Benzamide	-0.699	0.475	-4.46	-3.91	2.59E-03	1.12E-03	[8]
Bicalutamide	Benzamide	Chloroform		22.0	Benzamide	-0.699	0.475	-4.32	-3.91	2.77E-03	1.34E-03	[8]
Bicalutamide	Benzamide	Chloroform		30.0	Benzamide	-0.699	0.475	-4.06	-3.91	3.03E-03	3.03E-03	[8]
Bicalutamide	Salicylamide	Chloroform		22.0	Salicylamide	-1.350	0.374	-4.20	-4.51	2.47E-03	8.71E-04	[8]
Bicalutamide	Salicylamide	Chloroform		30.0	Salicylamide	-1.350	0.374	-4.00	-4.51	2.56E-03	1.15E-03	[8]
Arbidol	Benzoic Acid	EtOAc		25.0	Benzoic Acid	0.016	0.508	-2.28	-3.13	1.21E-02	5.54E-03	[18]
Arbidol	Benzoic Acid	EtOAc		30.0	Benzoic Acid	0.016	0.508	-2.13	-3.13	1.38E-02	7.05E-03	[18]
Arbidol	Benzoic Acid	EtOAc		35.0	Benzoic Acid	0.016	0.508	-1.98	-3.13	1.58E-02	9.29E-03	[18]
Theophylline	Acetylsalicylic Acid	Isopropyl		20.0	Theophylline	-0.526	0.781	-3.34	nd[g]	1.18E-02	1.30E-02	[21]
Theophylline	Acetylsalicylic Acid	Isopropyl		40.0	Theophylline	-0.526	0.781	-3.34	nd[g]	2.73E-02	3.12E-02	[21]

[a]Co-former for which it was obtained the correlation Eq (6) for calculation of $\ln X_{id}^{CC}(Cal)$ [22];

[b]Coefficients of Eq. (6);

[c] $\ln X_{id}^{CC}(Cal)$ and $\ln X_{id}^{CC}(Exp)$ calculated with account for $\Delta H_{fus}(CC) = Q \cdot MW(CC) = Q \cdot [MW_1 \cdot (m/(m+l)) + MW_2 \cdot (l/(m+l))]$

where MW(CC), MW_1 and MW_2 are molecular weights of the co-crystal, CF1, and CF2, respectively. Q [J/g] is a fusion heat effect. (CF1:CF2) is stoichiometry (l:m). In this case (stoichiometry 1:1), therefore in order to evaluate X_{cal}^{CC} and $X_{\exp}^{CC}$ the values of $\ln X_{id}^{CC}(Cal)$ and $\ln X_{id}^{CC}(Exp)$ should be multiplied in 2.

[d]Calculated by using $\ln X_{id}^{CC}(Cal)$ -values evaluated by Eq.(6)

[e]67THF-33H - 67%(V/V) THF +33% Heptane

[f]25THF-75H - 25%(V/V) THF +75% Heptane

[g]nd is not described in the paper;

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