Electronic Supplementary Information for CrystEngComm

Targeted crystallisation of novel carbamazepine solvates based on a retrospective Random Forest classification

S1 Random Forest Classification of carbamazepine physical form screen

The training data set used in RF classification[1] is shown in Table S1 with resultant forest and corresponding confusion matrix provided in Fig S1 and Table S2, respectively. The training set used 326 crystallization results from the previous screen (which totalled 594 recrystallizations) excluding replicates and 2-phenylethanol as a full complement of solvent descriptors were not available for this solvent. Hence the input data draw on crystallisations from 65 solvents under 5 distinct sets of conditions plus one crystallisation from one solvent (trifluoroethanol). The classified predictive probabilities for each solvent are listed in Tables S3.

S2 XRPD analysis

A small quantity (1 - 50 mg) of each recrystallized sample was analyzed using transmission foil XRPD data collected on a Bruker AXS D8-Advance transmission diffractometer equipped with θ/θ geometry, primary monochromated radiation (Cu $K\alpha_1$, λ= 1.54056 Å), a Braun 1D position sensitive detector (PSD) and an automated multi-position *x*-*y* sample stage.[5] Samples were mounted on a 28 position sample plate supported on a polyimide (Kapton, 7.5 μm thickness) film. Data were collected from each sample in the range 4 – 35 ^{o} 2θ with a 0.015 ^{o} 2θ step size and 1 sec. step^{-1} count time (data collection time per sample *ca*. 45 mins). Samples were oscillated ± 0.5 mm in the *x*-*y* plane at a speed of 0.3 mm sec.$^{-1}$ throughout data collection to maximize particle sampling and minimize preferred orientation effects. XRPD patterns were identified by a combination of standard procedures, including pattern matching (Eva),[6] unit cell indexing (DICVOL-91);[7] Topas v3.1)[8] and Pawley refinement (DASH v3).[9] Representative XRPD data, that have been Pawley fitted to the cells listed in Table 1 of the manuscript, are shown in Figure S2.

S3 Single Crystal Analysis

Single-crystal X-ray measurements were made with graphite monochromated MoKα_1 raditation (0.71073. Å). on a Nonius Kappa diffractometer equipped with a CCD detector and Oxford cryostream variable temperature device. All of the single-crystal structures were solved using SHELXS-97.[10] Initial atomic positions were located using direct methods and remaining non-hydrogen atom sites wre calculated using difference Fourier maps. Refinemement of atomic co-ordinates and thermal parameters was done by full-matrix least squares methods on $|F^2|$ within SHELX-97 and H-atoms were placed in calculated positions in a riding mode. Refinement was carried out against all reflections. The crystal structure information can be obtained in CIF format, free of charge, *via* www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Data set used in RF classification; in the first instance all data excluding the header row and solvent identity were used to train the forest and subsequently the final 15 rows were excluded and then used in the predict function.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
1,5-pentanediol	104.1	113.4	169.0	26.2	0.2	7	6	6	5.85	2.5	115	43.4	0.002	two	two	on	high	off	three
1-methylnapthalene	142.2	144.3	181.6	2.9	3.22	7.6	3.2	1.45	1.39	0	3.1	39.8	0.009	zero	zero	on	high	off	two
Dodecane	170.3	214.7	336.1	2.0	5.85	12	11	11.11	11	0	1.38	24.9	0.016	zero	zero	on	high	off	four
Nitrobenzene	123.1	107.8	138.5	35.6	1.72	7.1	3.2	2	1.55	4.22	1.86	41.7	0.03	two	zero	on	high	off	four
1-octanol	130.2	155.7	222.4	10.3	2.8	9	8	8	7.92	1.8	7.29	27.1	0.01	one	one	on	high	off	two
dimethylsulphoxide	78.1	72.6	109.7	47.2	-0.32	4	1.3	0	1.52	3.96	1.99	42.9	0.084	one	zero	on	high	off	five
Aniline	93.1	95.4	130.5	7.1	1.08	5.1	2.3	1.5	0.98	1.13	3.85	42.1	0.09	zero	two	on	high	off	zero
2-octanol	130.2	155.4	224.8	8.1	2.72	9	6.1	8	6.06	1.7	6.49	26.3	0.032	one	one	on	high	off	two
2-butoxyethanol	118.2	130.4	187.6	9.4	0.84	8	7	7.2	6.85	9.3	3.15	26.1	0.15	two	one	on	high	off	four
Furfural	96.1	84.0	111.6	42.1	1.55	5.1	2.3	1.19	0.94	3.5	1.59	43.1	0.29	two	zero	on	high	off	five
2-methoxyethylether	134.2	138.6	203.0	9.8	-0.21	9	8	8	7.77	2	0.989	27	0.315	three	zero	on	high	off	two
Cyclohexanol	100.2	110.3	154.3	16.4	1.5	5.1	2.3	1.5	1.69	1.61	57.5	32.9	0.1	one	one	on	high	off	two
1-hexanol	102.2	122.0	175.9	13.0	1.88	7	6	6	5.93	1.58	4.58	25.8	0.11	one	one	on	high	off	two
Anisole	108.1	109.5	145.6	4.3	1.81	6.1	3.1	1.8	1.65	1.38	1.06	35.1	0.47	one	zero	on	high	off	three
N,*N*-dimethylformamide	73.1	77.3	111.6	38.3	-1.17	5	2.3	4	1.57	3.82	0.79	37.1	0.439	one	zero	on	high	off	five
Pentylacetate	130.1	141.4	197.6	4.8	1.81	9	6.1	8	5.52	1.75	0.862	25.2	0.6	two	zero	on	high	off	two
Butylether	130.2	155.5	238.7	3.1	2.71	9	8	8	7.92	1.17	0.64	22.4	0.898	one	zero	on	high	off	two
Xylene	106.2	117.1	159.5	2.3	2.8	6.1	2.5	1.8	1.34	0	0.596	28.5	1.13	zero	zero	on	high	off	four
1-pentanol	88.1	104.6	159.1	15.1	1.43	6	5	5.33	4.93	1.7	3.62	36.5	0.259	one	one	on	high	off	two
2-ethoxyethanol	90.1	96.3	146.7	13.4	-0.14	6	5	5.33	4.85	2.1	1.85	28.4	0.71	two	one	on	high	off	two
3-methyl-1-butanol	88.1	105.1	152.7	23.7	1.22	6	3.2	5.33	3.14	1.8	3.69	23.7	0.315	one	one	on	high	off	two
Butylacetate	115.2	124.8	177.7	5.1	1.35	8	5.1	7.2	4.56	1.9	0.69	24.9	1.66	two	zero	on	high	off	two
diethyl carbonate	118.1	116.4	168.4	2.8	1.36	8	5.1	5	4.5	1.1	0.748	26.4	1.63	three	zero	on	high	off	zero
2-methoxyethanol	76.1	79.6	117.0	17.2	-0.49	5	4	4	3.86	2.36	1.6	30.8	1.31	two	one	on	high	off	four
tetrachloroethene	165.8	96.1	137.3	2.3	2.43	6	2.2	3	3.42	0	0.84	31.3	2.42	zero	zero	on	high	off	four
acetic acid	60.1	56.6	81.1	6.2	-0.2	4	1.3	0	0.92	1.7	1.06	27.1	2.07	two	one	on	high	off	five
2-pentanol	88.1	104.8	156.3	13.7	1.35	6	3.2	5.33	3.14	1.7	3.47	23.5	0.804	one	one	on	high	off	one
4-methyl-2-pentanone	100.2	115.9	168.7	13.1	1.27	7	3.1	6	2.65	2.81	4.07	23.6	2.64	one	zero	on	high	off	four
1-butanol	74.1	87.8	136.3	17.8	0.97	5	4	4	3.93	1.66	2.54	24.9	0.86	one	one	on	high	off	two

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
isobutyl acetate	116.2	124.9	178.4	5.1	1.21	8	3.9	7.2	3.44	1.9	0.676	23.1	2.39	two	zero	on	high	off	two
pyridine	79.1	79.3	108.5	13.3	0.68	4.2	2.2	1.33	0.87	2.22	0.88	36.6	2.76	one	zero	on	high	off	four
toluene	92.1	100.6	134.8	2.4	2.32	5.1	2.3	1.5	1.12	0.38	0.56	27.9	3.79	zero	zero	on	high	off	four
2-methyl-1-propanol	74.1	87.9	131.1	17.9	0.83	5	2.3	4	2.19	1.64	3.33	23	1.39	one	one	on	high	off	four
1,4-dioxan	88.1	85.9	118.7	2.2	-0.26	4.2	2.2	1.33	1.47	0	1.18	32.8	4.95	two	zero	on	high	off	five
water	18.0	19.6	36.3	80.0	-0.36	0	0	0	0	1.87	0.89	73	2.72	one	two	on	high	off	five
2,2,4-trimethylpentane	114.2	147.3	210.1	1.9	3.36	8	2.5	7.2	2.52	0	0.5404	18.3	6.5	zero	zero	on	high	off	one
heptane	100.2	130.2	207.4	1.9	3.57	7	6	6	6	0	0.39	19.7	6.09	zero	zero	on	high	off	zero
2-butanol	74.1	87.9	131.5	17.3	0.89	5	2.3	4	2.19	1.8	3.1	22.5	2.32	one	one	on	high	off	four
1-propanol	60.1	70.8	109.0	20.8	0.51	4	3	4	2.93	1.55	1.95	23.3	2.76	one	one	on	high	off	four
triethylamine	101.2	125.9	176.2	2.4	1.37	7	4.2	2.67	4.1	0.66	0.35	20.2	7.7	one	zero	on	high	off	two
trichloroethylene	131.4	81.8	121.9	3.4	1.74	5	2.3	4	3.17	0.8	0.55	28.8	9.91	zero	zero	on	high	off	two
1,2-dimethoxyethane	90.1	96.8	140.4	7.2	-0.08	6	5	5.33	4.85	0	0.455	24.6	9.93	two	zero	on	high	off	two
1,2-dichloroethane	99.0	73.6	111.2	10.4	1.51	4	3	4	4.1	1.8	0.78	31.9	10.6	zero	zero	on	high	off	two
2-propanol	60.1	70.8	112.2	20.2	0.37	4	1.3	0	1.28	1.56	2.04	20.9	6.02	one	one	on	high	off	four
acetonitrile	41.1	46.0	66.2	36.6	0.04	3	2	0	1.24	3.92	0.37	28.7	11.9	one	zero	on	high	off	three
cyclohexane	84.2	102.4	146.4	2.0	2.74	4.2	2.2	1.33	1.54	0	0.89	24.7	13	zero	zero	on	high	off	three
benzene	78.1	83.8	116.0	2.3	1.83	4.2	2.2	1.33	0.91	0	0.6	28.2	12.7	zero	zero	on	high	off	two
2-butanone	72.1	81.8	123.3	18.6	0.56	5	2.3	4	1.81	2.78	0.405	24	12.6	one	zero	on	high	off	four
1-chlorobutane	92.6	93.4	147.0	7.3	2.18	5	4	4	4.54	2.05	0.422	23.2	13.7	zero	zero	on	high	off	two
ethanol	46.1	54.2	86.1	25.3	-0.01	3	2	0	1.93	1.69	1.07	22	7.87	one	one	on	high	off	four
ethylacetate	87.1	90.7	131.0	6.1	0.37	6	3.2	5.33	2.67	1.78	0.42	23.4	12.6	two	zero	on	high	off	two
carbon tetrachloride	153.8	84.5	118.7	2.2	3.58	5	1	0	2.15	0	0.91	26.4	15.2	zero	zero	on	high	off	four
hexane	86.2	113.2	182.5	1.9	3.11	6	5	5.33	5	0	0.3	17.9	20.2	zero	zero	on	high	off	two
tetrahydrofuran	72.1	77.2	110.6	7.5	0.51	3.2	1.4	0.64	0.89	1.75	0.46	26.4	21.6	one	zero	on	high	off	two
methanol	32.0	37.4	59.3	32.6	-0.36	2	0	0	0	1.7	0.54	22.1	16.9	one	one	on	high	off	three
chloroform	119.4	70.9	102.7	4.8	1.62	4	1.3	0	2.59	1.04	0.54	26.7	26.2	zero	zero	on	high	off	two
methyl acetate	74.1	73.8	109.3	7.1	0.02	5	2.3	4	1.76	1.72	0.36	24.7	28.8	two	zero	on	high	off	two
acetone	58.1	65.1	95.7	21.0	-0.1	4	1.3	0	0.96	2.88	0.31	23.5	30.8	one	zero	on	high	off	five
2-methoxy-2-methylpropane	88.1	105.0	149.2	4.5	0.98	6	1.6	5.33	1.59	1.2	0.35	19.1	26.9	one	zero	on	high	off	three

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
cyclopentane	70.1	85.4	121.9	2.0	2.28	3.2	1.4	0.64	0.92	0	0.413	21.9	42.3	zero	zero	on	high	off	three
formamide	45.0	42.5	66.4	111.0	-1.58	3	2	0	1.21	3.73	3.34	57	0.002	one	two	on	high	off	five
methanoic acid	46.0	39.7	58.4	51.1	-0.96	3	2	0	1.43	1.41	1.61	37.1	5.75	two	one	on	high	off	five
1,5-pentanediol	104.1	113.4	169.0	26.2	0.2	7	6	6	5.85	2.5	115	43.4	0.002	two	two	off	high	off	three
1-methylnapthalene	142.2	144.3	181.6	2.9	3.22	7.6	3.2	1.45	1.39	0	3.1	39.8	0.009	zero	zero	off	high	off	four
dodecane	170.3	214.7	336.1	2.0	5.85	12	11	11.11	11	0	1.38	24.9	0.016	zero	zero	off	high	off	two
nitrobenzene	123.1	107.8	138.5	35.6	1.72	7.1	3.2	2	1.55	4.22	1.86	41.7	0.03	two	zero	off	high	off	zero
1-octanol	130.2	155.7	222.4	10.3	2.8	9	8	8	7.92	1.8	7.29	27.1	0.01	one	one	off	high	off	two
dimethylsulphoxide	78.1	72.6	109.7	47.2	-0.32	4	1.3	0	1.52	3.96	1.99	42.9	0.084	one	zero	off	high	off	five
aniline	93.1	95.4	130.5	7.1	1.08	5.1	2.3	1.5	0.98	1.13	3.85	42.1	0.09	zero	two	off	high	off	three
2-octanol	130.2	155.4	224.8	8.1	2.72	9	6.1	8	6.06	1.7	6.49	26.3	0.032	one	one	off	high	off	two
2-butoxyethanol	118.2	130.4	187.6	9.4	0.84	8	7	7.2	6.85	9.3	3.15	26.1	0.15	two	one	off	high	off	two
furfural	96.1	84.0	111.6	42.1	1.55	5.1	2.3	1.19	0.94	3.5	1.59	43.1	0.29	two	zero	off	high	off	five
2-methoxyethylether	134.2	138.6	203.0	9.8	-0.21	9	8	8	7.77	2	0.989	27	0.315	three	zero	off	high	off	two
cyclohexanol	100.2	110.3	154.3	16.4	1.5	5.1	2.3	1.5	1.69	1.61	57.5	32.9	0.1	one	one	off	high	off	two
1-hexanol	102.2	122.0	175.9	13.0	1.88	7	6	6	5.93	1.58	4.58	25.8	0.11	one	one	off	high	off	two
anisole	108.1	109.5	145.6	4.3	1.81	6.1	3.1	1.8	1.65	1.38	1.06	35.1	0.47	one	zero	off	high	off	two
N,N-dimethylformamide	73.1	77.3	111.6	38.3	-1.17	5	2.3	4	1.57	3.82	0.79	37.1	0.439	one	zero	off	high	off	five
pentylacetate	130.1	141.4	197.6	4.8	1.81	9	6.1	8	5.52	1.75	0.862	25.2	0.6	two	zero	off	high	off	two
butylether	130.2	155.5	238.7	3.1	2.71	9	8	8	7.92	1.17	0.64	22.4	0.898	one	zero	off	high	off	two
xylene	106.2	117.1	159.5	2.3	2.8	6.1	2.5	1.8	1.34	0	0.596	28.5	1.13	zero	zero	off	high	off	two
1-pentanol	88.1	104.6	159.1	15.1	1.43	6	5	5.33	4.93	1.7	3.62	36.5	0.259	one	one	off	high	off	two
2-ethoxyethanol	90.1	96.3	146.7	13.4	-0.14	6	5	5.33	4.85	2.1	1.85	28.4	0.71	two	one	off	high	off	two
3-methyl-1-butanol	88.1	105.1	152.7	23.7	1.22	6	3.2	5.33	3.14	1.8	3.69	23.7	0.315	one	one	off	high	off	two
butylacetate	115.2	124.8	177.7	5.1	1.35	8	5.1	7.2	4.56	1.9	0.69	24.9	1.66	two	zero	off	high	off	two
diethyl carbonate	118.1	116.4	168.4	2.8	1.36	8	5.1	5	4.5	1.1	0.748	26.4	1.63	three	zero	off	high	off	zero
2-methoxyethanol	76.1	79.6	117.0	17.2	-0.49	5	4	4	3.86	2.36	1.6	30.8	1.31	two	one	off	high	off	four
tetrachloroethene	165.8	96.1	137.3	2.3	2.43	6	2.2	3	3.42	0	0.84	31.3	2.42	zero	zero	off	high	off	two
acetic acid	60.1	56.6	81.1	6.2	-0.2	4	1.3	0	0.92	1.7	1.06	27.1	2.07	two	one	off	high	off	five
2-pentanol	88.1	104.8	156.3	13.7	1.35	6	3.2	5.33	3.14	1.7	3.47	23.5	0.804	one	one	off	high	off	four

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
4-methyl-2-pentanone	100.2	115.9	168.7	13.1	1.27	7	3.1	6	2.65	2.81	4.07	23.6	2.64	one	zero	off	high	off	four
1-butanol	74.1	87.8	136.3	17.8	0.97	5	4	4	3.93	1.66	2.54	24.9	0.86	one	one	off	high	off	four
isobutyl acetate	116.2	124.9	178.4	5.1	1.21	8	3.9	7.2	3.44	1.9	0.676	23.1	2.39	two	zero	off	high	off	two
pyridine	79.1	79.3	108.5	13.3	0.68	4.2	2.2	1.33	0.87	2.22	0.88	36.6	2.76	one	zero	off	high	off	zero
toluene	92.1	100.6	134.8	2.4	2.32	5.1	2.3	1.5	1.12	0.38	0.56	27.9	3.79	zero	zero	off	high	off	two
2-methyl-1-propanol	74.1	87.9	131.1	17.9	0.83	5	2.3	4	2.19	1.64	3.33	23	1.39	one	one	off	high	off	four
1,4-dioxan	88.1	85.9	118.7	2.2	-0.26	4.2	2.2	1.33	1.47	0	1.18	32.8	4.95	two	zero	off	high	off	five
water	18.0	19.6	36.3	80.0	-0.36	0	0	0	0	1.87	0.89	73	2.72	one	two	off	high	off	five
2,2,4-trimethylpentane	114.2	147.3	210.1	1.9	3.36	8	2.5	7.2	2.52	0	0.5404	18.3	6.5	zero	zero	off	high	off	zero
heptane	100.2	130.2	207.4	1.9	3.57	7	6	6	6	0	0.39	19.7	6.09	zero	zero	off	high	off	one
2-butanol	74.1	87.9	131.5	17.3	0.89	5	2.3	4	2.19	1.8	3.1	22.5	2.32	one	one	off	high	off	four
1-propanol	60.1	70.8	109.0	20.8	0.51	4	3	4	2.93	1.55	1.95	23.3	2.76	one	one	off	high	off	four
triethylamine	101.2	125.9	176.2	2.4	1.37	7	4.2	2.67	4.1	0.66	0.35	20.2	7.7	one	zero	off	high	off	two
trichloroethylene	131.4	81.8	121.9	3.4	1.74	5	2.3	4	3.17	0.8	0.55	28.8	9.91	zero	zero	off	high	off	two
1,2-dimethoxyethane	90.1	96.8	140.4	7.2	-0.08	6	5	5.33	4.85	0	0.455	24.6	9.93	two	zero	off	high	off	two
1,2-dichloroethane	99.0	73.6	111.2	10.4	1.51	4	3	4	4.1	1.8	0.78	31.9	10.6	zero	zero	off	high	off	two
2-propanol	60.1	70.8	112.2	20.2	0.37	4	1.3	0	1.28	1.56	2.04	20.9	6.02	one	one	off	high	off	four
acetonitrile	41.1	46.0	66.2	36.6	0.04	3	2	0	1.24	3.92	0.37	28.7	11.9	one	zero	off	high	off	two
cyclohexane	84.2	102.4	146.4	2.0	2.74	4.2	2.2	1.33	1.54	0	0.89	24.7	13	zero	zero	off	high	off	zero
benzene	78.1	83.8	116.0	2.3	1.83	4.2	2.2	1.33	0.91	0	0.6	28.2	12.7	zero	zero	off	high	off	zero
2-butanone	72.1	81.8	123.3	18.6	0.56	5	2.3	4	1.81	2.78	0.405	24	12.6	one	zero	off	high	off	zero
1-chlorobutane	92.6	93.4	147.0	7.3	2.18	5	4	4	4.54	2.05	0.422	23.2	13.7	zero	zero	off	high	off	zero
ethanol	46.1	54.2	86.1	25.3	-0.01	3	2	0	1.93	1.69	1.07	22	7.87	one	one	off	high	off	zero
ethylacetate	87.1	90.7	131.0	6.1	0.37	6	3.2	5.33	2.67	1.78	0.42	23.4	12.6	two	zero	off	high	off	zero
carbon tetrachloride	153.8	84.5	118.7	2.2	3.58	5	1	0	2.15	0	0.91	26.4	15.2	zero	zero	off	high	off	zero
hexane	86.2	113.2	182.5	1.9	3.11	6	5	5.33	5	0	0.3	17.9	20.2	zero	zero	off	high	off	zero
tetrahydrofuran	72.1	77.2	110.6	7.5	0.51	3.2	1.4	0.64	0.89	1.75	0.46	26.4	21.6	one	zero	off	high	off	zero
methanol	32.0	37.4	59.3	32.6	-0.36	2	0	0	0	1.7	0.54	22.1	16.9	one	one	off	high	off	zero
chloroform	119.4	70.9	102.7	4.8	1.62	4	1.3	0	2.59	1.04	0.54	26.7	26.2	zero	zero	off	high	off	zero
methyl acetate	74.1	73.8	109.3	7.1	0.02	5	2.3	4	1.76	1.72	0.36	24.7	28.8	two	zero	off	high	off	zero

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
acetone	58.1	65.1	95.7	21.0	-0.1	4	1.3	0	0.96	2.88	0.31	23.5	30.8	one	zero	off	high	off	five
2-methoxy-2-methylpropane	88.1	105.0	149.2	4.5	0.98	6	1.6	5.33	1.59	1.2	0.35	19.1	26.9	one	zero	off	high	off	zero
cyclopentane	70.1	85.4	121.9	2.0	2.28	3.2	1.4	0.64	0.92	0	0.413	21.9	42.3	zero	zero	off	high	off	zero
formamide	45.0	42.5	66.4	111.0	-1.58	3	2	0	1.21	3.73	3.34	57	0.002	one	two	off	high	off	five
methanoic acid	46.0	39.7	58.4	51.1	-0.96	3	2	0	1.43	1.41	1.61	37.1	5.75	two	one	off	high	off	five
1,5-pentanediol	104.1	113.4	169.0	26.2	0.2	7	6	6	5.85	2.5	115	43.4	0.002	two	two	on	low	off	zero
1-methylnapthalene	142.2	144.3	181.6	2.9	3.22	7.6	3.2	1.45	1.39	0	3.1	39.8	0.009	zero	zero	on	low	off	two
dodecane	170.3	214.7	336.1	2.0	5.85	12	11	11.11	11	0	1.38	24.9	0.016	zero	zero	on	low	off	four
nitrobenzene	123.1	107.8	138.5	35.6	1.72	7.1	3.2	2	1.55	4.22	1.86	41.7	0.03	two	zero	on	low	off	zero
1-octanol	130.2	155.7	222.4	10.3	2.8	9	8	8	7.92	1.8	7.29	27.1	0.01	one	one	on	low	off	four
dimethylsulphoxide	78.1	72.6	109.7	47.2	-0.32	4	1.3	0	1.52	3.96	1.99	42.9	0.084	one	zero	on	low	off	five
aniline	93.1	95.4	130.5	7.1	1.08	5.1	2.3	1.5	0.98	1.13	3.85	42.1	0.09	zero	two	on	low	off	zero
2-octanol	130.2	155.4	224.8	8.1	2.72	9	6.1	8	6.06	1.7	6.49	26.3	0.032	one	one	on	low	off	zero
2-butoxyethanol	118.2	130.4	187.6	9.4	0.84	8	7	7.2	6.85	9.3	3.15	26.1	0.15	two	one	on	low	off	three
furfural	96.1	84.0	111.6	42.1	1.55	5.1	2.3	1.19	0.94	3.5	1.59	43.1	0.29	two	zero	on	low	off	five
2-methoxyethylether	134.2	138.6	203.0	9.8	-0.21	9	8	8	7.77	2	0.989	27	0.315	three	zero	on	low	off	three
cyclohexanol	100.2	110.3	154.3	16.4	1.5	5.1	2.3	1.5	1.69	1.61	57.5	32.9	0.1	one	one	on	low	off	zero
1-hexanol	102.2	122.0	175.9	13.0	1.88	7	6	6	5.93	1.58	4.58	25.8	0.11	one	one	on	low	off	four
anisole	108.1	109.5	145.6	4.3	1.81	6.1	3.1	1.8	1.65	1.38	1.06	35.1	0.47	one	zero	on	low	off	two
N,N-dimethylformamide	73.1	77.3	111.6	38.3	-1.17	5	2.3	4	1.57	3.82	0.79	37.1	0.439	one	zero	on	low	off	five
pentylacetate	130.1	141.4	197.6	4.8	1.81	9	6.1	8	5.52	1.75	0.862	25.2	0.6	two	zero	on	low	off	two
butylether	130.2	155.5	238.7	3.1	2.71	9	8	8	7.92	1.17	0.64	22.4	0.898	one	zero	on	low	off	four
xylene	106.2	117.1	159.5	2.3	2.8	6.1	2.5	1.8	1.34	0	0.596	28.5	1.13	zero	zero	on	low	off	four
1-pentanol	88.1	104.6	159.1	15.1	1.43	6	5	5.33	4.93	1.7	3.62	36.5	0.259	one	one	on	low	off	three
2-ethoxyethanol	90.1	96.3	146.7	13.4	-0.14	6	5	5.33	4.85	2.1	1.85	28.4	0.71	two	one	on	low	off	zero
3-methyl-1-butanol	88.1	105.1	152.7	23.7	1.22	6	3.2	5.33	3.14	1.8	3.69	23.7	0.315	one	one	on	low	off	three
butylacetate	115.2	124.8	177.7	5.1	1.35	8	5.1	7.2	4.56	1.9	0.69	24.9	1.66	two	zero	on	low	off	one
diethyl carbonate	118.1	116.4	168.4	2.8	1.36	8	5.1	5	4.5	1.1	0.748	26.4	1.63	three	zero	on	low	off	zero
2-methoxyethanol	76.1	79.6	117.0	17.2	-0.49	5	4	4	3.86	2.36	1.6	30.8	1.31	two	one	on	low	off	four
tetrachloroethene	165.8	96.1	137.3	2.3	2.43	6	2.2	3	3.42	0	0.84	31.3	2.42	zero	zero	on	low	off	one

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
acetic acid	60.1	56.6	81.1	6.2	-0.2	4	1.3	0	0.92	1.7	1.06	27.1	2.07	two	one	on	low	off	five
2-pentanol	88.1	104.8	156.3	13.7	1.35	6	3.2	5.33	3.14	1.7	3.47	23.5	0.804	one	one	on	low	off	four
4-methyl-2-pentanone	100.2	115.9	168.7	13.1	1.27	7	3.1	6	2.65	2.81	4.07	23.6	2.64	one	zero	on	low	off	two
1-butanol	74.1	87.8	136.3	17.8	0.97	5	4	4	3.93	1.66	2.54	24.9	0.86	one	one	on	low	off	three
isobutyl acetate	116.2	124.9	178.4	5.1	1.21	8	3.9	7.2	3.44	1.9	0.676	23.1	2.39	two	zero	on	low	off	four
pyridine	79.1	79.3	108.5	13.3	0.68	4.2	2.2	1.33	0.87	2.22	0.88	36.6	2.76	one	zero	on	low	off	zero
toluene	92.1	100.6	134.8	2.4	2.32	5.1	2.3	1.5	1.12	0.38	0.56	27.9	3.79	zero	zero	on	low	off	four
2-methyl-1-propanol	74.1	87.9	131.1	17.9	0.83	5	2.3	4	2.19	1.64	3.33	23	1.39	one	one	on	low	off	three
1,4-dioxan	88.1	85.9	118.7	2.2	-0.26	4.2	2.2	1.33	1.47	0	1.18	32.8	4.95	two	zero	on	low	off	five
water	18.0	19.6	36.3	80.0	-0.36	0	0	0	0	1.87	0.89	73	2.72	one	two	on	low	off	five
2,2,4-trimethylpentane	114.2	147.3	210.1	1.9	3.36	8	2.5	7.2	2.52	0	0.5404	18.3	6.5	zero	zero	on	low	off	four
heptane	100.2	130.2	207.4	1.9	3.57	7	6	6	6	0	0.39	19.7	6.09	zero	zero	on	low	off	two
2-butanol	74.1	87.9	131.5	17.3	0.89	5	2.3	4	2.19	1.8	3.1	22.5	2.32	one	one	on	low	off	four
1-propanol	60.1	70.8	109.0	20.8	0.51	4	3	4	2.93	1.55	1.95	23.3	2.76	one	one	on	low	off	one
triethylamine	101.2	125.9	176.2	2.4	1.37	7	4.2	2.67	4.1	0.66	0.35	20.2	7.7	one	zero	on	low	off	two
trichloroethylene	131.4	81.8	121.9	3.4	1.74	5	2.3	4	3.17	0.8	0.55	28.8	9.91	zero	zero	on	low	off	three
1,2-dimethoxyethane	90.1	96.8	140.4	7.2	-0.08	6	5	5.33	4.85	0	0.455	24.6	9.93	two	zero	on	low	off	one
1,2-dichloroethane	99.0	73.6	111.2	10.4	1.51	4	3	4	4.1	1.8	0.78	31.9	10.6	zero	zero	on	low	off	one
2-propanol	60.1	70.8	112.2	20.2	0.37	4	1.3	0	1.28	1.56	2.04	20.9	6.02	one	one	on	low	off	one
acetonitrile	41.1	46.0	66.2	36.6	0.04	3	2	0	1.24	3.92	0.37	28.7	11.9	one	zero	on	low	off	zero
cyclohexane	84.2	102.4	146.4	2.0	2.74	4.2	2.2	1.33	1.54	0	0.89	24.7	13	zero	zero	on	low	off	zero
benzene	78.1	83.8	116.0	2.3	1.83	4.2	2.2	1.33	0.91	0	0.6	28.2	12.7	zero	zero	on	low	off	one
2-butanone	72.1	81.8	123.3	18.6	0.56	5	2.3	4	1.81	2.78	0.405	24	12.6	one	zero	on	low	off	three
1-chlorobutane	92.6	93.4	147.0	7.3	2.18	5	4	4	4.54	2.05	0.422	23.2	13.7	zero	zero	on	low	off	four
ethanol	46.1	54.2	86.1	25.3	-0.01	3	2	0	1.93	1.69	1.07	22	7.87	one	one	on	low	off	zero
ethylacetate	87.1	90.7	131.0	6.1	0.37	6	3.2	5.33	2.67	1.78	0.42	23.4	12.6	two	zero	on	low	off	three
carbon tetrachloride	153.8	84.5	118.7	2.2	3.58	5	1	0	2.15	0	0.91	26.4	15.2	zero	zero	on	low	off	two
hexane	86.2	113.2	182.5	1.9	3.11	6	5	5.33	5	0	0.3	17.9	20.2	zero	zero	on	low	off	zero
tetrahydrofuran	72.1	77.2	110.6	7.5	0.51	3.2	1.4	0.64	0.89	1.75	0.46	26.4	21.6	one	zero	on	low	off	zero
methanol	32.0	37.4	59.3	32.6	-0.36	2	0	0	0	1.7	0.54	22.1	16.9	one	one	on	low	off	zero

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form
chloroform	119.4	70.9	102.7	4.8	1.62	4	1.3	0	2.59	1.04	0.54	26.7	26.2	zero	zero	on	low	off	two
methyl acetate	74.1	73.8	109.3	7.1	0.02	5	2.3	4	1.76	1.72	0.36	24.7	28.8	two	zero	on	low	off	two
acetone	58.1	65.1	95.7	21.0	-0.1	4	1.3	0	0.96	2.88	0.31	23.5	30.8	one	zero	on	low	off	five
2-methoxy-2-methylpropane	88.1	105.0	149.2	4.5	0.98	6	1.6	5.33	1.59	1.2	0.35	19.1	26.9	one	zero	on	low	off	zero
cyclopentane	70.1	85.4	121.9	2.0	2.28	3.2	1.4	0.64	0.92	0	0.413	21.9	42.3	zero	zero	on	low	off	one
formamide	45.0	42.5	66.4	111.0	-1.58	3	2	0	1.21	3.73	3.34	57	0.002	one	two	on	low	off	five
methanoic acid	46.0	39.7	58.4	51.1	-0.96	3	2	0	1.43	1.41	1.61	37.1	5.75	two	one	on	low	off	five
1,5-pentanediol	104.1	113.4	169.0	26.2	0.2	7	6	6	5.85	2.5	115	43.4	0.002	two	two	on	mid	on	zero
1-methylnapthalene	142.2	144.3	181.6	2.9	3.22	7.6	3.2	1.45	1.39	0	3.1	39.8	0.009	zero	zero	on	mid	on	two
dodecane	170.3	214.7	336.1	2.0	5.85	12	11	11.11	11	0	1.38	24.9	0.016	zero	zero	on	mid	on	two
nitrobenzene	123.1	107.8	138.5	35.6	1.72	7.1	3.2	2	1.55	4.22	1.86	41.7	0.03	two	zero	on	mid	on	two
1-octanol	130.2	155.7	222.4	10.3	2.8	9	8	8	7.92	1.8	7.29	27.1	0.01	one	one	on	mid	on	two
dimethylsulphoxide	78.1	72.6	109.7	47.2	-0.32	4	1.3	0	1.52	3.96	1.99	42.9	0.084	one	zero	on	mid	on	five
aniline	93.1	95.4	130.5	7.1	1.08	5.1	2.3	1.5	0.98	1.13	3.85	42.1	0.09	zero	two	on	mid	on	zero
2-octanol	130.2	155.4	224.8	8.1	2.72	9	6.1	8	6.06	1.7	6.49	26.3	0.032	one	one	on	mid	on	two
2-butoxyethanol	118.2	130.4	187.6	9.4	0.84	8	7	7.2	6.85	9.3	3.15	26.1	0.15	two	one	on	mid	on	two
furfural	96.1	84.0	111.6	42.1	1.55	5.1	2.3	1.19	0.94	3.5	1.59	43.1	0.29	two	zero	on	mid	on	five
2-methoxyethylether	134.2	138.6	203.0	9.8	-0.21	9	8	8	7.77	2	0.989	27	0.315	three	zero	on	mid	on	two
cyclohexanol	100.2	110.3	154.3	16.4	1.5	5.1	2.3	1.5	1.69	1.61	57.5	32.9	0.1	one	one	on	mid	on	two
1-hexanol	102.2	122.0	175.9	13.0	1.88	7	6	6	5.93	1.58	4.58	25.8	0.11	one	one	on	mid	on	two
anisole	108.1	109.5	145.6	4.3	1.81	6.1	3.1	1.8	1.65	1.38	1.06	35.1	0.47	one	zero	on	mid	on	zero
N,N-dimethylformamide	73.1	77.3	111.6	38.3	-1.17	5	2.3	4	1.57	3.82	0.79	37.1	0.439	one	zero	on	mid	on	five
pentylacetate	130.1	141.4	197.6	4.8	1.81	9	6.1	8	5.52	1.75	0.862	25.2	0.6	two	zero	on	mid	on	two
butylether	130.2	155.5	238.7	3.1	2.71	9	8	8	7.92	1.17	0.64	22.4	0.898	one	zero	on	mid	on	two
xylene	106.2	117.1	159.5	2.3	2.8	6.1	2.5	1.8	1.34	0	0.596	28.5	1.13	zero	zero	on	mid	on	two
1-pentanol	88.1	104.6	159.1	15.1	1.43	6	5	5.33	4.93	1.7	3.62	36.5	0.259	one	one	on	mid	on	two
2-ethoxyethanol	90.1	96.3	146.7	13.4	-0.14	6	5	5.33	4.85	2.1	1.85	28.4	0.71	two	one	on	mid	on	zero
3-methyl-1-butanol	88.1	105.1	152.7	23.7	1.22	6	3.2	5.33	3.14	1.8	3.69	23.7	0.315	one	one	on	mid	on	two
butylacetate	115.2	124.8	177.7	5.1	1.35	8	5.1	7.2	4.56	1.9	0.69	24.9	1.66	two	zero	on	mid	on	two
diethyl carbonate	118.1	116.4	168.4	2.8	1.36	8	5.1	5	4.5	1.1	0.748	26.4	1.63	three	zero	on	mid	on	zero

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
2-methoxyethanol	76.1	79.6	117.0	17.2	-0.49	5	4	4	3.86	2.36	1.6	30.8	1.31	two	one	on	mid	on	zero
tetrachloroethene	165.8	96.1	137.3	2.3	2.43	6	2.2	3	3.42	0	0.84	31.3	2.42	zero	zero	on	mid	on	two
acetic acid	60.1	56.6	81.1	6.2	-0.2	4	1.3	0	0.92	1.7	1.06	27.1	2.07	two	one	on	mid	on	five
2-pentanol	88.1	104.8	156.3	13.7	1.35	6	3.2	5.33	3.14	1.7	3.47	23.5	0.804	one	one	on	mid	on	two
4-methyl-2-pentanone	100.2	115.9	168.7	13.1	1.27	7	3.1	6	2.65	2.81	4.07	23.6	2.64	one	zero	on	mid	on	two
1-butanol	74.1	87.8	136.3	17.8	0.97	5	4	4	3.93	1.66	2.54	24.9	0.86	one	one	on	mid	on	two
isobutyl acetate	116.2	124.9	178.4	5.1	1.21	8	3.9	7.2	3.44	1.9	0.676	23.1	2.39	two	zero	on	mid	on	two
pyridine	79.1	79.3	108.5	13.3	0.68	4.2	2.2	1.33	0.87	2.22	0.88	36.6	2.76	one	zero	on	mid	on	zero
toluene	92.1	100.6	134.8	2.4	2.32	5.1	2.3	1.5	1.12	0.38	0.56	27.9	3.79	zero	zero	on	mid	on	three
2-methyl-1-propanol	74.1	87.9	131.1	17.9	0.83	5	2.3	4	2.19	1.64	3.33	23	1.39	one	one	on	mid	on	three
1,4-dioxan	88.1	85.9	118.7	2.2	-0.26	4.2	2.2	1.33	1.47	0	1.18	32.8	4.95	two	zero	on	mid	on	five
water	18.0	19.6	36.3	80.0	-0.36	0	0	0	0	1.87	0.89	73	2.72	one	two	on	mid	on	five
2,2,4-trimethylpentane	114.2	147.3	210.1	1.9	3.36	8	2.5	7.2	2.52	0	0.5404	18.3	6.5	zero	zero	on	mid	on	two
heptane	100.2	130.2	207.4	1.9	3.57	7	6	6	6	0	0.39	19.7	6.09	zero	zero	on	mid	on	four
2-butanol	74.1	87.9	131.5	17.3	0.89	5	2.3	4	2.19	1.8	3.1	22.5	2.32	one	one	on	mid	on	three
1-propanol	60.1	70.8	109.0	20.8	0.51	4	3	4	2.93	1.55	1.95	23.3	2.76	one	one	on	mid	on	two
triethylamine	101.2	125.9	176.2	2.4	1.37	7	4.2	2.67	4.1	0.66	0.35	20.2	7.7	one	zero	on	mid	on	two
trichloroethylene	131.4	81.8	121.9	3.4	1.74	5	2.3	4	3.17	0.8	0.55	28.8	9.91	zero	zero	on	mid	on	two
1,2-dimethoxyethane	90.1	96.8	140.4	7.2	-0.08	6	5	5.33	4.85	0	0.455	24.6	9.93	two	zero	on	mid	on	two
1,2-dichloroethane	99.0	73.6	111.2	10.4	1.51	4	3	4	4.1	1.8	0.78	31.9	10.6	zero	zero	on	mid	on	two
2-propanol	60.1	70.8	112.2	20.2	0.37	4	1.3	0	1.28	1.56	2.04	20.9	6.02	one	one	on	mid	on	two
acetonitrile	41.1	46.0	66.2	36.6	0.04	3	2	0	1.24	3.92	0.37	28.7	11.9	one	zero	on	mid	on	four
cyclohexane	84.2	102.4	146.4	2.0	2.74	4.2	2.2	1.33	1.54	0	0.89	24.7	13	zero	zero	on	mid	on	two
benzene	78.1	83.8	116.0	2.3	1.83	4.2	2.2	1.33	0.91	0	0.6	28.2	12.7	zero	zero	on	mid	on	two
2-butanone	72.1	81.8	123.3	18.6	0.56	5	2.3	4	1.81	2.78	0.405	24	12.6	one	zero	on	mid	on	two
1-chlorobutane	92.6	93.4	147.0	7.3	2.18	5	4	4	4.54	2.05	0.422	23.2	13.7	zero	zero	on	mid	on	four
ethanol	46.1	54.2	86.1	25.3	-0.01	3	2	0	1.93	1.69	1.07	22	7.87	one	one	on	mid	on	two
ethylacetate	87.1	90.7	131.0	6.1	0.37	6	3.2	5.33	2.67	1.78	0.42	23.4	12.6	two	zero	on	mid	on	two
carbon tetrachloride	153.8	84.5	118.7	2.2	3.58	5	1	0	2.15	0	0.91	26.4	15.2	zero	zero	on	mid	on	two
hexane	86.2	113.2	182.5	1.9	3.11	6	5	5.33	5	0	0.3	17.9	20.2	zero	zero	on	mid	on	one

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
tetrahydrofuran	72.1	77.2	110.6	7.5	0.51	3.2	1.4	0.64	0.89	1.75	0.46	26.4	21.6	one	zero	on	mid	on	two
methanol	32.0	37.4	59.3	32.6	-0.36	2	0	0	0	1.7	0.54	22.1	16.9	one	one	on	mid	on	zero
chloroform	119.4	70.9	102.7	4.8	1.62	4	1.3	0	2.59	1.04	0.54	26.7	26.2	zero	zero	on	mid	on	two
methyl acetate	74.1	73.8	109.3	7.1	0.02	5	2.3	4	1.76	1.72	0.36	24.7	28.8	two	zero	on	mid	on	two
acetone	58.1	65.1	95.7	21.0	-0.1	4	1.3	0	0.96	2.88	0.31	23.5	30.8	one	zero	on	mid	on	five
2-methoxy-2-methylpropane	88.1	105.0	149.2	4.5	0.98	6	1.6	5.33	1.59	1.2	0.35	19.1	26.9	one	zero	on	mid	on	two
cyclopentane	70.1	85.4	121.9	2.0	2.28	3.2	1.4	0.64	0.92	0	0.413	21.9	42.3	zero	zero	on	mid	on	two
formamide	45.0	42.5	66.4	111.0	-1.58	3	2	0	1.21	3.73	3.34	57	0.002	one	two	on	mid	on	five
methanoic acid	46.0	39.7	58.4	51.1	-0.96	3	2	0	1.43	1.41	1.61	37.1	5.75	two	one	on	mid	on	five
1,5-pentanediol	104.1	113.4	169.0	26.2	0.2	7	6	6	5.85	2.5	115	43.4	0.002	two	two	off	mid	off	three
1-methylnapthalene	142.2	144.3	181.6	2.9	3.22	7.6	3.2	1.45	1.39	0	3.1	39.8	0.009	zero	zero	off	mid	off	four
dodecane	170.3	214.7	336.1	2.0	5.85	12	11	11.11	11	0	1.38	24.9	0.016	zero	zero	off	mid	off	zero
nitrobenzene	123.1	107.8	138.5	35.6	1.72	7.1	3.2	2	1.55	4.22	1.86	41.7	0.03	two	zero	off	mid	off	four
1-octanol	130.2	155.7	222.4	10.3	2.8	9	8	8	7.92	1.8	7.29	27.1	0.01	one	one	off	mid	off	two
dimethylsulphoxide	78.1	72.6	109.7	47.2	-0.32	4	1.3	0	1.52	3.96	1.99	42.9	0.084	one	zero	off	mid	off	five
aniline	93.1	95.4	130.5	7.1	1.08	5.1	2.3	1.5	0.98	1.13	3.85	42.1	0.09	zero	two	off	mid	off	two
2-octanol	130.2	155.4	224.8	8.1	2.72	9	6.1	8	6.06	1.7	6.49	26.3	0.032	one	one	off	mid	off	two
2-butoxyethanol	118.2	130.4	187.6	9.4	0.84	8	7	7.2	6.85	9.3	3.15	26.1	0.15	two	one	off	mid	off	four
furfural	96.1	84.0	111.6	42.1	1.55	5.1	2.3	1.19	0.94	3.5	1.59	43.1	0.29	two	zero	off	mid	off	five
2-methoxyethylether	134.2	138.6	203.0	9.8	-0.21	9	8	8	7.77	2	0.989	27	0.315	three	zero	off	mid	off	two
cyclohexanol	100.2	110.3	154.3	16.4	1.5	5.1	2.3	1.5	1.69	1.61	57.5	32.9	0.1	one	one	off	mid	off	four
1-hexanol	102.2	122.0	175.9	13.0	1.88	7	6	6	5.93	1.58	4.58	25.8	0.11	one	one	off	mid	off	two
anisole	108.1	109.5	145.6	4.3	1.81	6.1	3.1	1.8	1.65	1.38	1.06	35.1	0.47	one	zero	off	mid	off	four
N,N-dimethylformamide	73.1	77.3	111.6	38.3	-1.17	5	2.3	4	1.57	3.82	0.79	37.1	0.439	one	zero	off	mid	off	five
pentylacetate	130.1	141.4	197.6	4.8	1.81	9	6.1	8	5.52	1.75	0.862	25.2	0.6	two	zero	off	mid	off	two
butylether	130.2	155.5	238.7	3.1	2.71	9	8	8	7.92	1.17	0.64	22.4	0.898	one	zero	off	mid	off	four
xylene	106.2	117.1	159.5	2.3	2.8	6.1	2.5	1.8	1.34	0	0.596	28.5	1.13	zero	zero	off	mid	off	three
1-pentanol	88.1	104.6	159.1	15.1	1.43	6	5	5.33	4.93	1.7	3.62	36.5	0.259	one	one	off	mid	off	four
2-ethoxyethanol	90.1	96.3	146.7	13.4	-0.14	6	5	5.33	4.85	2.1	1.85	28.4	0.71	two	one	off	mid	off	four
3-methyl-1-butanol	88.1	105.1	152.7	23.7	1.22	6	3.2	5.33	3.14	1.8	3.69	23.7	0.315	one	one	off	mid	off	three

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
butylacetate	115.2	124.8	177.7	5.1	1.35	8	5.1	7.2	4.56	1.9	0.69	24.9	1.66	two	zero	off	mid	off	four
diethyl carbonate	118.1	116.4	168.4	2.8	1.36	8	5.1	5	4.5	1.1	0.748	26.4	1.63	three	zero	off	mid	off	zero
2-methoxyethanol	76.1	79.6	117.0	17.2	-0.49	5	4	4	3.86	2.36	1.6	30.8	1.31	two	one	off	mid	off	four
tetrachloroethene	165.8	96.1	137.3	2.3	2.43	6	2.2	3	3.42	0	0.84	31.3	2.42	zero	zero	off	mid	off	zero
acetic acid	60.1	56.6	81.1	6.2	-0.2	4	1.3	0	0.92	1.7	1.06	27.1	2.07	two	one	off	mid	off	five
2-pentanol	88.1	104.8	156.3	13.7	1.35	6	3.2	5.33	3.14	1.7	3.47	23.5	0.804	one	one	off	mid	off	four
4-methyl-2-pentanone	100.2	115.9	168.7	13.1	1.27	7	3.1	6	2.65	2.81	4.07	23.6	2.64	one	zero	off	mid	off	four
1-butanol	74.1	87.8	136.3	17.8	0.97	5	4	4	3.93	1.66	2.54	24.9	0.86	one	one	off	mid	off	three
isobutyl acetate	116.2	124.9	178.4	5.1	1.21	8	3.9	7.2	3.44	1.9	0.676	23.1	2.39	two	zero	off	mid	off	zero
pyridine	79.1	79.3	108.5	13.3	0.68	4.2	2.2	1.33	0.87	2.22	0.88	36.6	2.76	one	zero	off	mid	off	zero
toluene	92.1	100.6	134.8	2.4	2.32	5.1	2.3	1.5	1.12	0.38	0.56	27.9	3.79	zero	zero	off	mid	off	zero
2-methyl-1-propanol	74.1	87.9	131.1	17.9	0.83	5	2.3	4	2.19	1.64	3.33	23	1.39	one	one	off	mid	off	four
1,4-dioxan	88.1	85.9	118.7	2.2	-0.26	4.2	2.2	1.33	1.47	0	1.18	32.8	4.95	two	zero	off	mid	off	five
water	18.0	19.6	36.3	80.0	-0.36	0	0	0	0	1.87	0.89	73	2.72	one	two	off	mid	off	five
2,2,4-trimethylpentane	114.2	147.3	210.1	1.9	3.36	8	2.5	7.2	2.52	0	0.5404	18.3	6.5	zero	zero	off	mid	off	zero
heptane	100.2	130.2	207.4	1.9	3.57	7	6	6	6	0	0.39	19.7	6.09	zero	zero	off	mid	off	zero
2-butanol	74.1	87.9	131.5	17.3	0.89	5	2.3	4	2.19	1.8	3.1	22.5	2.32	one	one	off	mid	off	four
1-propanol	60.1	70.8	109.0	20.8	0.51	4	3	4	2.93	1.55	1.95	23.3	2.76	one	one	off	mid	off	four
triethylamine	101.2	125.9	176.2	2.4	1.37	7	4.2	2.67	4.1	0.66	0.35	20.2	7.7	one	zero	off	mid	off	four
trichloroethylene	131.4	81.8	121.9	3.4	1.74	5	2.3	4	3.17	0.8	0.55	28.8	9.91	zero	zero	off	mid	off	four
1,2-dimethoxyethane	90.1	96.8	140.4	7.2	-0.08	6	5	5.33	4.85	0	0.455	24.6	9.93	two	zero	off	mid	off	two
1,2-dichloroethane	99.0	73.6	111.2	10.4	1.51	4	3	4	4.1	1.8	0.78	31.9	10.6	zero	zero	off	mid	off	one
2-propanol	60.1	70.8	112.2	20.2	0.37	4	1.3	0	1.28	1.56	2.04	20.9	6.02	one	one	off	mid	off	two
acetonitrile	41.1	46.0	66.2	36.6	0.04	3	2	0	1.24	3.92	0.37	28.7	11.9	one	zero	off	mid	off	four
cyclohexane	84.2	102.4	146.4	2.0	2.74	4.2	2.2	1.33	1.54	0	0.89	24.7	13	zero	zero	off	mid	off	zero
benzene	78.1	83.8	116.0	2.3	1.83	4.2	2.2	1.33	0.91	0	0.6	28.2	12.7	zero	zero	off	mid	off	four
2-butanone	72.1	81.8	123.3	18.6	0.56	5	2.3	4	1.81	2.78	0.405	24	12.6	one	zero	off	mid	off	four
1-chlorobutane	92.6	93.4	147.0	7.3	2.18	5	4	4	4.54	2.05	0.422	23.2	13.7	zero	zero	off	mid	off	zero
ethanol	46.1	54.2	86.1	25.3	-0.01	3	2	0	1.93	1.69	1.07	22	7.87	one	one	off	mid	off	four
ethylacetate	87.1	90.7	131.0	6.1	0.37	6	3.2	5.33	2.67	1.78	0.42	23.4	12.6	two	zero	off	mid	off	four

Table S1 continued.

Solvent [a]	MW [b]	Vm [c]	Area [d]	DC [e]	AlogP 98 [f]	K 1 [g]	K 2 [h]	K 3 [i]	PHI [j]	DM [k]	V [l]	ST [m]	VP [n]	HB A [o]	HB D [p]	Vortex [q]	T_{sat} [r]	Vacuum [s]	Form [t]
carbon tetrachloride	153.8	84.5	118.7	2.2	3.58	5	1	0	2.15	0	0.91	26.4	15.2	zero	zero	off	mid	off	zero
Hexane	86.2	113.2	182.5	1.9	3.11	6	5	5.33	5	0	0.3	17.9	20.2	zero	zero	off	mid	off	zero
tetrahydrofuran	72.1	77.2	110.6	7.5	0.51	3.2	1.4	0.64	0.89	1.75	0.46	26.4	21.6	one	zero	off	mid	off	two
Methanol	32.0	37.4	59.3	32.6	-0.36	2	0	0	0	1.7	0.54	22.1	16.9	one	one	off	mid	off	three
Chloroform	119.4	70.9	102.7	4.8	1.62	4	1.3	0	2.59	1.04	0.54	26.7	26.2	zero	zero	off	mid	off	two
methyl acetate	74.1	73.8	109.3	7.1	0.02	5	2.3	4	1.76	1.72	0.36	24.7	28.8	two	zero	off	mid	off	three
Acetone	58.1	65.1	95.7	21.0	-0.1	4	1.3	0	0.96	2.88	0.31	23.5	30.8	one	zero	off	mid	off	five
2-methoxy-2-methylpropane	88.1	105.0	149.2	4.5	0.98	6	1.6	5.33	1.59	1.2	0.35	19.1	26.9	one	zero	off	mid	off	three
Cyclopentane	70.1	85.4	121.9	2.0	2.28	3.2	1.4	0.64	0.92	0	0.413	21.9	42.3	zero	zero	off	mid	off	zero
Formamide	45.0	42.5	66.4	111.0	-1.58	3	2	0	1.21	3.73	3.34	57	0.002	one	two	off	mid	off	five
methanoic acid	46.0	39.7	58.4	51.1	-0.96	3	2	0	1.43	1.41	1.61	37.1	5.75	two	one	off	mid	off	five
trifluoroethanol	100.0	69.1	99.0	27.7	0.65	6	1.6	5.33	1.4	4.8	1.99	21.1	9.87	one	one	off	mid	off	five
N-methylpyrrolidone	99.1	99.9	145.0	32.2	-0.16	5.1	1.9	0.96	1.01	4.1	1.67	58.6	0.04	one	zero	on	high	off	three
N-methylpyrrolidone	99.1	99.9	145.0	32.2	-0.16	5.1	1.9	0.96	1.01	4.1	1.67	58.6	0.04	one	zero	off	high	off	zero
N-methylpyrrolidone	99.1	99.9	145.0	32.2	-0.16	5.1	1.9	0.96	1.01	4.1	1.67	58.6	0.04	one	zero	on	low	off	zero
N-methylpyrrolidone	99.1	99.9	145.0	32.2	-0.16	5.1	1.9	0.96	1.01	4.1	1.67	58.6	0.04	one	zero	on	mid	on	zero
N-methylpyrrolidone	99.1	99.9	145.0	32.2	-0.16	5.1	1.9	0.96	1.01	4.1	1.67	58.6	0.04	one	zero	off	mid	off	three
N,N-dimethylacetamide	87.1	94.3	137.2	38.9	-0.42	6	2.2	3	1.64	3.7	1.96	32.4	0.075	one	zero	on	high	off	one
N,N-dimethylacetamide	87.1	94.3	137.2	38.9	-0.42	6	2.2	3	1.64	3.7	1.96	32.4	0.075	one	zero	off	high	off	zero
N,N-dimethylacetamide	87.1	94.3	137.2	38.9	-0.42	6	2.2	3	1.64	3.7	1.96	32.4	0.075	one	zero	on	low	off	zero
N,N-dimethylacetamide	87.1	94.3	137.2	38.9	-0.42	6	2.2	3	1.64	3.7	1.96	32.4	0.075	one	zero	on	mid	on	zero
N,N-dimethylacetamide	87.1	94.3	137.2	38.9	-0.42	6	2.2	3	1.64	3.7	1.96	32.4	0.075	one	zero	off	mid	off	three
Nitromethane	61.0	52.8	77.5	37.3	0.29	4	1.3	0	0.85	3.46	0.63	36.5	4.79	two	zero	on	high	off	four
Nitromethane	61.0	52.8	77.5	37.3	0.29	4	1.3	0	0.85	3.46	0.63	36.5	4.79	two	zero	off	high	off	four
Nitromethane	61.0	52.8	77.5	37.3	0.29	4	1.3	0	0.85	3.46	0.63	36.5	4.79	two	zero	on	low	off	four
Nitromethane	61.0	52.8	77.5	37.3	0.29	4	1.3	0	0.85	3.46	0.63	36.5	4.79	two	zero	on	mid	on	two
nitromethane	61.0	52.8	77.5	37.3	0.29	4	1.3	0	0.85	3.46	0.63	36.5	4.79	two	zero	off	mid	off	two

[a] Solvent used for recrystallization [7]; [b] molecular weight (g $mole^{-1}$); [c] molecular volume / cm^3 mol^{-1} (calculated); [d] accessible surface area / $Å^2$ (calculated); [e] dielectric constant (literature and calculated); [f] AlogP98 (calculated); [g] Kappa1 (calculated); [h] Kappa2 (calculated); [i] Kappa3 (calculated); [j] Phi (calculated); [k] dipole moment / D (calculated and literature); [l] viscosity / mPA (literature); [m] surface tension / mNm^{-1} (literature); [n] vapor pressure / kPa (literature); [o] number of potential hydrogen bond

acceptors; [p] number of potential hydrogen bond donors; [q] Vortexing of solutions during crystallisation; [2 r] Temperature at which solutions were saturated prior to filtration and subsequent crystallization[2]; [s] Vacuum applied during crystallisation [2]; [t] Outcome of crystallization [2]. All literature values obtained from reference 3. Calculated parameters generated using Cerius[2] Descriptors+ module.[4]

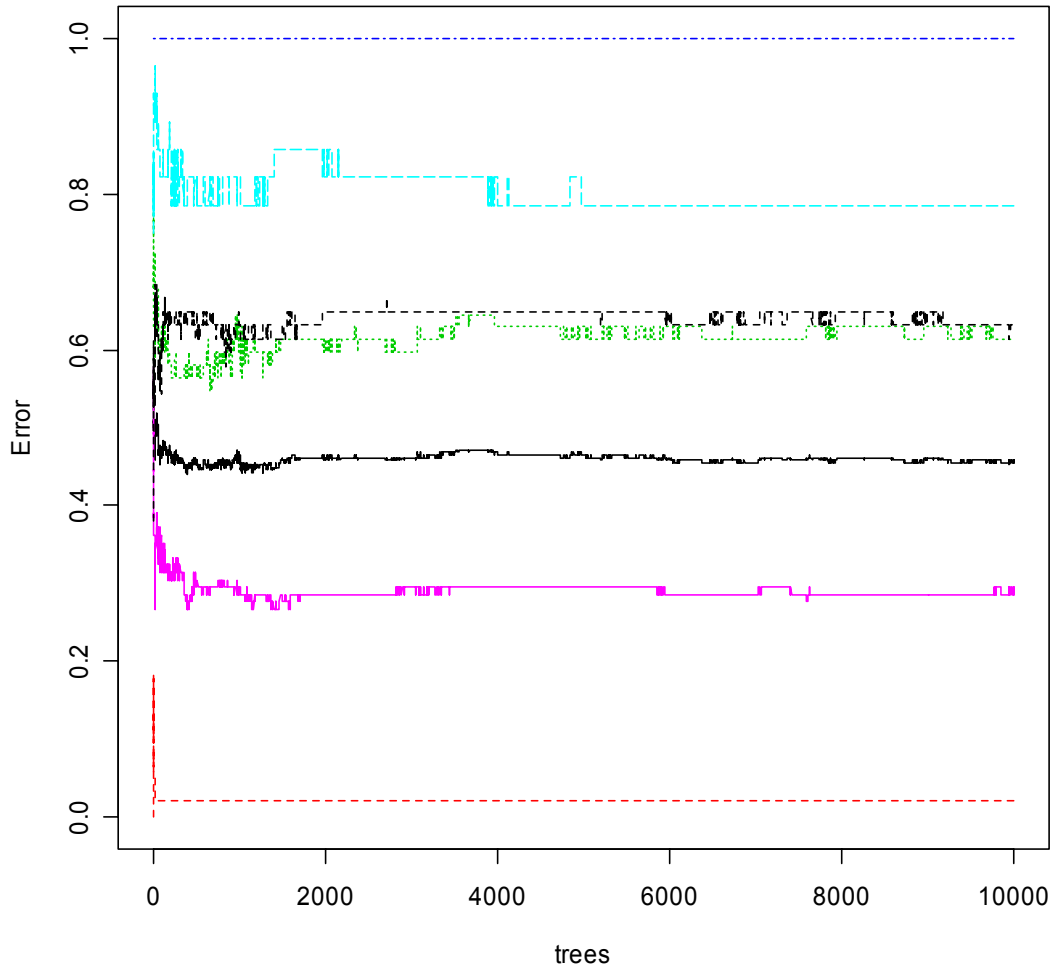

Fig. S1 Plot of Random Forest classification for data set presented in Table S1

Table S2. Confusion matrix from random forest analysis on all CBZ results from polymorph screen.

	Five	**four**	**one**	**three**	**two**	**zero**	**class.error**
Five	45	1	0	0	0	0	0.02173913
Four	0	24	1	2	26	9	0.61290323
One	3	5	0	0	5	3	1.00000000
Three	0	7	0	6	8	7	0.78571429
Two	0	18	2	3	74	8	0.29523810
Zero	0	11	3	8	14	21	0.63157895

Table S3 . Predicted probabilities (percentage votes) of CBZ recrystallizing as any of the defined outcomes from NM, DMA and NMP.

Solvent	**Outcomes**					
	Zero	**Form I**	**Form II**	**Form III**	**Mixed Phase**	**Solvate**
NM	0.12	0.007	0.14	0.05	0.16	**0.50**
DMA	0.07	0.005	0.12	0.06	0.16	**0.58**
NMP	0.19	0.003	0.1	0.1	0.16	**0.45**

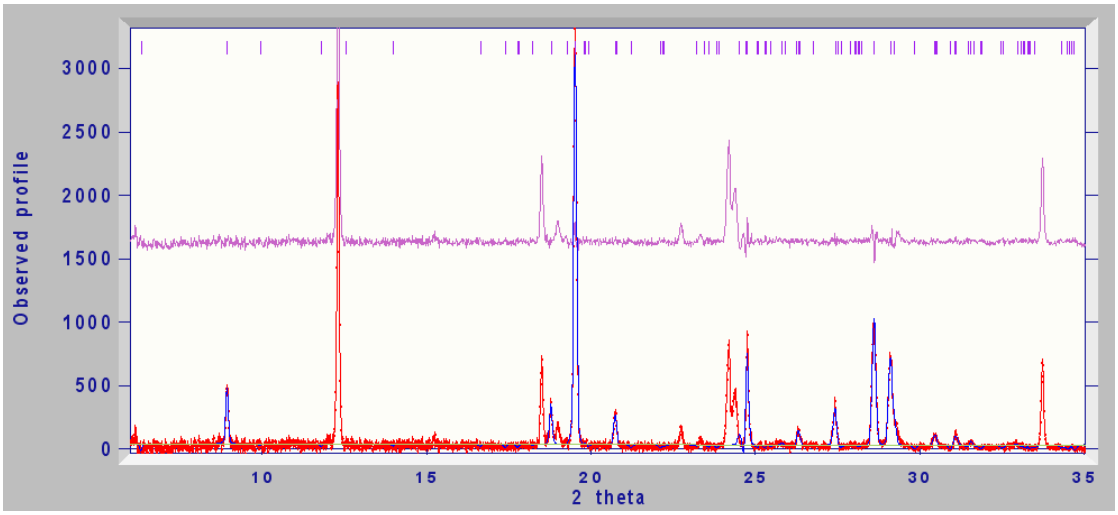

Figure S2a Carbamazepine – NM solvate. Refined unit cell parameters *a*, *b*, *c* (Å) = 10.20, 5.22, 28.95; α, β, γ (°) = 90.00, 99.70, 90.00 (P21/c); Pawley χ^2 = 15.6. The relatively high Pawley χ^2 value and significant misfit evident from the difference plot (pink) results from the presence of form I in the sample, due to partial desolvation during data collection.

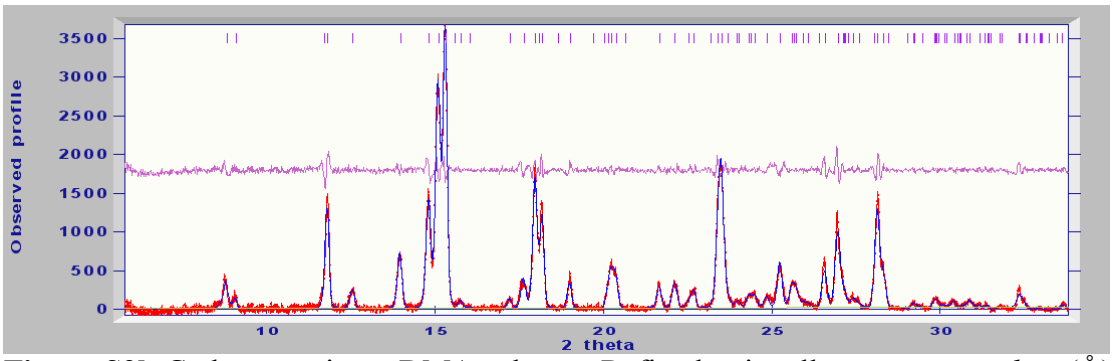

Figure S2b Carbamazepine – DMA solvate. Refined unit cell parameters *a*, *b*, *c* (Å) = 7.619, 19.535, 11.823; α, β, γ (°) = 90.00, 96.36, 90.00 (P21/c); Pawley χ^2 = 2.83.

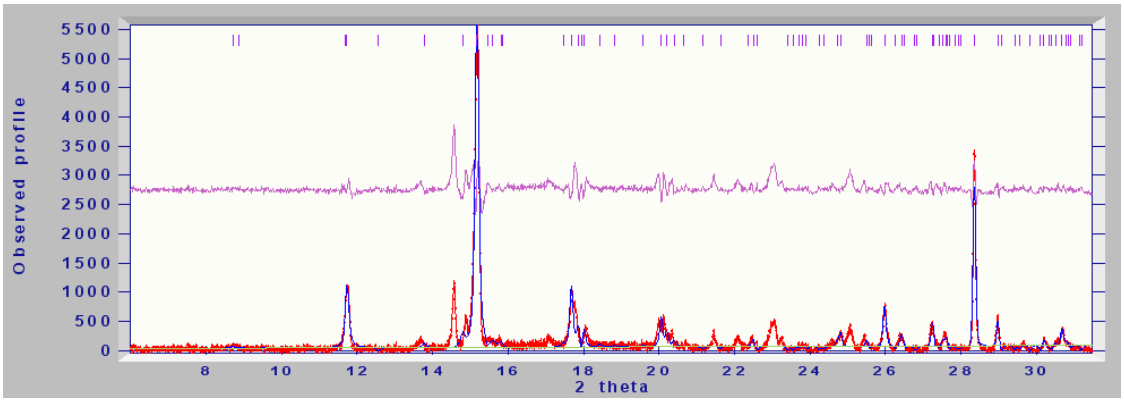

Figure S2c Carbamazepine – NMP solvate. Refined unit cell parameters *a*, *b*, *c* (Å) = 7.481, 19.481, 11.626; α, β, γ (°) = 90.00, 98.38, 90.00 (P21/c); Pawley χ^2 = 8.36. The relatively high Pawley χ^2 value and significant misfit evident from the difference

plot (pink) (e.g. in the following ranges of the pattern 14-15 and 22 - 24 $^{o}2\theta$) results from the presence of form I in the sample, due to partial desolvation.

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