Electronic Supplementary Material (ESI) for Digital Discovery.

SI 1: Scree plot for PCA of DrugBank dataset

Below is presented the accompanying scree plot for the PCA detailed in the main text. The large number of PCs required to capture the variance is a reflection of the rich information content of the feature set; indeed, it would reflect poorly on it if it could be easily reduced to a small number of dimensions.

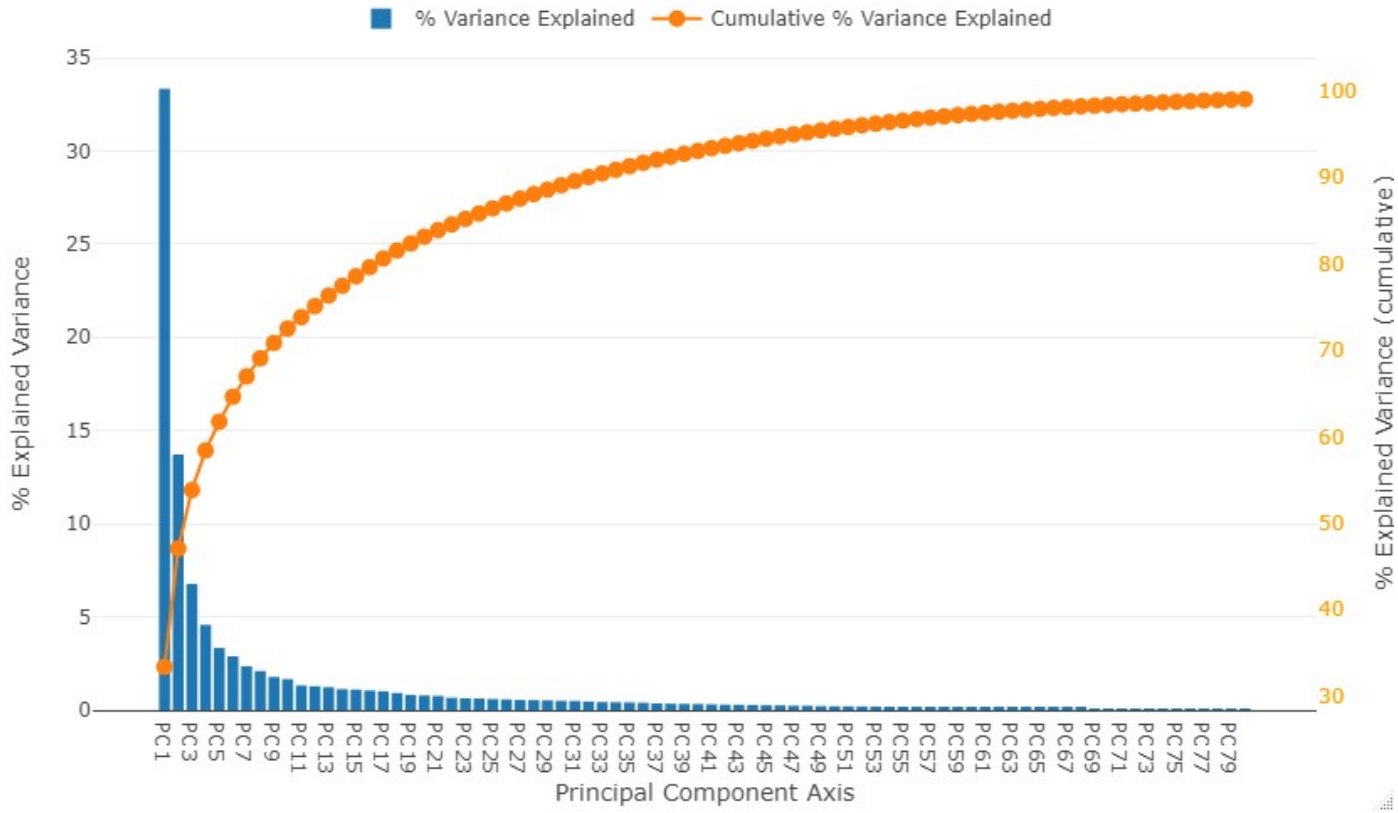


Figure SI-1. Accompanying scree plot for the PCA detailed in the main text.

SI 2: High error results

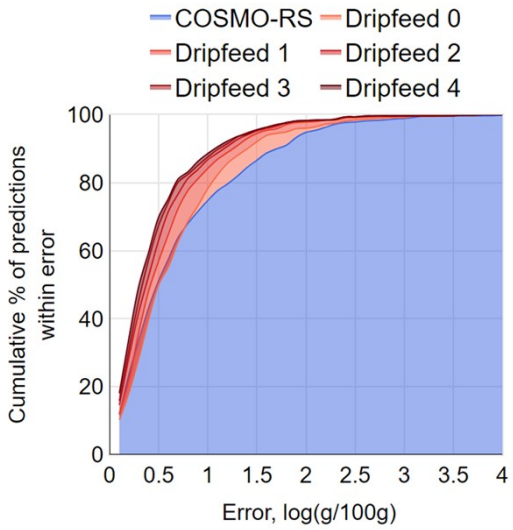
Readers may be interested in examining individual systems poorly predicted by COSMO-RS and our RF-based models. Below are listed i) the 50 highest-error COSMO-RS predictions for our dataset and ii) the 50 highest-error RF-hybrid (10-fold CV) predictions for our dataset. All solubility values are in $\log_{10}$(g/100g). These data are included in the repository at https://github.com/AntonyVass/cmac_solpred_cosmo_rf.

Solvent Name	Solute Name	Exp. Solubility	COSMO Solubility	COSMO abs. error	RF Solubility	RF Abs. Error
Tetrahydrofuran	hydrocortisone	-1.9615	1.9971	**3.9586**	-0.1635	1.7980
2-Propanol	Sulfapyridine	-0.6518	2.5258	**3.1777**	-0.0349	0.6169
Acetonitrile	glibenclamide	-2.9626	0.2058	**3.1683**	-1.5324	1.4302
Methanol	2-aminoacetic acid	-3.3979	-0.2381	**3.1599**	-0.7616	2.6363
Ethyl Acetate	ascorbic acid	-1.5850	1.5090	**3.0940**	-0.4038	1.1812
Tetrahydrofuran	paracetamol	-1.4318	1.4971	**2.9289**	1.1767	2.6085
Ethanol	2-aminoacetic acid	-3.5229	-0.6261	**2.8967**	-1.1155	2.4073
Formamide	ibuprofen	-0.1825	2.6561	**2.8386**	1.6192	1.8017
Acetonitrile	ascorbic acid	-0.9872	1.8183	**2.8055**	-0.2224	0.7647
Acetonitrile	3-pyridinecarboxylic acid	-1.2558	1.5327	**2.7885**	0.5552	1.8110
1-Octanol	Sulfapyridine	-1.8214	0.9644	**2.7859**	-0.2375	1.5839
Methanol	glibenclamide	-2.7258	-0.0181	**2.7077**	-1.7453	0.9806
Acetone	glibenclamide	-1.9780	0.7219	**2.6998**	-0.8647	1.1133
Propionic Acid	2,2-dichloro-n-((1s,2r)-1-(fluoromethyl)-2-hydroxy-2-(4-(methylsulfonyl)phenyl)ethyl) acetamide	-0.5655	2.0158	**2.5813**	0.5046	1.0701
Chloroform	hydrocortisone	-0.5653	1.9364	**2.5017**	-0.3387	0.2266
Acetone	311-03-5	-0.5925	1.6738	**2.2663**	0.0880	0.6805
Methanol	haloperidol	0.2547	2.5144	**2.2597**	0.8929	0.6382
1,2-Dichloroethane	311-03-5	-0.5659	1.6921	**2.2580**	-0.0758	0.4901
2-Propanol	ascorbic acid	-0.7338	1.4295	**2.1633**	-0.3955	0.3383
Ethyl Acetate	hydrocortisone	-0.5061	1.6545	**2.1606**	-0.4556	0.0504
Benzene	hydrocortisone	-1.8296	0.3029	**2.1325**	-1.1609	0.6687
Ethanol	glibenclamide	-2.6345	-0.5781	**2.0564**	-2.0751	0.5594
Acetone	(2R,3R,4R,5S)-hexane-1,2,3,4,5,6-hexol	-0.9213	1.1125	**2.0338**	-0.3484	0.5730
Acetone	3-((6-O-(6-deoxy-??-L-mannopyranosyl)-??-D-glucopyranosyl)oxy)-2-(3,4-dihydroxyphenol)-5,7-dihydroxy-4H-1-benzopyran-4-one	-0.5452	1.4576	**2.0029**	0.3576	0.9028
Ethyl Acetate	lamivudine	-2.2007	-0.2210	**1.9797**	-0.5668	1.6338
Isopropyl Acetate	hydrocortisone	-0.7947	1.1719	**1.9666**	-0.6089	0.1858
Tetrahydrofuran	sulfamethoxypyridazine	-1.8083	0.1313	**1.9395**	-0.2467	1.5616
Dichloromethane	311-03-5	-0.0228	1.8862	**1.9090**	-0.2027	0.1799
Methyl Acetate	hydrocortisone	-0.2017	1.7041	**1.9058**	-0.3011	0.0994
Benzene	ibuprofen	1.3882	3.2879	**1.8997**	1.1579	0.2302
Tetrahydrofuran	311-03-5	-0.1482	1.7505	**1.8987**	-0.0762	0.0720
Benzene	piroxicam	-1.5139	0.3769	**1.8908**	-0.9281	0.5858
Chloroform	311-03-5	-0.0835	1.7866	**1.8700**	0.1051	0.1886
acetophenone	ibuprofen	-0.2772	1.5601	**1.8372**	1.4695	1.7467
Ethanol	ascorbic acid	0.0202	1.8523	**1.8322**	0.0480	0.0278
Dichloromethane	n-(1-oxopentyl)-n-((2-(1h-tetrazol-5-yl)(1,1-biphenyl)-4-yl)methyl)-l-valine	0.2925	2.1225	**1.8300**	0.1268	0.1657
2-Propanol	glibenclamide	-2.7055	-0.9017	**1.8038**	-2.0492	0.6564
Ethyl Acetate	glibenclamide	-1.4915	0.3093	**1.8008**	-1.6030	0.1115
Chloroform	n-(1-oxopentyl)-n-((2-(1h-tetrazol-5-yl)(1,1-biphenyl)-4-yl)methyl)-l-valine	0.1913	1.9882	**1.7969**	0.4732	0.2819
Acetone	haloperidol	0.3023	2.0944	**1.7921**	0.9224	0.6201

Solvent Name	Solute Name	Exp. Solubility	COSMO Solubility	COSMO abs. Error	RF Solubility	RF Abs. Error
Water	2-aminoacetic acid	1.3813	0.1143	-1.2670	-1.5556	**2.9369**
Methanol	2-aminoacetic acid	-3.3979	-0.2381	3.1599	-0.7616	**2.6363**
Tetrahydrofuran	paracetamol	-1.4318	1.4971	2.9289	1.1767	**2.6085**
Water	(2S)-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-2,3-dihydrochromen-4-one	-3.8539	-2.7924	1.0615	-1.4012	**2.4527**
Water	indomethacin	-4.0000	-4.1367	-0.1367	-1.5902	**2.4098**
Ethanol	2-aminoacetic acid	-3.5229	-0.6261	2.8967	-1.1155	**2.4073**
Water	gsk-B	-3.0969	-4.9208	-1.8239	-0.8189	**2.2781**
Hexane	4-Hydroxybenzoic acid	-3.3038	-3.8327	-0.5289	-1.4269	**1.8769**
Acetonitrile	3-pyridinecarboxylic acid	-1.2558	1.5327	2.7885	0.5552	**1.8110**
Formamide	ibuprofen	-0.1825	2.6561	2.8386	1.6192	**1.8017**
Tetrahydrofuran	hydrocortisone	-1.9615	1.9971	3.9586	-0.1635	**1.7980**
Cyclohexane	hydrocortisone	-3.9700	-3.6882	0.2818	-2.2090	**1.7610**
acetophenone	ibuprofen	-0.2772	1.5601	1.8372	1.4695	**1.7467**
Chloroform	2-hydroxypropane-1,2,3-tricarboxylic acid	-2.1549	-4.0555	-1.9006	-0.4637	**1.6912**
Tetrahydrofuran	2,2-dichloro-n-((1s,2r)-1-(fluoromethyl)-2-hydroxy-2-(4-(methylsulfonyl)phenyl)ethyl)acetamide	1.3137	0.7614	-0.5523	-0.3557	**1.6694**
Formamide	sclareol	-0.9996	-0.1116	0.8880	0.6458	**1.6454**
Ethyl Acetate	lamivudine	-2.2007	-0.2210	1.9797	-0.5668	**1.6338**
1-Octanol	Sulfapyridine	-1.8214	0.9644	2.7859	-0.2375	**1.5839**
Tetrahydrofuran	sulfadiazine	-3.1808	-3.0555	0.1253	-1.6037	**1.5771**
Tetrahydrofuran	sulfamethoxypyridazine	-1.8083	0.1313	1.9395	-0.2467	**1.5616**
N,N-Dimethylformamide	sulfadiazine	1.4178	0.5734	-0.8444	-0.1277	**1.5455**
Water	naproxen	-3.1549	-2.8136	0.3413	-1.6369	**1.5181**
Carbon Tetrachloride	hydrocortisone	-3.1899	-2.5923	0.5977	-1.6920	**1.4979**
Water	d-(-)fructose	2.4680	1.6708	-0.7972	1.0009	**1.4672**
Acetonitrile	glibenclamide	-2.9626	0.2058	3.1683	-1.5324	**1.4302**
Water	lamivudine	1.9289	2.4048	0.4759	0.5723	**1.3566**
Acetonitrile	n-(1-oxopentyl)-n-((2-(1h-tetrazol-5-yl)(1,1-biphenyl)-4-yl)methyl)-l-valine	1.1949	1.6570	0.4621	-0.1415	**1.3364**
Heptane	gsk-Z	0.8732	-0.7103	-1.5834	-0.4214	**1.2946**
Ethanol	(benzyldisulfanyl)methyl benzene	-0.1614	0.8082	0.9695	1.1326	**1.2939**
Chloroform	haloperidol	1.7776	1.7329	-0.0447	0.5169	**1.2607**
Heptane	gsk-B	1.6317	-0.7109	-2.3426	0.3758	**1.2559**
Methanol	piroxicam	-1.6716	-0.2128	1.4588	-0.4305	**1.2411**
Hexane	mefenamic acid	-0.4384	-1.7544	-1.3161	-1.6592	**1.2208**
Ethyl Formate	salicylic acid	0.1536	1.6827	1.5290	1.3462	**1.1926**
2-Methoxy-2-Methylpropane	gsk-A	-2.1249	-0.6711	1.4539	-0.9407	**1.1843**
Ethyl Acetate	ascorbic acid	-1.5850	1.5090	3.0940	-0.4038	**1.1812**
Diethylether	diclofenac	-0.0741	1.5651	1.6392	1.1048	**1.1789**
Hexane	acetanilide	-2.6939	-1.1767	1.5173	-1.5264	**1.1675**
2-Propanol	3-((6-O-(6-deoxy-??-L-mannopyranosyl)-??-D-glucopyranosyl)oxy)-2-(3,4-dihydroxyphenol)-5,7-dihydroxy-4H-1-benzopyran-4-one	0.2034	-0.7320	-0.9354	-0.9518	**1.1552**
Diethylether	naproxen	-0.0306	1.5269	1.5576	1.1239	**1.1545**

SI 2: Drip-feeding CV of RF-pure

Drip-feeding CV was also performed using the RF-pure method (i.e. excluding COSMO-RS predictions). The results were as expected, adding little to the interpretation and conclusions of an already dense presentation, and so are excluded from the main text; for completeness, they are presented here.



Model	RMSE	MAE	FI
COSMO-RS	0.97	0.71	NA
Dripfeed 0	0.89	0.67	0.47
Dripfeed 1	0.76	0.56	0.54
Dripfeed 2	0.71	0.51	0.61
Dripfeed 3	0.68	0.48	0.63
Dripfeed 4	0.67	0.46	0.64

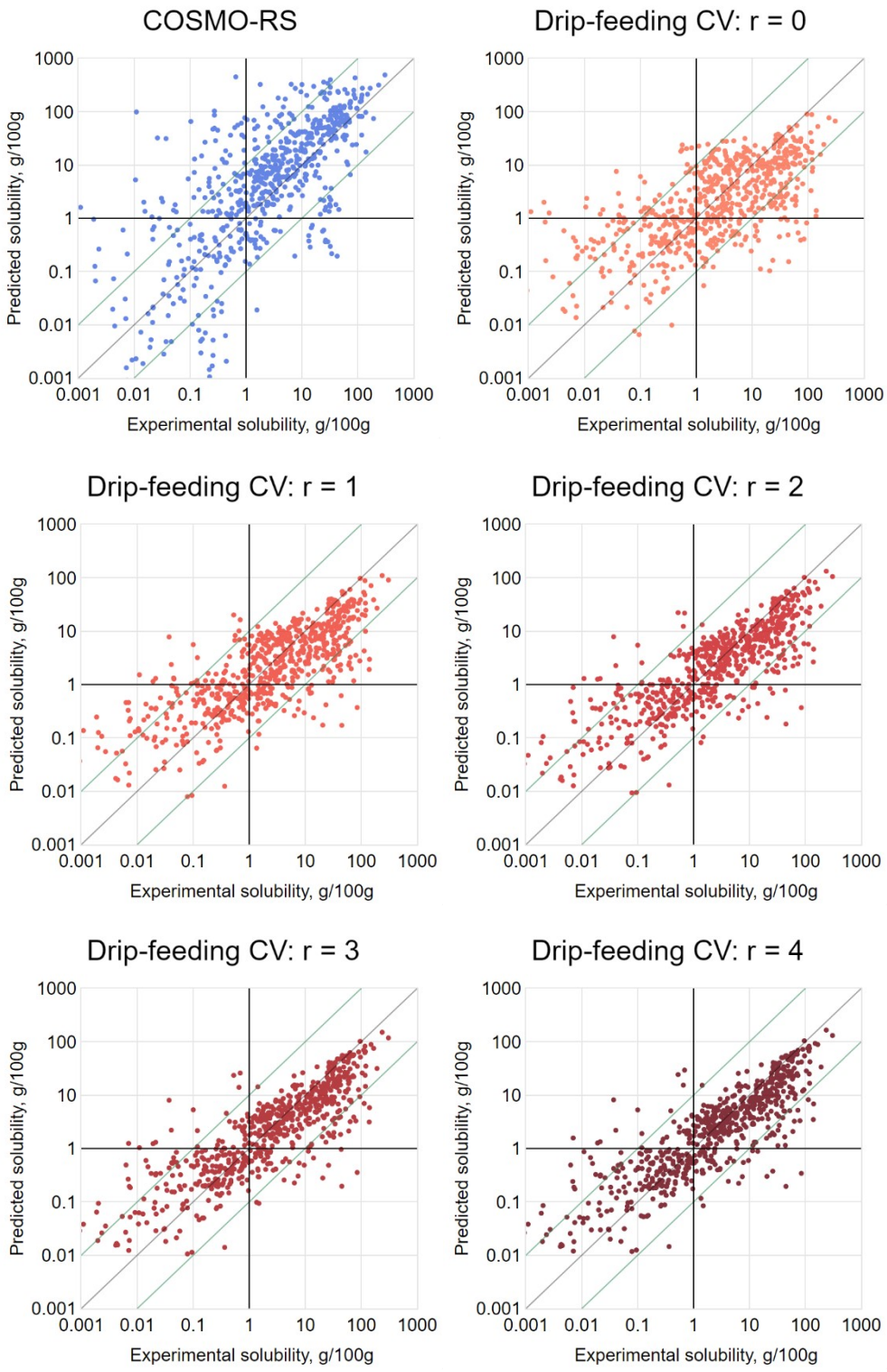


Figure SI-2. The results of drip-feeding CV for RF-pure, for *r* values of 0 to 4. Predictions were only made for solutes appearing in the dataset 5+ times to keep the plots comparable (658 of 714 instances). COSMO-RS prediction errors were recalculated for this subset for reference.

SI 3: Solvent list

Solvent ID	Solvent Name
1	1,2-dichloroethane
2	1,4-dioxane
3	1-butanol
4	1-heptanol
5	1-hexanol
6	1-octanol
7	1-pentanol
8	1-propanol
9	2-butanol
10	2-butanone
11	2-methoxy-2-methylpropane
12	2-methyltetrahydrofuran
13	2-propanol
14	4-methyl-2-pentanone
15	acetone
16	acetonitrile
17	acetophenone
18	anisole
19	benzene
20	carbon tetrachloride
21	chlorobenzene
22	chloroform
23	cyclohexane
24	cyclohexanone
25	dichloromethane
26	dimethylformamide
27	diethyl ether
28	dodecane
29	ethanol
30	ethyl acetate
31	ethyl formate
32	ethylene glycol
33	formamide
34	hexane
35	isobutanol
36	isopentanol
37	isopropyl acetate
38	methanol
39	methyl acetate
40	methylcyclohexane
41	n-butyl acetate
42	n-heptane
43	n-propyl acetate
44	octane
45	propionic acid
46	propylene glycol
47	tetrahydrofuran
48	toluene
49	water

SI 4: Solute list

Solute ID	Chemical Name	ΔH_{fus} (kj/mol)	Melting point (°C)	Reference
1	2-(2-bromoethoxy)-1,3,5-trichlorobenzene	24.05	50.9	[1]
2	2-[(6-oxobenzo[c][2,1]benzoxaphosphinin-6-yl)methyl]butanedioic acid	43.63	188	[2]
3	2-aminopyridine	15.31	58.15	[3]
4	2-hydroxy-1,2-diphenylethanone	40.3	135	[4]
5	3,4-dimethoxybenzoic acid	29.62	179.97	[3]
6	3-[bis(3-hydroxypropyl)phosphoryl]propan-1-ol	34.21	114.61	[5]
7	4-aminobenzoic acid	20.93	186	[3]
8	4-hydroxy-3-methoxybenzaldehyde	21.36	81.75	[3]
9	4-hydroxybenzoic acid	32.5	216.25	[6]
10	acetanilide	21.65	114.3	[3]
11	ascorbic acid	19.72	192	[3]
12	benzoic acid	17.452	122.4	[3]
13	benzyl disulfide	44.69	68.57	[7]
14	butylparaben	24.57	67.57	[3]
15	carbamazepine	26.33	190.2	[8]
16	citric acid	40.32	153.85	[9]
17	D-fructose	36.06	104	[3]
18	D-sorbitol	35	92.7	[10]
19	diclofenac	40.4	179.45	[11]
20	diphenylamine	19.5	325.6	[12]
21	florfenicol	18.98	152	[13]
22	frambinone	22.75	84.43	[14]
23	fumaric acid	33.3	287	[15]
24	glibenclamide	52.9	173.33	[16]
25	glycine	28.4	262	[15]
26	haloperidol	22.44	151.5	[15]
27	hesperetin	35.9	226.07	[17]
28	hexanedioic acid	34.85	153.4	[3]
29	hydrocortisone	33.9	86.1	[18]
30	hydroquinone	27.11	171.95	[19]
31	ibuprofen	25.5	74	[20]
32	indomethacin	36.85	160.1	[21]
33	iodopropynyl butylcarbamate	22.69	68.26	[3]
34	isoniazid	28.15	172.89	[3]
35	ketoprofen	28.25	94.5	[3]
36	lamivudine	20.84	178.6	[22]
37	lovastatin	43.14	172.35	[23]
38	maltol	21.23	160.25	[24]
39	mefenamic acid	38.7	230.5	[15]
40	metacetamol	28.8	146.85	[25]
41	m-phthalic acid	43.2	344.26	[26]
42	N-(pyridin-3-ylmethylideneamino)pyridin-2-amine	34	175.85	[27]
43	naproxen	31.75	155.85	[3]
44	nicotinic acid	13.01	236.01	[28]
45	octadecanoic acid	56.4	69.6	[29]
46	oxolane-2,5-dione	20.4	119	[3]
47	paracetamol	28.1	168.6	[30]
48	phenacetin	31.27	135	[3]
49	phenylphosphinic acid	12.8	356	[31]
50	piroxicam	35.52	202.1	[32]
51	propylparaben	28.01	96.05	[3]
52	pyridoxine	31.15	160.4	[33]
53	pyrrolidine-2,5-dione	15.17	128.7	[34]
54	quercetin	32.9	318	[35]
55	rutin	82.3	177	[17]
56	salicylic acid	23.2	158.85	[36]
57	sclareol	28.7	103.3	[35]
58	sulfadiazine	44.3	255.5	[15]
59	sulfamethoxazole	33.76	167.5	[37]
60	sulfamethoxypyridazine	22.3	182.5	[15]
61	sulfapyridine	5.39	192	[38]

62	testosterone	28.2	426.45	[39]
63	testosterone propionate	22.14	120	[15]
64	theophylline	30.91	273.1	[40]
65	triclosan	17.76	57.95	[3]
66	trimethoprim	49.8	472.85	[39]
67	tris(1,2-dioxyphenyl)cyclotriphosphazene	19.54	249.05	[41]
68	valsartan	11.9	358.14	[42]
69	gsk-Q	58.42	242	*
70	gsk-A	18.59	245.7	*
71	gsk-H	33.14	147	*
72	gsk-S	18.98	52.7	*
73	gsk-Z	27.99	161.4	*
74	gsk-E	33.04	202	*
75	gsk-B	32.06	225	*

* Melting temperature and fusion enthalpy were obtained from Differential Scanning Calorimetry with a TA Instruments Q100 DSC, using a 10°C/min ramp and a maximum temperature of 300°C per default for a DSC scan. Solute identity withheld due to commercial sensitivity.

SI 5: Solubility Dataset

The following table is also available as a .csv file.

Solute id	Solute Name	Solvent id	Solvent Name	Solubility (g/100g)	Reference
1	2-(2-bromoethoxy)-1,3,5-trichlorobenzene	8	1-propanol	6.6716	[43]
		13	2-propanol	6.0484	
		15	acetone	89.6024	
		16	acetonitrile	23.2484	
		29	ethanol	7.2141	
		38	methanol	8.5503	
		42	n-heptane	27.822	
2	2-[(6-oxobenzo[c][2,1]benzoxaphosphinin-6-yl)methyl]butanedioic acid	2	1,4-dioxane	0.7695**	[44]
		8	1-propanol	1.5078	
		19	benzene	0.1463	
		23	cyclohexane	0.0947	
		29	ethanol	3.1778	
		30	ethyl acetate	0.4564	
		38	methanol	6.2608	
		47	tetrahydrofuran	1.7834	
		48	toluene	0.3052**	
3	2-aminopyridine	15	acetone	85.515	[19]
		22	chloroform	32.761	
		29	ethanol	121.1282	
		30	ethyl acetate	48.0374	
		41	n-butyl acetate	25.0209	
4	2-hydroxy-1,2-diphenylethanone	3	1-butanol	0.6699	[45]
		8	1-propanol	0.828	
		13	2-propanol	0.5614	
		15	acetone	4.6894	
		16	acetonitrile	3.4742	
		23	cyclohexane	0.3429	
		29	ethanol	1.1093	
		30	ethyl acetate	3.2595	
		35	isobutanol	0.552	
		38	methanol	1.6148	
		41	n-butyl acetate	1.9893	
		48	toluene	1.2774	
5	3,4-dimethoxybenzoic acid	3	1-butanol	1.4089	[46]
		8	1-propanol	2.014	
		10	2-butanone	3.0685	
		13	2-propanol	1.9219	
		29	ethanol	2.948	
		30	ethyl acetate	1.4995	
		35	isobutanol	1.0118	
		39	methyl acetate	1.9832	

6	3-[bis(3-hydroxypropyl)phosphoryl]propan-1-ol	3	1-butanol	3.3616	[5]
		8	1-propanol	14.2959	
		13	2-propanol	5.8822	
		15	acetone	0.3903	
		29	ethanol	11.2647	
		35	isobutanol	4.716	
		38	methanol	38.9079	
7	4-aminobenzoic acid	2	1,4-dioxane	11.712	[47]
		3	1-butanol	5.9958	
		4	1-heptanol	2.7498	
		5	1-hexanol	3.6734	
		6	1-octanol	2.2456	
		7	1-pentanol	4.2021	
		9	2-butanol	5.3453	
		13	2-propanol	7.5876	
		15	acetone	12.433	[48]
		19	benzene	0.0702	[49]
		29	ethanol	15.8719	[47]
		35	isobutanol	3.2973	
		38	methanol	21.5602	[50]
		47	tetrahydrofuran	32.5448	
		49	water	0.5409	
8	4-hydroxy-3-methoxybenzaldehyde	8	1-propanol	36.7084	[51]
		29	ethanol	274.41	[52]
		49	water	0.9917	[53]
9	4-hydroxybenzoic acid	6	1-octanol	17.1225	[54]
		13	2-propanol	34.4479	[20]
		14	4-methyl-2-pentanone	15.2063	
		22	chloroform	0.0191	[55]
		29	ethanol	40.0603	
		30	ethyl acetate	12.4719	[56]
		34	hexane	0.0005	[54]
		38	methanol	54.2084	[56]
		48	toluene	0.1651	[20]
		49	water	0.744	[57]
10	acetanilide	6	1-octanol	17.8864	[54]
		11	2-methoxy-2-methylpropane	3.025	#
		13	2-propanol	19.57	
		14	4-methyl-2-pentanone	13.1	
		16	acetonitrile	21.435	
		18	anisole	3	
		22	chloroform	16.8501	[58]
		23	cyclohexane	0.0339	[59]
		28	dodecane	0.19	
		29	ethanol	33.2195	#
		34	hexane	0.002	[54]
		36	isopentanol	16.5567	#
		37	isopropyl acetate	8.955	
		42	n-heptane	0.06	
		48	toluene	0.845	
		49	water	0.3313	
11	ascorbic acid	13	2-propanol	0.1846	[60]
		16	acetonitrile	0.103	
		29	ethanol	1.0475	
		30	ethyl acetate	0.026	
		49	water	32.3572	
12	benzoic acid	1	1,2-dichloroethane	9.2173	[61]
		3	1-butanol	41.9647	[62]
		5	1-hexanol	30.0675	
		6	1-octanol	13.8886	
		7	1-pentanol	40.4525	
		9	2-butanol	39.9084	[63]
		13	2-propanol	48.8187	[61]
		16	acetonitrile	16.9477	[64]
		19	benzene	11.569	[61]
		20	carbon tetrachloride	4.1257	
		21	chlorobenzene	10.2347	

		22	chloroform	15.0566	
		23	cyclohexane	1.4953	
		27	diethyl ether	37.0771	
		29	ethanol	57.7567	
		32	ethylene glycol	19.0798	
		33	formamide	48.7885	
		34	hexane	1.3592	
		35	isobutanol	29.6238	
		38	methanol	74.3314	
		41	n-butyl acetate	21.5181	
		42	n-heptane	1.4428	
		45	propionic acid	38.3433	
13	benzyl disulfide	22	chloroform	54.3717	[65]
		29	ethanol	0.6897**	
		30	ethyl acetate	29.7846	
		34	hexane	2.1299	
		48	toluene	41.324**	
14	butylparaben	3	1-butanol	149.9717	[66]
		5	1-hexanol	111.1637	
		6	1-octanol	73.7917	
		29	ethanol	237.1531	
		38	methanol	306.7349	
15	carbamazepine	3	1-butanol	1.7086	[67]
		10	2-butanone	3.4286	[68]
		13	2-propanol	1.2675	
		15	acetone	1.5171	
		16	acetonitrile	4.1141	
		22	chloroform	11.3271	
		25	dichloromethane	11.9245	
		29	ethanol	3.0925	
		30	ethyl acetate	1.1863	
		38	methanol	9.7092	
16	citric acid	2	1,4-dioxane	30.8055	[69]
		3	1-butanol	23.4759	[70]
		7	1-pentanol	14.0859	[69]
		22	chloroform	0.007	[71]
		29	ethanol	73.7287	[72]
		30	ethyl acetate	1.3475	[69]
		32	ethylene glycol	66.575	
		33	formamide	61.623	
		38	methanol	94.459	
		46	propylene glycol	11.3393	
		49	water	140.9947	[73]
17	D-fructose	29	ethanol	1.7238	[74]
		38	methanol	13.4464	
		49	water	293.7709	[75]
18	D-Sorbitol	3	1-butanol	0.2202	[76]
		8	1-propanol	0.3758	
		15	acetone	0.1199	
		16	acetonitrile	0.0923	
		38	methanol	3.3472	
19	diclofenac	1	1,2-dichloroethane	1.2109	[48]
		2	1,4-dioxane	39.6463	
		6	1-octanol	3.4726	
		7	1-pentanol	4.3796	
		15	acetone	15.8773	
		17	acetophenone	11.5429	
		19	benzene	1.0342	
		21	chlorobenzene	0.9717	
		22	chloroform	2.3518	
		23	cyclohexane	0.0216	
		27	diethyl ether	0.8432	
		29	ethanol	5.6614	
		30	ethyl acetate	7.8747	
		31	ethyl formate	1.6176	
		32	ethylene glycol	0.811	
		33	formamide	1.1586	

		38	methanol	5.4569	
		42	n-heptane	0.0177	
		45	propionic acid	3.9621	
		46	propylene glycol	1.9213	
20	diphenylamine	3	1-butanol	43.0394	
		9	2-butanol	41.6423	[63]
		36	isopentanol	28.781	
21	Florfenicol	3	1-butanol	0.5419	
		8	1-propanol	1.2855	
		13	2-propanol	0.7956	[13]
		29	ethanol	2.4125	
		35	isobutanol	0.2963	
		36	isopentanol	0.3901	
		38	methanol	12.9488	[77]
		45	propionic acid	0.272	[13]
		47	tetrahydrofuran	20.5918	[78]
		49	water	0.1092	
22	frambinone	3	1-butanol	57.8619	
		8	1-propanol	60.1412	
		9	2-butanol	37.6299	
		13	2-propanol	67.3298	
		15	acetone	116.2637	[14]
		29	ethanol	96.8699	
		30	ethyl acetate	39.7248	
		39	methyl acetate	49.3838	
23	fumaric acid	19	benzene	0.0045	
		22	chloroform	0.02	[79]
		49	water	0.6998	
24	glibenclamide	3	1-butanol	0.0043	
		13	2-propanol	0.002	
		14	4-methyl-2-pentanone	0.0501	
		15	acetone	0.0105	
		16	acetonitrile	0.0011	[80]
		29	ethanol	0.0023	
		30	ethyl acetate	0.0323	
		38	methanol	0.0019	
25	glycine	26	dimethylformamide	0.0464	
		29	ethanol	0.0003	[81]
		38	methanol	0.0004	
		49	water	24.0616	[82]
26	haloperidol	2	1,4-dioxane	2.4154	
		3	1-butanol	3.971	
		7	1-pentanol	1.3946	
		13	2-propanol	7.3404	
		15	acetone	2.0059	
		19	benzene	5.2437	
		22	chloroform	59.9185	[83]
		26	dimethylformamide	21.6883	
		29	ethanol	4.6772	
		30	ethyl acetate	4.3397	
		38	methanol	1.7975	
		41	n-butyl acetate	1.6084	
		46	propylene glycol	0.445	
27	Hesperetin	3	1-butanol	1.3808	[84]
		15	acetone	12.9931	
		16	acetonitrile	1.5202	
		29	ethanol	2.9156	[85]
		30	ethyl acetate	2.3881	
		38	methanol	3.5678	
		49	water	0.0001	[84]
28	hexanedioic acid	3	1-butanol	5.9939	[86]
		13	2-propanol	7.3003	[87]
		15	acetone	4.2448	[88]
		19	benzene	0.02	[87]
		22	chloroform	0.2565	[88]
		30	ethyl acetate	0.8233	[89]
		48	toluene	0.0072	[88]

		49	water	2.3701	[90]
29	hydrocortisone	6	1-octanol	0.4115	[91]
		19	benzene	0.0148	
		20	carbon tetrachloride	0.0006	
		22	chloroform	0.2721	
		23	cyclohexane	0.0001	
		30	ethyl acetate	0.3118	
		34	hexane	0.0005	
		37	isopropyl acetate	0.1604	
		39	methyl acetate	0.6285	
		41	n-butyl acetate	0.2175	
		46	propylene glycol	1.6094	
		47	tetrahydrofuran	0.0109	
30	hydroquinone	29	ethanol	56.5762	[92]
		41	n-butyl acetate	12.5969	
31	ibuprofen	2	1,4-dioxane	9.0429	[93]
		7	1-pentanol	38.6346	[94]
		9	2-butanol	71.3233	
		13	2-propanol	104.5087	
		14	4-methyl-2-pentanone	62.75	[95]
		15	acetone	191.9609	[93]
		17	acetophenone	0.5282	
		19	benzene	24.4442	
		21	chlorobenzene	3.7644	
		22	chloroform	58.7729	
		23	cyclohexane	43.9589	
		26	dimethylformamide	41.3183	
		27	diethyl ether	6.3261	
		29	ethanol	41.0192	
		30	ethyl acetate	117.8434	
		31	ethyl formate	26.1583	
		32	ethylene glycol	6.4508	
		33	formamide	0.6569	
		34	hexane	9.61	[95]
		35	isobutanol	70.0541	[94]
		38	methanol	16.2917	[93]
		41	n-butyl acetate	58.89	[95]
		42	n-heptane	12.2085	[93]
		45	propionic acid	73.9792	
		46	propylene glycol	25.4709	
		47	tetrahydrofuran	57.446**	[20]
		48	toluene	65.17	[95]
32	indomethacin	2	1,4-dioxane	11.7761	[96]
		35	isobutanol	1.1973	[97]
		49	water	0.0001	[98]
33	iodopropynyl butylcarbamate	3	1-butanol	90.1139	[99]
		4	1-heptanol	44.3722	
		5	1-hexanol	56.7472	
		7	1-pentanol	71.9053	
		8	1-propanol	119.1368	
		29	ethanol	167.1137	
34	isoniazid	15	acetone	1.8612**	[100]
		29	ethanol	1.4307**	
		30	ethyl acetate	0.2228**	
		38	methanol	4.1301**	
35	ketoprofen	3	1-butanol	32.6079	[101]
		4	1-heptanol	15.8149	
		5	1-hexanol	22.053	
		6	1-octanol	14.494	[101]
		7	1-pentanol	24.2685	[102]
		8	1-propanol	35.8786	
		9	2-butanol	59.5923	
		13	2-propanol	61.4996	
		27	diethyl ether	38.149	
		29	ethanol	41.6094	
		30	ethyl acetate	52.1339	
		35	isobutanol	38.4992	

		38	methanol	32.7219	[101]
36	lamivudine	3	1-butanol	0.6667	[103]
		8	1-propanol	0.8966	
		9	2-butanol	0.495	
		13	2-propanol	0.6242	
		15	acetone	0.1188	
		16	acetonitrile	0.218	[104]
		26	dimethylformamide	20.258	
		29	ethanol	1.4449	[103]
		30	ethyl acetate	0.0063	
		38	methanol	3.5777	
		47	tetrahydrofuran	0.4303	[104]
		49	water	84.9	[103]
37	lovastatin	5	1-hexanol	1.8094	[105]
		6	1-octanol	1.2906**	[23]
		10	2-butanone	6.5327	[105]
		15	acetone	8.6955	[106]
		29	ethanol	3.1099	
		30	ethyl acetate	2.6248	
		37	isopropyl acetate	1.9784	[105]
		38	methanol	3.9857	[106]
		39	methyl acetate	2.452	[105]
		41	n-butyl acetate	1.8483	[106]
		43	n-propyl acetate	2.3388	[105]
38	maltol	1	1,2-dichloroethane	2.2567	[24]
		3	1-butanol	1.9829	
		8	1-propanol	2.5101	
		9	2-butanol	1.9132	
		13	2-propanol	2.1925	
		15	acetone	2.9581	
		16	acetonitrile	3.3163	
		29	ethanol	3.4651	
		30	ethyl acetate	2.2255	
		35	isobutanol	1.8524	
		38	methanol	7.4185	
		41	n-butyl acetate	1.4032	
		43	n-propyl acetate	1.6238	
39	mefenamic acid	8	1-propanol	0.75	[63]
		13	2-propanol	0.8046	[107]
		15	acetone	1.7271	[108]
		23	cyclohexane	0.2583	[107]
		26	dimethylformamide	5.743	
		29	ethanol	0.997	
		30	ethyl acetate	1.0722	
		34	hexane	0.3645	
		42	n-heptane	0.2652	
		46	propylene glycol	0.1187	[109]
40	metacetamol	11	2-methoxy-2-methylpropane	0.85	#
		13	2-propanol	19.48	
		14	4-methyl-2-pentanone	6.94	
		16	acetonitrile	8.05	
		18	anisole	0.24	
		28	dodecane	0.115	
		37	isopropyl acetate	2.455	
		42	n-heptane	0.03	
		48	toluene	0.11	
41	m-phthalic acid	3	1-butanol	0.7574	[110]
		4	1-heptanol	0.4209	
		5	1-hexanol	0.4958	
		6	1-octanol	0.357	
		7	1-pentanol	0.5984	
		8	1-propanol	0.9983	
		9	2-butanol	0.8224	
		13	2-propanol	1.1557	
		15	acetone	5.9599	[111]
		30	ethyl acetate	1.1083**	
		35	isobutanol	0.537	[110]

		36	isopentanol	0.5519	
		38	methanol	1.996	
42	N-(pyridin-3-ylmethylideneamino)pyridin-2-amine	6	1-octanol	1.7241	[27]
		34	hexane	0.0068	
		49	water	0.0139	
43	naproxen	1	1,2-dichloroethane	3.1347	[112]
		2	1,4-dioxane	30.3348	[113]
		3	1-butanol	4.462	
		4	1-heptanol	3.8564	
		5	1-hexanol	3.8111	
		6	1-octanol	2.8823	
		7	1-pentanol	3.4459	
		9	2-butanol	4.4684	
		13	2-propanol	5.1804	
		15	acetone	29.4826	[112]
		16	acetonitrile	2.5355	[114]
		17	acetophenone	80.3036	[112]
		19	benzene	2.1507	
		21	chlorobenzene	1.8352	
		22	chloroform	6.0239	
		23	cyclohexane	0.0328	
		27	diethyl ether	0.9319	
		29	ethanol	7.6115	[114]
		30	ethyl acetate	6.9764	
		31	ethyl formate	4.1876	[112]
		32	ethylene glycol	1.4335	
		33	formamide	3.3655	
		35	isobutanol	2.7074	[113]
		38	methanol	10.6326	[112]
		39	methyl acetate	8.7764	[113]
		41	n-butyl acetate	4.7539	
		42	n-heptane	0.0069	[114]
		45	propionic acid	9.1888	[112]
		46	propylene glycol	2.3389	
		47	tetrahydrofuran	52.7637	[113]
		49	water	0.0007	[115]
44	nicotinic acid	16	acetonitrile	0.0555	[116]
		27	diethyl ether	0.1352	
		49	water	1.6619	[117]
45	octadecanoic acid	15	acetone	3.8008	[118]
		34	hexane	2.4276	
		42	n-heptane	1.5127	
46	oxolane-2,5-dione	13	2-propanol	14.3424	[119]
		15	acetone	28.6563	
		16	acetonitrile	41.7409	
		30	ethyl acetate	9.4886	
47	paracetamol	2	1,4-dioxane	5.562	[69]
		3	1-butanol	8.327	[120]
		6	1-octanol	2.9397	[54]
		7	1-pentanol	11.932	[120]
		8	1-propanol	11.932	[121]
		13	2-propanol	12.115	[120]
		14	4-methyl-2-pentanone	1.66	[121]
		15	acetone	9.938	[120]
		16	acetonitrile	2.754	
		18	anisole	0.05	[121]
		19	benzene	0.0213	[69]
		22	chloroform	0.0405	
		23	cyclohexane	0.0054	[58]
		28	dodecane	0.065	[121]
		29	ethanol	20.991	[120]
		30	ethyl acetate	0.945	
		33	formamide	63.6745	[69]
		34	hexane	0.0007	[54]
		36	isopentanol	5.4872	[121]
		37	isopropyl acetate	0.75	
		38	methanol	33.211	[120]

		45	propionic acid	2.2925	[69]
		46	propylene glycol	25.8261	
		47	tetrahydrofuran	0.037	[120]
		48	toluene	0.037	[118]
		49	water	1.49	[121]
48	phenacetin	2	1,4-dioxane	3.49	[122]
		3	1-butanol	6.9872	[123]
		7	1-pentanol	4.0384	
		8	1-propanol	5.3587	
		19	benzene	0.4483	
		22	chloroform	5.2131	[58]
		23	cyclohexane	0.0218	
		29	ethanol	7.1486	[123]
		30	ethyl acetate	2.3379	
		34	hexane	0.0041	[54]
		38	methanol	11.3327	[123]
		47	tetrahydrofuran	8.1868	
		49	water	0.0787	[122]
49	phenylphosphinic acid	38	methanol	120.8774	[31]
		48	toluene	4.4432	
		49	water	7.5109	
50	piroxicam	1	1,2-dichloroethane	2.9877	[124]
		2	1,4-dioxane	1.8678	
		6	1-octanol	0.0763	
		7	1-pentanol	0.093	
		15	acetone	1.6102	
		17	acetophenone	0.0564	
		19	benzene	0.0306	
		21	chlorobenzene	0.0207	
		22	chloroform	6.4167	
		23	cyclohexane	0.007	
		26	dimethylformamide	7.7252	
		27	diethyl ether	0.0226	
		29	ethanol	0.1016	
		30	ethyl acetate	0.9215	
		31	ethyl formate	3.9912	
		32	ethylene glycol	0.0747	
		33	formamide	0.3676	
		38	methanol	0.0213	
		42	n-heptane	0.0045	
		45	propionic acid	0.7181	
		46	propylene glycol	0.1179	
51	propylparaben	3	1-butanol	63.0751	[66]
		5	1-hexanol	46.8818	
		6	1-octanol	34.5933	
		7	1-pentanol	50.47	
		29	ethanol	95.9628	
		38	methanol	116.8251	
52	pyridoxine	15	acetone	0.3704	[33]
		29	ethanol	1.3379	
		38	methanol	8.5035	
		47	tetrahydrofuran	0.5645	
53	pyrrolidine-2,5-dione	13	2-propanol	2.9882	[34]
		15	acetone	14.8157	
		29	ethanol	5.4247	
		30	ethyl acetate	3.8622	
		38	methanol	18.3454	
		47	tetrahydrofuran	11.4643	
54	quercetin	8	1-propanol	2.6694	[35]
		13	2-propanol	2.7749	
		16	acetonitrile	1.1122	
		29	ethanol	3.3058	
55	rutin	3	1-butanol	0.2851	[125]
		8	1-propanol	1.8238	
		13	2-propanol	1.5975	
		15	acetone	0.285	
		29	ethanol	5.81	

		30	ethyl acetate	0.7527	
		38	methanol	5.7985	
56	salicylic acid	1	1,2-dichloroethane	1.0663	[48]
		3	1-butanol	36.7155	[126]
		6	1-octanol	24.235	[54]
		6	1-octanol	24.235	[127]
		7	1-pentanol	28.6855	[48]
		9	2-butanol	42.8331	[126]
		13	2-propanol	50.0766	
		16	acetonitrile	10.2057	[56]
		17	acetophenone	20.7246	[48]
		19	benzene	0.9691	
		20	carbon tetrachloride	0.2999	[128]
		21	chlorobenzene	0.8274	[48]
		22	chloroform	0.1689	
		23	cyclohexane	0.1269	[129]
		27	diethyl ether	33.4357	[48]
		29	ethanol	50.8461	[130]
		31	ethyl formate	1.4244	[48]
		32	ethylene glycol	20.6973	
		33	formamide	13.6578	
		34	hexane	0.0787	[54]
		35	isobutanol	31.0935	[126]
		38	methanol	63.2867	[56]
		41	n-butyl acetate	18.7647	[126]
		42	n-heptane	0.154	[48]
		45	propionic acid	13.2051	
		46	propylene glycol	23.2643	
57	sclareol	8	1-propanol	13.1222	[131]
		15	acetone	17.9245	
		16	acetonitrile	4.0583	
		23	cyclohexane	21.5067	
		26	dimethylformamide	5.042	
		29	ethanol	15.2074	
		30	ethyl acetate	12.9944	
		33	formamide	0.1001	
		34	hexane	1.626	
		38	methanol	7.6426	
		48	toluene	15.3403	
58	sulfadiazine	2	1,4-dioxane	0.1406	[32]
		3	1-butanol	0.0107	[132]
		6	1-octanol	0.0027	
		7	1-pentanol	0.0075	
		13	2-propanol	0.0131	[32]
		15	acetone	0.4495	
		19	benzene	0.0009	
		26	dimethylformamide	26.1715	
		29	ethanol	0.0417	[132]
		30	ethyl acetate	0.0338	[32]
		32	ethylene glycol	0.1293	
		35	isobutanol	0.0091	
		38	methanol	0.1828	
		41	n-butyl acetate	0.0126	
		46	propylene glycol	0.1181	
		47	tetrahydrofuran	0.0007	
59	sulfamethoxazole	6	1-octanol	0.187	[133]
		13	2-propanol	1.1293	[134]
		19	benzene	0.0576	
		22	chloroform	0.1545	
		38	methanol	11.3991	
60	sulfamethoxypyridazine	2	1,4-dioxane	7.7899	[135]
		3	1-butanol	0.2763	
		6	1-octanol	0.0667	
		7	1-pentanol	0.2642	
		13	2-propanol	0.252	
		15	acetone	4.4715	
		19	benzene	0.0215	

		22	chloroform	0.3033	
		29	ethanol	0.7676	
		30	ethyl acetate	0.6535	
		32	ethylene glycol	2.2511	
		35	isobutanol	0.1627	
		38	methanol	2.5795	
		41	n-butyl acetate	0.2125	
		46	propylene glycol	1.9664	
		47	tetrahydrofuran	0.0156	
61	Sulfapyridine	6	1-octanol	0.0151	[133]
		13	2-propanol	0.2229	[134]
62	Testosterone	4	1-heptanol	13.3115	[136]
		5	1-hexanol	14.7633	
		6	1-octanol	13.3623	
		7	1-pentanol	15.418	
		42	n-heptane	0.0446	
		44	octane	0.0452	
63	Testosterone propionate	19	benzene	139.269	[137]
		20	carbon tetrachloride	42.6574	
		21	chlorobenzene	113.199	
		23	cyclohexane	4.9716	
		34	hexane	2.0088	
		42	n-heptane	2.0056	
		44	octane	2.4627	
		47	tetrahydrofuran	119.4384	
64	theophylline	3	1-butanol	0.2888	[138]
		8	1-propanol	0.3656	[50]
		13	2-propanol	0.3909	[138]
		15	acetone	0.3436	[139]
		16	acetonitrile	0.1878	[140]
		22	chloroform	0.2573	[138]
		29	ethanol	0.5343	[139]
		30	ethyl acetate	0.1519	[50]
		38	methanol	0.3542	[141]
		47	tetrahydrofuran	0.5221	[50]
		49	water	0.7421	[142]
65	triclosan	22	chloroform	169.9449	[143]
		42	n-heptane	8.5075	
66	trimethoprim	3	1-butanol	0.2488	[144]
		7	1-pentanol	0.2232	
		9	2-butanol	0.2204	
		13	2-propanol	0.1558	
		15	acetone	0.4451	
		29	ethanol	0.4293	
		38	methanol	1.5684	
		47	tetrahydrofuran	0.472	
67	tris(1,2-dioxyphenyl)cyclotriphosphazene	1	1,2-dichloroethane	0.2717	[145]
		15	acetone	0.2555	
		22	chloroform	0.8251	
		25	dichloromethane	0.949	
		29	ethanol	0.1169	
		47	tetrahydrofuran	0.7109	
		48	toluene	0.4329	
68	valsartan	16	acetonitrile	15.664	[146]
		22	chloroform	1.5534	
		25	dichloromethane	1.9612	
69	gsk-Q	10	2-butanone	2.0621	##
		11	2-methoxy-2-methylpropane	0.1486	##
		16	acetonitrile	0.1426	##
		30	ethyl acetate	0.9756	##
		37	isopropyl acetate	0.8028	##
		48	toluene	0.046	##
70	gsk-A	1	1,2-dichloroethane	1.438	##
		2	1,4-dioxane	0.3226	##
		3	1-butanol	0.0592	##
		8	1-propanol	0.0504	##
		9	2-butanol	0.0427	##

		10	2-butanone	1.4214	##
		11	2-methoxy-2-methylpropane	0.0075	##
		12	2-methyltetrahydrofuran	0.1624	##
		13	2-propanol	0.0539	##
		14	4-methyl-2-pentanone	0.3232	##
		15	acetone	2.4343	##
		16	acetonitrile	4.1959	##
		18	anisole	0.3236	##
		21	chlorobenzene	0.0638	##
		25	dichloromethane	2.6862	##
		29	ethanol	0.1442	##
		30	ethyl acetate	0.2776	##
		32	ethylene glycol	0.2643	##
		37	isopropyl acetate	0.1843	##
		38	methanol	0.5194	##
		39	methyl acetate	0.9211	##
		40	methylcyclohexane	0.0062	##
		41	n-butyl acetate	0.211	##
		42	n-heptane	0.0072	##
		43	n-propyl acetate	0.2441	##
		47	tetrahydrofuran	0.7466	##
		48	toluene	0.0281	##
		49	water	0.4711	##
71	gsk-H	1	1,2-dichloroethane	10.3363	##
		21	chlorobenzene	2.4416	##
		25	dichloromethane	3.7823	##
		40	methylcyclohexane	0.0425	##
		42	n-heptane	0.0411	##
		48	toluene	4.3255	##
72	gsk-S	3	1-butanol	25.5876	##
		13	2-propanol	31.4802	##
		18	anisole	10.0299	##
		24	cyclohexanone	24.5607	##
		30	ethyl acetate	32.4112	##
		37	isopropyl acetate	29.1601	##
		40	methylcyclohexane	45.0723	##
		49	water	0.0143	##
73	gsk-Z	12	2-methyltetrahydrofuran	8.0148	##
		15	acetone	7.9983	##
		16	acetonitrile	2.1316	##
		40	methylcyclohexane	0.3326	##
		42	n-heptane	7.4675	##
		47	tetrahydrofuran	7.7727	##
		48	toluene	1.4353	##
74	gsk-E	10	2-butanone	3.6522	##
		11	2-methoxy-2-methylpropane	1.4857	##
		16	acetonitrile	1.5377	##
		30	ethyl acetate	3.1818	##
		37	isopropyl acetate	2.7294	##
		48	toluene	2.9425	##
75	gsk-B	3	1-butanol	26.333	##
		9	2-butanol	26.8157	##
		10	2-butanone	32.4269	##
		11	2-methoxy-2-methylpropane	40.67	##
		12	2-methyltetrahydrofuran	31.0638	##
		13	2-propanol	26.6172	##
		14	4-methyl-2-pentanone	26.8182	##
		15	acetone	45.9522	##
		16	acetonitrile	24.6449	##
		18	anisole	21.4686	##
		24	cyclohexanone	24.8217	##
		29	ethanol	29.1992	##
		30	ethyl acetate	32.9241	##
		37	isopropyl acetate	31.4965	##
		38	methanol	32.2754	##
		40	methylcyclohexane	34.182	##
		42	n-heptane	42.8235	##

		47	tetrahydrofuran	33.4494	##
		48	toluene	25.8603	##
		49	water	0.0008	##

** Using all temperature points within the data source, solubility at 25°C was determined using the Van't Hoff equation for solubility.

Solubility values determined experimentally using a Technobis Crystal16 via turbidity measurements. Heating rate = 0.2°C/min, cooling rate = 0.4°C/min. Cycling four times per sample. Solubility at 25°C was determined using the Van't Hoff equation for solubility.

Solubility data generated with the automated FreeSlate CM3 platform in a 96 well format using solids in excess, operating in isothermal mode. The HPLC used for determining solute concentration is calibrated prior to sample analysis to identify the specific response factor for the given solute, using the same input material as used in the samples. Only analytical data within the linear calibration range is taken forward.

SI 5: References

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