

Table S3 Full data set and descriptors employed

Name	oct	chcl	cyc	TSA	ASA (scaled)	BSA (scaled)	PSA (scaled)	ASA (unscaled)
Acetamide	-1.09	-2.00	-4.88	103.10	6.17	44.39	50.56	8.23
Trimethylphosphate	-0.52	0.76	-2.22	183.69	0.00	81.23	81.23	0.00
Nitromethane	-0.35	0.44	-0.93	97.02	0.00	20.50	20.50	0.00
Acetonitrile	-0.34	0.40	-1.46	88.87	0.00	28.23	28.23	0.00
Aceticacid	-0.17	-1.60	-3.05	100.20	7.84	30.06	37.90	4.36
Imidazole	-0.08	-0.83	-3.70	106.85	2.57	44.10	46.67	4.08
1-Propanol	0.25	-0.30	-1.49	123.99	4.99	27.88	32.87	4.38
t-Butanol	0.35	-0.04	-1.15	144.18	4.94	25.23	30.16	4.33
Benzamide	0.64	0.11	-1.92	166.82	5.31	41.02	46.33	7.09
Pyrrole	0.75	0.91	-0.36	118.09	0.00	34.49	34.49	0.00
2-Butanol	0.76	0.30	-0.96	146.57	4.96	24.87	29.83	4.35
Triethylphosphate	0.80	2.28	-0.14	261.44	0.00	76.05	76.05	0.00
Nitropropane	0.87	1.91	0.53	145.51	0.00	19.59	19.59	0.00
Benzylamine	1.09	1.18	-0.12	168.53	2.04	49.49	51.54	8.51
2-Methylpyridine	1.11	1.79	0.23	152.99	0.00	30.25	30.25	0.00
Acetanilide	1.16	0.78	-1.51	196.64	6.05	26.25	32.30	4.03
3-Methylpyridine	1.20	1.89	0.27	152.33	0.00	31.76	31.76	0.00
4-Methylpyridine	1.22	1.77	0.21	152.34	0.00	31.85	31.85	0.00
o-Toluidine	1.32	1.96	0.61	166.96	2.71	21.68	24.39	7.54
4-Hydroxyacetophenone	1.45	0.08	-2.16	186.62	6.66	47.74	54.39	4.11
Benzaldehyde	1.47	2.25	1.13	158.25	0.00	28.02	28.02	0.00
Benzonitrile	1.56	2.71	1.11	157.26	0.00	28.24	28.24	0.00
4-Hydroxybenzoicacid	1.58	-2.00	-1.77	172.02	14.44	49.23	63.67	8.43
Acetophenone	1.58	2.78	1.27	179.23	0.00	26.63	26.63	0.00
2-Hydroxybenzaldehyde	1.81	2.43	1.37	164.05	0.61	21.74	22.35	4.06
Nitrobenzene	1.85	2.93	1.69	161.73	0.00	18.84	18.84	0.00
Tripropylphosphate	1.87	3.67	1.18	334.92	0.00	75.69	75.69	0.00
Isoquinoline	2.08	3.07	1.11	179.93	0.00	31.70	31.70	0.00
Methylbenzoate	2.12	3.01	2.08	193.44	0.00	24.09	24.09	0.00
Indole	2.14	2.95	0.79	167.14	2.57	9.11	11.68	4.07
4-Ethylphenol	2.47	1.47	0.37	189.36	6.63	21.17	27.80	4.09
4-Bromophenol	2.59	1.07	-0.09	166.09	6.65	21.14	27.79	4.10
1-Heptanol	2.72	2.41	1.12	220.03	4.99	27.89	32.88	4.38
Chlorobenzene	2.89	3.37	3.13	154.09	0.00	0.00	0.00	0.00

4-Iodophenol	2.91	1.56	0.57	172.60	6.65	21.14	27.79	4.11
Iodobenzene	3.25	3.70	3.54	165.20	0.00	0.00	0.00	0.00
Naphthalene	3.30	4.18	3.50	185.69	0.00	0.00	0.00	0.00
Biphenyl	4.01	4.67	4.16	221.43	0.00	0.00	0.00	0.00
2,4-Dimethylphenol	2.30	1.50	0.59	187.90	4.81	20.65	25.45	2.97
2,5-Dimethylphenol	2.33	1.59	0.57	187.99	4.80	20.63	25.44	2.96
2-Bromophenol	2.33	1.64	1.16	164.70	4.58	20.64	25.23	2.83
2-Fluorophenol	1.71	0.57	-0.30	146.87	6.02	21.14	27.16	3.71
2-Hydroxybenzoicacid	2.26	0.58	-0.46	169.93	8.08	23.43	31.51	6.30
2-Iodophenol	2.65	1.97	1.26	171.02	4.23	20.56	24.79	2.61
2-Methylphenol	1.98	1.23	-0.04	164.49	4.80	20.64	25.44	2.96
3,5-Dimethylphenol	2.35	1.60	0.38	189.13	6.60	21.16	27.76	4.07
3-Ethylphenol	2.50	1.41	0.36	189.36	6.60	21.17	27.76	4.07
3-Methylphenol	1.98	0.89	-0.34	165.71	6.60	21.17	27.77	4.08
4-Methylphenol	1.97	1.06	-0.35	165.72	6.62	21.17	27.80	4.09
Butanoicacid	0.79	-0.27	-1.76	148.74	7.83	28.15	35.98	4.35
Butylacetate	1.82	3.05	1.75	203.50	0.00	26.06	26.06	0.00
Butylamine	0.97	0.78	-0.29	150.91	2.04	52.66	54.70	8.51
Diethylamine	0.58	0.76	-0.34	158.20	1.03	36.13	37.16	4.28
Ethylamine	-0.13	-0.35	-1.80	103.11	2.04	52.85	54.89	8.51
Methylhexanoate	2.42	3.48	2.39	225.64	0.00	24.22	24.22	0.00
Methylpentanoate	1.87	3.01	1.81	201.65	0.00	24.22	24.22	0.00
Methylpropanoate	0.76	1.87	0.57	153.59	0.00	24.40	24.40	0.00
Propanone.mol	-0.24	0.50	-0.96	116.95	0.00	29.24	29.24	0.00
Butanone.mol	0.29	1.15	-0.25	140.80	0.00	26.91	26.91	0.00
Methanol.mol	-0.77	-1.33	-2.49	73.58	5.00	29.52	34.52	4.39
Ethanol.mol	-0.31	-0.87	-1.89	99.77	4.99	28.02	33.01	4.38
Butan-1-ol.mol	0.84	0.42	-0.87	146.32	4.87	24.75	29.62	4.27
pentanol.mol	1.56	1.05	-0.26	172.03	4.99	27.89	32.88	4.38
Benzoicacid.mol	1.87	0.60	-0.85	164.66	7.79	28.14	35.93	4.33
Phenol.mol	1.47	0.32	-0.93	142.27	6.62	21.16	27.78	4.09
m-Chlorophenol.mol	2.50	1.02	-0.12	161.49	6.63	21.14	27.77	4.09
p-Chlorophenol.mol	2.39	1.07	-0.35	161.52	6.64	21.15	27.79	4.10
triethylamine.mol	1.44	1.86	1.10	199.60	0.00	35.14	35.14	0.00
Propylamine.mol	0.47	0.25	-0.98	126.93	2.04	52.66	54.70	8.51
Pentanoicacid.mol	1.39	0.32	-1.10	172.74	7.83	28.17	36.00	4.35

p-Toluidine.mol	1.39	1.95	0.56	168.92	3.03	23.04	26.07	8.41
Ethylacetate.mol	0.73	1.82	0.34	155.11	0.00	26.05	26.05	0.00
Aniline.mol	0.90	1.35	0.05	145.43	3.03	23.03	26.06	8.41
Resorcinol.mol	0.80	-1.34	-3.79	149.68	13.25	42.28	55.52	8.18
o-Nitroaniline.mol	1.85	1.83	0.36	169.55	2.21	33.41	35.62	6.54
m-Nitroaniline.mol	1.37	1.60	-0.42	172.14	3.02	41.79	44.80	8.39
p-Nitroaniline.mol	1.39	1.26	-1.00	172.07	2.99	41.75	44.74	8.30
Methylacetate.mol	0.18	1.16	-0.19	129.17	0.00	26.20	26.20	0.00
Pyridine.mol	0.65	1.29	-0.31	128.62	0.00	31.81	31.81	0.00
2-Nitrophenol.mol	1.85	2.53	1.45	167.10	0.31	29.44	29.75	2.09
3-Nitrophenol.mol	2.00	0.50	-0.51	167.10	0.31	29.44	29.75	2.09
4-Nitrophenol.mol	1.91	0.20	-2.05	169.07	6.68	39.91	46.58	4.12
o-Methoxyphenol.mol	1.32	1.70	0.47	174.82	2.48	27.32	29.79	3.30
Benzene.mol	2.13	2.76	2.35	134.83	0.00	0.00	0.00	0.00
Toluene.mol	2.73	3.41	2.99	158.28	0.00	0.00	0.00	0.00
hexanol.mol	2.03	1.69	0.45	196.04	4.99	27.89	32.88	4.38
Diethylether.mol	0.89	1.88	0.93	154.89	0.00	17.23	17.23	0.00
2-Naphthol.mol	2.70	1.74	0.29	193.08	6.70	21.06	27.76	4.13
Phenylaceticacid.mol	1.00	0.57	-1.23	192.25	7.82	29.19	37.01	4.34
atropine.mol	1.83	2.44	-1.02	372.70	5.00	90.42	95.42	4.38
Aspirin.mol	0.90	0.63	-2.00	224.44	7.78	51.94	59.72	4.32
nicotine.mol	1.17	1.89	0.36	242.92	0.00	63.22	63.22	0.00
1-Naphthylamine.mol	2.25	2.60	1.26	194.24	2.64	21.73	24.36	7.32
1-Naphthol.mol	2.84	1.50	0.58	191.54	3.95	20.81	24.76	2.44
Ephedrine.mol	1.13	1.10	-0.44	244.87	4.64	50.17	54.81	7.46
o-Chlorophenol.mol	2.15	1.36	0.87	160.21	4.61	20.69	25.30	2.84
Quinine.mol	3.47	2.29	0.04	393.19	4.34	123.61	127.95	3.81
Propranolol	3.48	1.03	-0.64	355.15	5.83	72.22	78.05	8.05
Tetracaine	3.51	2.90	2.05	391.74	1.50	78.65	80.14	4.16
Papaverine	2.95	4.28	2.56	417.10	0.00	94.45	94.45	0.00
Tryptamine	2.15	1.53	-0.60	226.44	4.61	61.68	66.29	12.59
Diclofenac	4.51	2.97	1.88	323.01	8.49	35.48	43.97	6.14
Chlorpromazine	5.40	6.21	5.24	376.42	0.00	71.61	71.61	0.00
Ibuprofen	3.97	3.03	1.88	298.29	7.84	25.65	33.49	4.36
Lidocaine	2.44	4.08	1.23	340.30	5.09	54.53	59.62	3.39
Deprenyl	2.90	4.29	2.81	284.83	3.39	23.61	27.01	0.00

Desipramine	4.21	5.33	3.38	359.54	1.03	41.22	42.24	4.27
Fluoxetine	3.75	5.48	3.62	383.09	1.03	49.48	50.50	4.28
Procaine	2.14	2.13	-0.13	337.98	3.01	80.79	83.80	8.36
Miconazole	5.34	5.42	4.69	438.78	0.00	45.61	45.61	0.00

BSA (unscaled)	PSA (unscaled)	BenSA	HalSA	Predicted oct	Predicted chl	Predicted cyc
41.57	49.79	0.00	0.00	-0.26	-1.36	-3.11
46.93	46.93	0.00	0.00	-0.37	0.16	-2.13
50.69	50.69	0.00	0.00	0.27	0.98	-0.25
25.44	25.44	0.00	0.00	-0.08	0.52	-0.87
41.74	46.09	0.00	0.00	0.16	-1.25	-2.75
27.82	31.90	23.74	0.00	0.01	-0.25	-1.97
19.36	23.74	0.00	0.00	0.50	-0.03	-1.44
17.52	21.85	0.00	0.00	0.86	0.46	-0.87
38.70	45.78	52.29	0.00	1.30	0.50	-1.16
15.33	15.33	38.16	0.00	0.57	1.06	-0.45
17.27	21.62	0.00	0.00	0.90	0.51	-0.81
45.17	45.17	0.00	0.00	0.86	1.80	-0.31
48.67	48.67	0.00	0.00	0.96	1.91	0.74
18.33	26.84	51.50	0.00	1.00	0.99	-0.79
13.44	13.44	44.87	0.00	1.25	1.92	0.52
26.25	30.28	53.00	0.00	2.17	1.47	0.11
14.11	14.11	44.39	0.00	1.19	1.84	0.41
14.16	14.16	44.34	0.00	1.19	1.84	0.41
18.06	25.60	49.17	0.00	1.80	1.89	0.63
39.27	43.38	49.19	0.00	1.36	0.25	-1.53
20.76	20.76	52.43	0.00	1.48	2.15	0.80
25.44	25.44	52.27	0.00	1.46	2.13	0.76
57.68	66.11	49.77	0.00	1.26	-1.96	-3.88
19.73	19.73	51.78	0.00	1.80	2.59	1.28
37.95	42.01	50.28	0.00	1.73	2.35	1.11
47.14	47.14	53.23	0.00	1.81	2.59	1.41
44.95	44.95	0.00	0.00	1.88	3.17	1.14
14.09	14.09	78.34	0.00	1.96	2.58	1.15
27.03	27.03	52.35	0.00	2.08	2.96	1.71
12.15	16.22	73.22	0.00	2.45	2.59	1.54
19.61	23.70	47.77	0.00	2.18	1.36	0.09
19.58	23.68	49.09	43.64	2.16	0.86	-0.14
19.37	23.74	0.00	0.00	1.82	1.74	0.44
0.00	0.00	51.58	39.15	2.52	3.12	2.55

19.58	23.68	48.54	51.16	2.30	0.97	0.02
0.00	0.00	51.14	51.19	2.74	3.30	2.83
0.00	0.00	85.95	0.00	3.08	4.00	3.17
0.00	0.00	100.82	0.00	3.74	4.76	3.95
19.12	22.09	44.94	0.00	2.11	1.78	0.54
19.11	22.07	44.85	0.00	2.11	1.78	0.54
19.12	21.94	49.49	42.67	2.12	1.36	0.39
19.58	23.29	52.74	19.28	1.77	0.73	-0.46
55.89	62.19	50.04	0.00	1.89	0.57	-0.78
19.04	21.65	48.98	50.13	2.25	1.55	0.64
19.11	22.07	49.76	0.00	1.84	1.38	0.11
19.59	23.66	44.53	0.00	2.14	1.34	0.07
19.60	23.67	47.75	0.00	2.18	1.37	0.10
19.60	23.67	49.40	0.00	1.87	0.94	-0.36
19.61	23.69	49.40	0.00	1.87	0.94	-0.36
40.22	44.57	0.00	0.00	0.88	-0.27	-1.69
29.46	29.46	0.00	0.00	1.56	2.72	1.49
19.50	28.02	0.00	0.00	0.08	0.19	-1.62
10.04	14.32	0.00	0.00	0.65	1.23	-0.24
19.57	28.08	0.00	0.00	-0.59	-0.70	-2.56
29.16	29.16	0.00	0.00	1.92	3.20	2.03
29.17	29.17	0.00	0.00	1.59	2.76	1.57
29.29	29.29	0.00	0.00	0.93	1.87	0.62
21.66	21.66	0.00	0.00	0.28	1.00	-0.38
19.94	19.94	0.00	0.00	0.67	1.53	0.22
20.50	24.89	0.00	0.00	-0.24	-1.03	-2.52
19.46	23.83	0.00	0.00	0.17	-0.48	-1.92
17.19	21.46	0.00	0.00	0.90	0.54	-0.78
19.37	23.74	0.00	0.00	1.16	0.86	-0.50
38.15	42.48	52.36	0.00	1.70	0.37	-1.07
19.60	23.68	54.24	0.00	1.60	0.54	-0.79
19.57	23.67	48.98	39.12	2.07	0.79	-0.25
19.58	23.68	48.99	39.13	2.07	0.79	-0.25
3.91	3.91	0.00	0.00	1.24	2.29	0.88
19.50	28.01	0.00	0.00	-0.25	-0.25	-2.08
40.22	44.57	0.00	0.00	1.21	0.17	-1.23

19.20	27.62	48.51	0.00	1.79	1.79	0.50
29.54	29.54	0.00	0.00	0.90	1.83	0.55
19.19	27.60	53.38	0.00	1.52	1.39	0.07
39.15	47.32	51.65	0.00	1.16	-1.79	-3.59
63.41	69.95	50.25	0.00	1.49	1.60	0.12
66.22	74.61	49.83	0.00	1.28	1.11	-0.53
66.22	74.53	49.73	0.00	1.28	1.12	-0.52
30.74	30.74	0.00	0.00	0.54	1.34	0.04
14.14	14.14	49.43	0.00	0.93	1.44	-0.02
64.61	66.70	50.98	0.00	1.55	2.17	0.80
64.61	66.70	50.98	0.00	1.55	2.17	0.80
66.61	70.74	50.64	0.00	1.37	0.25	-1.41
29.97	33.27	50.34	0.00	1.75	1.87	0.52
0.00	0.00	56.84	0.00	2.05	2.87	2.01
0.00	0.00	51.99	0.00	2.32	3.27	2.44
19.37	23.74	0.00	0.00	1.49	1.30	-0.03
10.44	10.44	0.00	0.00	1.16	2.18	1.07
19.50	23.63	83.39	0.00	2.64	1.65	0.35
40.86	45.21	50.49	0.00	2.03	0.82	-0.62
43.29	47.67	48.71	0.00	2.60	2.39	0.01
63.56	67.88	47.62	0.00	1.75	0.50	-1.33
17.61	17.61	41.13	0.00	1.46	2.24	0.31
18.11	25.43	82.76	0.00	2.56	2.63	1.37
19.27	21.71	46.33	0.00	2.15	2.06	0.83
24.35	31.81	49.46	0.00	2.05	1.72	-0.02
19.16	22.00	49.36	38.15	2.03	1.28	0.27
46.59	50.39	64.60	0.00	2.05	1.71	-1.28
35.02	43.07	82.07	0.00	3.30	2.81	0.72
39.78	43.94	47.65	0.00	3.14	4.05	1.96
53.08	53.08	105.92	0.00	3.65	4.64	2.24
31.61	44.20	65.12	0.00	1.63	1.03	-0.96
43.48	49.63	86.03	72.58	4.54	2.93	1.96
8.12	8.12	87.78	39.01	3.83	4.61	2.89
37.91	42.27	40.36	0.00	3.48	2.85	1.60
26.56	29.96	43.77	0.00	3.18	3.16	1.44
2.62	2.62	49.52	0.00	3.38	3.82	2.64

12.87	17.15	89.14	0.00	4.29	5.34	3.89
17.27	21.55	96.14	55.53	4.81	5.39	4.19
48.41	56.77	48.85	0.00	2.38	2.61	0.41
21.00	21.00	102.52	148.71	6.37	6.71	6.27