For submission to CrystEngComm theme issue on "Functional Co-Crystals"

Supplementary Materials

Table S1 – Multi-component HBP screening results summary for paracetamol with potential co-former molecules ranked in order of their MC Score. Each computed MC score also has an associated estimated uncertainty based on Chi^2 statistics resulting from model fitting. The size of the uncertainty is related to the amount of contributory data from the CSD.

Rank	Co-Former	MC Score	Statistical Uncertainty	Most Likely Interaction	Co-Crystal	Refcode
1	caffeine	0.22	0.10	A:B	no	-
2	4,4-trimethylene-dipyridine	0.21	0.07	A:B	unclear*	N/A
3	pyrazine	0.21	0.09	A:B	no	-
4	1,2-bis-4-pyridyl-ethane	0.20	0.07	A:B	yes	KETZAM
5	4,4-bipyridine	0.19	0.07	A:B	yes	MUPQAP
6	1,4-di-4-pyridyl-ethylene	0.19	0.07	A:B	yes	KETYUF
7	phenazine	0.19	0.15	A:B	yes	LUJSOZ
8	citric acid	0.15	0.05	B:A	yes	AMUBAM
9	malic acid	0.12	0.04	B:A	no	-
10	malonic acid	0.12	0.05	B:A	no	-
11	N-methyl-morpholine	0.12	0.12	A:B	yes	MUPPOC
12	adipic acid	0.11	0.06	B:A	no	-
13	2,5-dihydroxy-benzoic acid	0.11	0.07	B:A	no	-
14	benzoic acid	0.11	0.07	B:A	no	-
15	piperazine	0.11	0.07	B:A	yes	MUPPUI
16	1,4-diaminocyclohexane	0.10	0.08	B:A	yes	WIGCEW
17	theobromine	0.10	0.12	A:B	no	-
18	succinic acid	0.09	0.06	B:A	no	-
19	fumaric acid	0.09	0.07	B:A	no	-
20	maleic acid	0.09	0.07	B:A	no	-
21	morpholine	0.06	0.05	B:A	yes	MUPQET
22	N,N-dimethyl-piperazine	0.05	0.07	A:B	yes	MUPPIW
23	saccharin	0.03	0.20	B:A	no	-
24	melamine	0.02	0.11	B:A	no	-
25	resorcinol	0.00	0.09	A:A	no	-
26	theophylline	0.00	0.11	B:B	yes	KIGLUI
27	ascorbic acid	-0.03	0.06	B:B	no	-
28	imidazole	-0.03	0.10	B:B	no	-
29	oxalic acid	-0.06	0.14	A:A	yes	LUJTAM
30	1,4-dioxane	-0.07	0.07	A:A	yes	MUPPES
31	1-naphthol	-0.07	0.09	A:A	no	-
32	nicotinamide	-0.11	0.04	B:B	no	-
33	isonicotinamide	-0.12	0.04	B:B	no	-
34	3S-cis-3,6-dimethyl-1,4-dioane-2,5-dione	-0.21	0.10	A:A	no	-
35	3-isochromanone	-0.40	0.08	A:A	no	-

* V. K. Srirambhatla, A. Kraft, S. Watt and A. V. Powell, Cryst. Growth Des., 2012, 12, 4870-4879.