New solid forms of artemisinin obtained through cocrystallisation

Supplementary Material

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Figure S35. Cocrystallisation of art and L-glutamine, from top to bottom: PXRD patterns of art, L-glutamine, LAG product.



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Figure S59. Cocrystallisation of art and benzenesulfonic acid, from top to bottom: PXRD patterns of art, benzenesulfonic acid, LAG product.



Figure S60. Cocrystallisation of art and L-aspartic acid, from top to bottom: PXRD patterns of art, L-aspartic acid, LAG product.



Figure S61. Cocrystallisation of art and L-arginine, from top to bottom: PXRD patterns of art, L-arginine, LAG product.



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Figure S63. Cocrystallisation of art and acetic acid, from top to bottom: PXRD patterns of art and the LAG product.



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Figure S65. Cocrystallisation of art and 3-ap, from top to bottom: PXRD patterns of art, 3-ap, LAG product.



Figure S66. Cocrystallisation of **art** and 3,5-diaminobenzoic acid, from top to bottom: PXRD patterns of **art**, 3,5-diaminobenzoic acid, LAG product.



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Figure S68. Cocrystallisation of art and 1,3-pda, from top to bottom: PXRD patterns of art, 1,3-pda, LAG product.



Figure S69. Cocrystallisation of **art** and 1,3-dihydroxynaphthalene, from top to bottom: PXRD patterns of **art**, 1,3-dihydroxynaphthalene, LAG product.



Figure S70. Cocrystallisation of art and olivetol, from top to bottom: PXRD patterns of art, olivetol, LAG product.



Figure S71. Cocrystallisation of art and orotic acid, from top to bottom: PXRD patterns of art, orotic acid, LAG product.



Figure S72. Cocrystallisation of art and piperazine, from top to bottom: PXRD patterns of art, piperazine, LAG product.



Figure S73. Cocrystallisation of art and L-tyrosine, from top to bottom: PXRD patterns of art, L-tyrosine, LAG product.



Figure S74. Cocrystallisation of **art** and succinic acid, from top to bottom: PXRD patterns of **art**, succinic acid, LAG product. Mechanochemical reaction resulted in conversion of **art** to triclinic form.



Figure S75. Cocrystallisation of art and phenol, from top to bottom: PXRD patterns of art, phenol, LAG product.



Figure S76. Reflectance FT-IR spectra (top to bottom) for res, art and (art)₂ (res).



Figure S77. Reflectance FT-IR spectra (top to bottom) for orc, art and (art) (orc).



Figure S78. DSC thermogram for $(art)_2$ (res) cocrystal obtained by LAG.



Figure S79. DSC thermogram for (art) (orc) cocrystal obtained by LAG.

						Predicted
entry	co-former	S/L	M/L	FNO	Dipole	cocrystallisation
1	phloroglucinol	0.41	0.93	0.33	1.19	Y
2	phenol	0.44	0.88	0.14	0.98	Y
3	orc	0.50	0.95	0.22	1.03	Y
4	res	0.39	0.84	0.25	1.88	Y
5	3-aminophenol	0.45	0.91	0.25	2.52	Y
6	1,3-phenylenediamine	0.40	0.83	0.25	1.6	Y
7	tyrosine	0.66	0.71	0.31	16.11	Ν
8	glutamine	0.68	0.68	0.50	15.38	Ν
9	saccharin	0.61	0.87	0.33	3.21	Y
10	ascorbic acid	0.60	0.76	0.50	4.52	Y
11	glycolic acid	0.59	0.76	0.60	2.98	Ν
12	gentisic acid	0.39	0.86	0.36	2.5	Y
13	tartaric acid ^(a)	0.69	0.69	0.60	4.68	Ν
14	lysine	0.45	0.57	0.40	14.77	Ν
15	mannitol	0.62	0.66	0.50	2.49	Y
16	N-methylglucamine	0.59	0.68	0.46	2.02	Y
17	pyridoxine	0.46	0.94	0.33	4.83	Y
18	nicotinamide	0.41	0.69	0.33	1.96	Y
19	glucose	0.59	0.89	0.50	2.51	Y
20	citric acid	0.56	0.65	0.54	5.67	Y
21	acetic acid	0.65	0.88	0.50	2.35	Y
22	sorbitol	0.64	0.69	0.50	2.66	Y
23	arginine	0.57	0.59	0.50	<u>29.75</u>	Ν
24	fructose	0.80	0.93	0.50	2.69	Y
25	caffeine	0.42	0.86	0.43	3.42	Y
26	sucrose	0.78	0.87	0.48	4.82	Y
27	glycine	0.62	0.79	0.60	<u>15</u>	Ν
28	hippuric acid	0.46	0.56	0.31	4.22	Ν
29	lactose	0.48	0.73	0.48	5.65	Y
30	cysteine	0.86	0.98	0.43	<u>14.4</u>	Ν
31	aspartic acid	0.63	0.72	0.56	<u>13.56</u>	Ν
32	lactic acid	0.69	0.83	0.50	3.58	Y
33	malic acid ^(a)	0.57	0.64	0.56	2.66	Ν
34	ethylenediamine	0.61	0.71	0.50	<u>0</u>	Ν
35	succinic acid	0.44	0.60	0.50	<u>0</u>	Ν
36	fumaric acid	0.38	0.65	0.50	<u>0</u>	Ν
37	maleic acid	0.38	0.69	0.50	3.53	Y
38	malonic acid	0.63	0.69	0.57	3.76	Ν
39	orotic acid	0.37	0.82	0.55	3.57	Ν
40	mandelic acid ^(a)	0.73	0.74	0.27	1.72	Y
41	urea	0.54	0.88	<u>0.75</u>	3.68	Ν
42	tromethamine	0.60	0.92	0.36	2.35	Y
43	glucuronic acid	0.63	0.78	0.54	2.48	Y
44	benzenesulfonic acid	0.58	0.72	0.30	2.04	Y
45	piperazine	0.67	0.94	0.33	0	N

Table S1. Calculated descriptors for potential cocrystal formers^(a,b) (orc and res are highlighted in bold and values outside the range are underlined).

-		-		2		
46	ibuprofen	0.47	0.54	0.13	2.15	Ν
47	paracetamol	0.36	0.60	0.27	5.41	Ν
48	benzoic acid	0.37	0.73	0.22	2.51	Y
49	theophylline	0.43	0.88	0.46	3.26	Y
50	theobromine	0.43	0.81	0.46	4.18	Y
51	camphorsulfonic acid	0.77	0.78	0.27	5.91	Y
52	1,3-dihydroxynaphthalene	0.35	0.83	0.17	1.07	Y
53	3,5-diaminobeznoic acid	0.36	0.91	0.36	3.31	Y
54	5-aminosalicylic acid	0.36	0.80	0.36	3.38	Y
55	alanine ^(a)	0.77	0.97	0.50	14.99	Ν
56	L-serine	0.78	0.98	0.57	16.03	Ν
57	cyanuric acid	0.44	0.98	0.67	0.04	Ν
58	ethanedisulfonic acid	0.51	0.52	0.60	<u>0</u>	Ν
59	galacturonic acid	0.55	0.78	0.54	4.83	Y
60	hexylresorcinol	0.36	0.55	0.14	1.57	Ν
61	hydroquinone	0.39	0.79	0.25	<u>0</u>	Ν
62	lactobionic acid	0.56	0.92	0.50	3.89	Y
63	methanesulfonic acid	0.80	0.85	0.60	1.95	Ν
64	olivetol	0.44	0.64	0.15	2.72	Y
65	phenylalanine ^(a)	0.61	0.65	0.25	15.26	Ν
66	sulfamide	0.75	0.87	0.80	2.51	Ν
67	theophylline-7-acetic acid	0.53	0.82	0.47	4.34	Y

Continuation of Table 1

(a) Descriptors for chiral and racemic forms of a compound are identical; (b) cyclodextrin inclusion hosts are excluded.