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Melting points of one- and two-component molecular crystals as effective characteristics for rational design of pharmaceutical systems

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Table S1 Coefficients of correlation equation (1) for the clusters including the considered compound as one from the components of the two-component crystal

№	API	(API:CF)			A	B	R[a]	σ[b]	n[c]	T_{fus} /°C
1	1,2-phenylenediamine	1:1			-286±190	1.767±0.445	0.9420	38.90	4	102.1
2	1-hydroxy-2-naphthoic acid	1:1			202±59	0.525±0.136	0.8246	23.30	9	192.0
3	2,3,5,6-F-4-I-BA	1:1			31±77	1.065±0.211	0.9458	12.00	5	151.0
4	2,4-OH-BA	1:1			119±41	0.717±0.089	0.9309	15.90	12	213.0
5	2-Acetaminopyridine	2:1			150±46	0.579±0.104	0.8922	20.50	10	69.0
6	2-OH-BZA	1:1			214±36	0.441±0.080	0.9006	10.90	9	140.8
7	2-Pyridone	1:1			105±51	0.657±0.121	0.9121	16.80	8	107.8
8	3,5-OH-BA	1:1			255±39	0.522±0.081	0.9335	19.10	8	237.5
9	3-OH-BA	1:1			241±22	0.404±0.047	0.9032	15.20	19	203.0
10	4-Bromobenzamide	2:1			142±115	0.704±0.271	0.7576	19.80	7	191.5
11	4-nitro-Phenol	1:1	2:1		175±39	0.612±0.097	0.9031	19.30	11	113.5
12	4-Phenylpyridine	1:1	2:1		182±44	0.449±0.111	0.8964	14.40	6	69.5
13	p-toluenesulfonic acid	1:1			17±20	0.988±0.040	0.9967	5.60	6	106.5
14	Aakeroy_1	1:2			251±39	0.421±0.099	0.8854	12.20	7	158.5
15	Acetazolamide	1:1	1:2	2:1	162±39	0.698±0.940	0.9339	15.70	10	258.5
16	Acridine	1:1			8±55	0.905±0.122	0.8988	18.00	15	108.5
17	AMG517	1:1			207±35	0.593±0.089	0.8871	15.60	14	230.0
18	Arbidol	1:1	2:1		329±28	0.190±0.061	0.8728	8.02	5	124.8
19	Benzamide	1:1			151±39	0.561±0.082	0.9215	13.10	9	128.5
20	Benzoic Acid	1:1			97±45	0.701±0.701	0.8319	27.40	24	122.0
21	Benzotrifuroxan	1:1			231±38	0.545±0.091	0.9488	12.50	6	197.4
22	1,2-bis(4-pyridyl)propane	1:1			252±32	0.361±0.072	0.8455	17.50	12	54.5
23	trans-Cinnamic acid	1:1			168±36	0.523±0.079	0.9469	9.56	7	134.0
24	Clotrimazole	1:1	2:1		210±41	0.461±0.091	0.9298	7.36	6	148.0
25	Dapson	1:1	2:1	1:2	208±36	0.484±0.087	0.9407	10.80	6	177.5
26	Edaravone	1:1			165±29	0.421±0.099	0.9690	11.50	7	128.0
27	Febuxostat	1:1			328±31	0.266±0.070	0.8400	9.28	7	201.0
28	Flufenamic Acid	1:1			190±37	0.544±0.083	0.9563	11.60	6	133.9
29	Furosemide	1:1			264±24	0.406±0.055	0.8870	19.40	17	203.0
30	Gabapentin	1:1			205±31	0.470±0.071	0.9198	6.74	10	161.0
31	Glycolic Acid	1:1			209±34	0.414±0.069	0.9492	8.62	6	75.0
32	Imatinib mesylate	1:1	1:2		375±12	0.175±0.022	0.9397	4.30	10	223.3
33	Indomethacin	1:1			181±37	0.548±0.081	0.9490	10.20	7	160.8

34	Lamotrigine	1:1			45±12	0.980±0.027	0.9988	2.83	5	217.3
35	Lornoxicam	1:1			364±24	0.246±0.057	0.9274	5.88	5	227.5
36	Maleic Acid	1:1			166±30	0.585±0.064	0.9127	15.80	19	139.0
37	L-Malic Acid	1:1	1:2		131±55	0.678±0.117	0.9215	14.00	8	101.0
38	Malonic acid	1:1			168±49	0.541±0.100	0.8632	17.40	12	136.0
39	Methyl-Paraben	1:1			-15±18	0.911±0.039	0.9956	4.55	7	126.5
40	Meloxicam	1:1			251±37	0.508±0.087	0.8688	14.50	13	254.0
41	Nicotinic acid	1:1			46±38	0.873±0.079	0.9724	15.90	9	232.0
42	Norfloxacin	1:1			245±52	0.485±0.114	0.8493	22.50	9	220.6
43	p-Coumaric acid	1:1			296±18	0.338±0.040	0.9535	7.22	9	211.5
44	Paracetamol	1:1			297±17	0.272±0.037	0.9338	6.97	10	170.0
45	Phenazine	1:1	1:2	2:1	16±83	0.968±0.178	0.9252	25.90	7	177.0
46	Pimelic Acid	1:1	1:2		144±46	0.592±0.110	0.8626	13.30	12	104.0
47	Pyrazinamide	1:1			145±29	0.609±0.062	0.8569	13.50	37	189.0
48	Resorcinol	1:1			235±45	0.474±0.097	0.8786	14.30	9	110.5
49	Saccharin	1:1			242±21	0.459±0.047	0.8504	13.50	39	227.9
50	2-OH-BA	1:1			189±35	0.533±0.073	0.8305	20.20	26	159.0
51	Sulfadimidine	1:1			337±28	0.284±0.060	0.7036	12.80	25	197.0
52	Tefagur	1:1			288±58	0.262±0.126	0.7683	15.50	5	171.7
53	Tenoxicam	1:1			324±72	0.341±0.182	0.7348	7.76	5	209.5
54	Theophylline	1:1			197±33	0.571±0.075	0.8079	18.50	33	273.6
55	2,4,6-Trinitrotoluene	1:1			242±27	0.331±0.063	0.8451	14.60	13	80.5
56	Urea	1:1			210±42	0.504±0.088	0.8041	17.40	20	134.3
57	Vanillic Acid	1:1	2:1	1:2	285±26	0.308±0.053	0.9104	10.90	9	209.2
58	Adefovir dipivoxil	1:1			234±55	0.375±0.126	0.8303	15.30	6	93.3
59	Diethylstilbestrol	1:1	1:2		35±39	0.997±0.144	0.9516	13.50	7	182.1
60	Itraconazole	1:1	2:1	1:2	87±44	0.780±0.104	0.9424	11.20	9	166.2
61	Resveratrol	1:1	1:2		252±57	0.457±0.125	0.9034	16.40	5	267.7
62	Stanozolol	1:1			282±99	0.416±0.214	0.7466	19.00	5	244.3
63	4-Aminobenzoic acid	1:1			156±22	0.621±0.047	0.9396	13.60	25	189.0
64	Flurbiprofen	1:1			117±45	0.629±0.096	0.8914	16.90	13	109.3
65	Glutaric acid		1:2		254±38	0.372±0.078	0.9217	15.70	6	96.5
66	Oxalic Acid		1:2		144±56	0.695±0.123	0.8528	25.10	14	189.0
67	Pyrazine		1:2		1±19	0.997±0.045	0.9929	11.60	9	52.0
68	Quercetin		1:2		204±84	0.567±0.159	0.8032	24.50	9	321.4
69	D- or L-Tartaric Acid	1:1			59±23	0.801±0.047	0.9881	5.18	9	166.0
70	Sebacic acid	1:1			233±53	0.465±0.127	0.8532	17.70	7	132.0
1	1,4-diiodotetrafluorobenzene	1:1			106±32	0.738±0.083	0.9168	20.70	17	109.0
	1,4-diiodotetrafluorobenzene		1:2		271±62	0.306±0.171	0.4313	25.40	16	109.0

2	4-OH-BA	1:1			128±24	0.702±0.054	0.9228	14.60	31	214.5
	4-OH-BA		2:1		295±40	0.446±0.097	0.8990	19.10	7	214.5
3	Adipic acid	1:1			156±43	0.644±0.098	0.9003	15.00	12	152.1
	Adipic acid		1:2		148±35	0.628±0.077	0.9040	17.00	17	152.1
4	1,2-bis(4-pyridyl)ethylene	1:1			262±41	0.419±0.089	0.8561	16.50	10	151.5
	1,2-bis(4-pyridyl)ethylene		1:2		212±28	0.535±0.063	0.9370	18.40	12	151.5
5	1,2-bis-(4-pyridyl)ethane	1:1			300±22	0.305±0.049	0.8396	14.30	18	112.0
	1,2-bis-(4-pyridyl)ethane		1:2		236±33	0.402±0.078	0.8906	14.80	9	112.0
6	Caffeine	1:1			132±21	0.673±0.045	0.9512	16.00	26	227.0
	Caffeine		2:1		223±30	0.445±0.063	0.9623	10.20	6	227.0
7	Carbamazepine	1:1			245±15	0.415±0.032	0.8990	11.50	42	190.1
	Carbamazepine		2:1		275±61	0.369±0.142	0.6544	18.30	11	190.1
8	CL20		1:2		114±78	0.743±0.176	0.9039	24.10	6	244.0
	CL20			2:1	118±22	0.712±0.044	0.9963	7.93	4	244.0
9	Fumaric Acid	1:1			303±30	0.324±0.065	0.7802	17.80	18	287.0
	Fumaric Acid		1:2		103±28	0.772±0.063	0.9261	19.10	27	287.0
10	Gallic Acid	1:1			236±62	0.547±0.138	0.8318	15.40	9	250.0
	Gallic Acid		1:2		164±27	0.638±0.064	0.9807	6.31	6	250.0
11	Hydrochlorothiazide	1:1			104±44	0.839±0.105	0.9428	16.40	10	269.0
	Hydrochlorothiazide		1:2		272±24	0.385±0.061	0.9642	7.37	5	269.0
12	Isoniazid	1:1			195±23	0.495±0.052	0.8782	14.50	29	171.5
	Isoniazid		2:1		271±30	0.316±0.063	0.8582	12.80	11	171.5
13	Isonicotinamide	1:1			243±26	0.420±0.059	0.7533	21.90	41	156.0
	Isonicotinamide		2:1		265±23	0.400±0.051	0.8919	14.30	18	156.0
	Isonicotinamide			1:2	220±27	0.513±0.064	0.9704	7.36	6	156.0
14	D- or L-Proline	1:1			258±14	0.413±0.030	0.9394	11.80	27	228.0
	D- or L-Proline			1:2	246±34	0.475±0.084	0.9423	4.22	6	228.0
15	Naproxen	1:1			135±32	0.604±0.069	0.9407	10.70	12	155.6
	Naproxen		2:1		263±27	0.349±0.063	0.9413	7.62	6	155.6
16	Nicotinamide	1:1			178±15	0.514±0.033	0.8936	15.60	63	128.4
	Nicotinamide		1:2		-73±71	1.086±0.151	0.9381	16.80	9	128.4
	Nicotinamide			2:1	268±28	0.322±0.058	0.8907	14.30	10	128.4
17	Riluzole	1:1			319±45	0.216±0.102	0.6237	12.60	9	118.0
	Riluzole		2:1		165±58	0.555±0.140	0.8706	11.60	7	118.0
18	Succinic acid	1:1			276±24	0.371±0.053	0.7952	20.90	31	184.0
	Succinic acid		1:2		155±30	0.624±0.067	0.8666	17.00	31	184.0

[a] Pair correlation coefficient; [b] Standard deviation; [c] A number of points in the cluster;

3-OH-BA – 3-hydroxybenzoic acid;

2-OH-BA – 2-hydroxybenzoic acid;

2,4-OH-BA – 2,4-dihydroxybenzoic acid;

3,5-OH-BA – 3,5-dihydroxybenzoic acid;

2,3,5,6-F-4-I-BA - 4-iodotetrafluorobenzoic acid;

2-OH-BZA - 2-hydroxybenzamide (Salicylamide);

Table S2 Correlation equation (1) is not observed for the clusters including the considered compound as one from the components of the two-component crystal

№	API	(API:CF)			n[a]	T_{fus} /°C
1	4,4'-bipyridine	1:1	1:2		75	111.8
2	Glutaric acid	1:1			34	96.5
3	4-NH2-SA	1:1	2:1	1:2	27	150.5
4	Suberic acid	1:1	1:2		24	142.5
5	Ciprofloxacin	1:1	2:1		23	271.7
6	Citric acid	1:1	1:2		20	155.2
7	Curcumin	1:1			18	183.2
8	Quercetin	1:1			16	321.4
9	Diflunisal	1:1	2:1		14	211.8
10	tetra-Me-pyrazine	1:1	1:2	2:1	14	85.0
11	Naringenin	1:1	1:2		14	252.4
12	2,5-OH-BA	1:1			13	205.0
13	4-OH-BZA	1:1	1:2		13	161.5
14	HMX	1:1			13	279.0
15	Nitrofurantoin	1:1			13	268.4
16	Metaxalone	1:1	2:1		13	124.0
17	4,4'-azopyridine	1:1			12	105.5
18	Sertraline	1:1			12	247.5
19	DL-Tartaric Acid	1:1			11	205.0
20	Mandelic acid	1:1			10	132.6
21	3,3'-azopyridine	1:1			10	133.0
22	5-Fluorocytosine	1:1			10	297.8
23	4-DMA-Py	1:1			10	111.5
24	D- or L-Proline		2:1		10	228.0
25	Azelaic Acid	1:1	2:1		9	106.5
26	Amoxapine	1:1			9	183.1
27	Flurbiprofen		2:1		9	109.3
28	Ketoconazole	1:1			8	148.0
29	Minoxidil	1:1			8	273.0
30	Voriconazole	1:1			8	129.6
31	Pefloxacin	1:1			8	273.0
32	Theobromine	1:1			8	357.0
33	4-NH2-BA		1:2		8	189.0
34	Agomelatine	1:1			7	113.0
35	Phloroglucinol	1:1	2:1		7	216.0

36	Albendazole	1:1			7	204.5
37	Lesinurad	1:1			7	175.6
38	Oxalic Acid	1:1			7	189.0
39	Sebacic acid		1:2		7	132.0
40	Sildenafil	1:1			7	188.7
41	Sildenafil		2:1		7	188.7
42	2-NH2-BA	1:1			6	146.0
43	Hydroquinone	1:1			6	173.5
44	MMP	1:1	2:1		6	195.0
45	Niclosamide	1:1			6	229.5
46	Sorbic acid	1:1			6	133.5
47	Temozolomide	1:1	2:1		6	210.0
48	11-Azaartemisinin	1:1			6	159.0
49	Entacapone	1:1			6	163.0
50	4-Br-BA	1:2	1:4		5	234.0
51	Acyclovir	1:1			5	253.6
52	DL-Proline	1:1	2:1	1:2	5	208.0
53	Pyrazine	1:1			5	52.0
54	Sulfacetamide	1:1	1:2		5	184.0
55	Celecoxib	1:1			5	157.8
56	4-DMA-Py		1:2		4	111.5
57	4-DMA-Py			2:1	4	111.5

[a] A number of points in the cluster;

HMX - octahydro-1,3,5,7-tertranitro-1,3,5,7-tetrazocine;

MMP - 3-(6-Methoxypyridin-3-yl)-5-(4-methylsulfonyl phenyl)-pyridin-2-amine;

4-DMA-Py – 4-(dimethylamino)pyridine;

4-NH2-BA – 4-Aminobenzoic acid;

4-NH2-SA (PASA) - p-Aminosalicylic acid;

Table S3 The melting points of the two-component crystals having the same composition but different stoichiometry[a]

№	API	CF	(API:CF)	$T_{fus}(API)/°C$	$T_{fus}(CF)/°C$	$T_{fus}(CC)/°C$
1	Isonicotinamide	Salicylic acid	1:2	156.0	158.6	141.1
			1:1			120.0
			1:1			132.5
			1:1			131.7
2	Pimelic Acid	Isonicotinamide	1:2	105.0	156.0	140.0
			1:1			111.0
3	Suberic Acid	Isonicotinamide	1:2	142.5	156.0	170.0
			1:1			169.0
4	Azelaic acid	Isonicotinamide	1:2	106.5	156.0	141.0
			1:1			142.0
5	Adipic acid	Isonicotinamide	1:2	151.5	156.0	178.0
			1:1			164.0
6	Glutaric acid	Isonicotinamide	1:2	98.0	156.0	149.0
			1:1			134.5
7	Benzoic acid	Isonicotinamide	1:1	122.0	156.0	166.0
			1:1			162.6
			1:1			163.5
			2:1			143.1
8	Isonicotinamide	Furosemide	1:2	156.0	220.7	204.3
			1:1			196.0 (P)
			1:1			154.0 (P)
9	4-Aminobenzoic acid	Carbamazepine	***1:4***	189.0	191.0	***120.0***
			1:2			186.0
			1:2			157.0
			1:1			148.0
10	Carbamazepine	Succinic acid	1:2	191.0	192.1	188.9
			1:2			188.9
			1:1			188.6
11	Glutaric acid	Carbamazepine	1:2	98.0	191.0	125.0
			1:1			124.6
			1:1			125.9
12	Malonic acid	Carbamazepine	1:2	134.0	191.0	142.0
			1:1			143.4
13	Carbamazepine	Oxalic acid	1:2	191.0	192.1	164.7

			1:1			157.7
14	Carbamazepine	2,3-OH-BA	1:1	191.0	204.0	140.5
			2:1			158.0
15	**Urea**	**Succinic acid**	**1:1**	**134.3**	**192.1**	**140.0**
			2:1			**150.0**
16	3-Cyanophenol	Bipyete	1:1	81.5	151.5	124.5
			2:1			113.0
17	4-Cyanophenol	Bipyete	1:1	111.5	151.5	154.5
			2:1			141.5
18	4,4’-bipyridine	Carprofen	1:2	111.8	212.3	176.0
			1:1			167.0
			2:1			106.0
19	**4,4’-bipyridine**	**p-Aminosalicylic acid**	**1:2**	**111.8**	**150.5**	**157.0**
			3:2			**162.0**
20	Bipyeta	p-Aminosalicylic acid	1:2	112.0	150.5	142.0
			1:1			145.0 (P)
			1:1			140.0 (P)
21	2-Methoxy-4-nitrophenol	4-dimethylamino pyridine	1:1	101.5	111.5	116.5
			2:1			100.0
22	2-Methoxy-5-nitrophenol	4-dimethylamino pyridine	1:1	104.5	111.5	75.0
			2:1			60.0
23	Fluconazole	Fumaric acid	1:1	139.0	287.0	185.4
			2:1			130.5
24	Maleic Acid	Caffeine	1:2	139.0	236.0	119.0
			1:1			105.0
			1:1			99.0
25	Dmpz	Salicylic acid	1:2	106.5	158.6	78.6
			2:1			76.3
26	Nicotinamide	Fumaric acid	1:1	129.5	287.0	176.0
			2:1			170.0
27	Citric acid	Ciprofloxacin	1:2	155.2	269.5	225.0
			1:1			210.8
28	Ciprofloxacin	Fumaric acid	1:1	269.5	287.0	203.8
			2:1			230.0
29	Ciprofloxacin	Fumaric acid	1:1	269.5	287.0	227.8
			2:1			226.7
30	Succinic acid	Ciprofloxacin	1:2	192.1	269.5	228.1
			1:1			214.8

31	Phenazine	Phloroglucinol	3:2	177.0	216.0	241.0
			3.5:2			240.0
			2:1			237.0
32	Malonic acid	AMG517	1:2	134.0	230.0	197.0
			1:1			186.0
33	1-hydroxy-2-naphthoic acid	Minoxidil	1:1	192.0	273.0	154.0
			2:1			164.0
34	**p-Coumaric acid**	**Caffeine**	**1:2**	**211.5**	**236.0**	**177.8**
			1:1			**181.4**
35	**2,4,6-Trinitrotoluene**	**Anthranilic acid**	**1:2**	**81.0**	**99.0**	**139.3**
			1:1			**151.7**
36	Nicotinamide	(R)-mandelic acid	1:2	129.5	131.7	66.8
			1:1			89.1 (P)
			1:1			85.2 (P)
			4:1			98.3
37	**4,4'-bipyridine**	**Felodipine**	**1:2**	**111.8**	**143.8**	**128.9**
			1:1			**141.8 (P)**
			1:1			**138.8 (P)**
38	Nicotinamide	p-Coumaric Acid	1:2	128.0	211.5	174.0
			1:1			154.0 (P)
			1:1			158.0 (P)
			1:1			160.0 (P)
			1:1			161.0
39	Metaxalone	Maleic Acid	1:1	123.7	139.0	128.1
			2:1			125.0
40	**4-dimethylamino pyridine**	**Salicylic acid**	**1:2**	**111.5**	**158.6**	**107.5**
			1:1			**175.5**
41	Voriconazole	Oxalic acid	2:3	129.6	192.1	158.0
			1:1			154.5
42	Methyl Paraben	Ezetimibe	1:3	127.3	164.4	111.0
			2:3			110.0
			1:1			109.0
43	2-Pyridone	Acetazolamide	1:1	107.8	258.5	180.0
			2:1			160.0
44	Pyrazinamide	4-Nitrobenzoic acid	1:1	190.0	237.0	181.0
			2:1			171.0
45	Pyrazine	4-Aminosalicylic acid	1:2	53.0	150.5	167.0
			1:1			139.0

46	3-Aminopyridine	4-Aminosalicylic acid	1:1	65.0	150.5	158.0
			2:1			118.0
47	2,6-OH-BA	Isoniazid	1:1	164.0	171.0	193.8
			2:1			189.2
48	Isoniazid	4-Aminobenzoic acid	1:2	171.0	189.0	152.6 (P)
			1:2			130.5 (P)
			1:1			122.8
49	4,4'-bipyridine	N-bromosuccinimide	1:2	111.8	208.0	136.0
			1:1			131.0
50	Benzamide	Salicylic acid	1:1	123.7	158.6	138.3
			2:1			130.1
51	Hydroxyquinol	Curcumin	1:1	140.0	183.2	163.2
			2:1			160.2
52	Norfloxacin	Fumaric acid	1:1	220.0	287.0	229.0 (P)
			1:1			201.8 (P)
			2:1			227.1
53	Progesterone	4-OH-BA	1:2	129.8	215.0	180.4
			1:1			141.3 (P)
			1:1			137.5 (P)
			2:1			142.3
54	Resorcinol	Sildenafil	1:1	110.0	188.7	117.0
			2:1			152.0
55	2-Picolinic	Leflunomide	1:1	137.4	165.6	135.4
			2:1			125.4
56	Quinoxaline	N-triphenylacetyl-l-tyrosine	1:2	28.0	205.0	145.0
			1:1			120.0
57	**Pyrazine**	**CL20**	**3:2**	**53.0**	**219.0**	**225.0**
			2:1			**233.0**
58	**4-aminopyridine**	**Orotic Acid**	**1:2**	**154.4**	**300.0**	**278.0**
			1:1			**285.0**
59	Nicotinamide	Diethylstilbestrol	1:1	129.3	182.1	157.2
			2:1			156.6
60	Nicotinamide	Zaltoprofen	1:1	123.0	134.0	128.0
			2:1			121.0
61	TDZ	Gallic Acid	1:1	114.0	272.0	155.0
			2:1			130.0
62	**R-Flurbiprofen**	**L-Proline**	**1:3**	**108.0**	**226.6**	**156.3**
			1:2			**137.7**
			1:1			**144.9**

			2:1			**156.5**
63	**R-Flurbiprofen**	**D-Proline**	**1:1**	**108.0**	**226.6**	**143.6**
			2:1			**152.1**
64	R-Flurbiprofen	DL-Proline	1:1	108.0	207.8	146.9
			2:1			147.6
65	RS-Flurbiprofen	D-Proline	1:1	114.0	226.6	142.6 (P)
			1:1			185.4 (P)
			2:1			154.0
66	RS-Flurbiprofen	L-Proline	1:1	114.0	226.6	149.7 (P)
			1:1			188.3 (P)
			1:1			151.6 (P)
			2:1			160.4

[a](P) is polymorphic form;

2,6-OH-BA – 2,6-dihydroxybenzoic acid;

Bipyeta – 1,2-bis-(4-pyridyl)ethane;

Bipyete -1,2-bis(4-pyridyl)ethylene;

Dmpz - 3,5-Dimethyl-1H-pyrazole;

TDZ - (1-[5-(3-Chloro-phenylamino)-1,2,4-thiadiazol-3-yl]-propan-2-ol);

Table S4 Melting points of the two-component crystals based on racemates and enantiomersa

№	API	CF	(API:CF)	$T_{fus}(API)/°C$	$T_{fus}(CF)/°C$	$T_{fus}(CC)/°C$
1	(RS)-Ibuprofen	4,4'-bipyridine	2:1	113.3	111.8	121.4
	(S)-Ibuprofen	4,4'-bipyridine	2:1	51.4	111.8	75.1
2	(RS)-Ibuprofen	Nicotinamide	1:1	74.0	129.5	89.5
	(S)-Ibuprofen	Nicotinamide	1:1	51.4	129.5	80.3
3	Meloxicam	DL-Malic acid	2:1	254.0	131.0	215.0
	Meloxicam	L-Malic acid	2:1	254.0	101.0	200.0
4	CBZ	DL-Tartaric acid	1:1	191.0	205.0	170.0
	CBZ	L-Tartaric acid	1:1	191.0	169.0	159.7
5	CBZ	DL-Malic acid	1:1	191.0	131.0	135.3
	CBZ	L-Malic acid	1:1	191.0	101.0	91.1
6	Acyclovir	DL-Tartaric acid	1:1	250.0	205.0	163.0
	Acyclovir	L-Tartaric acid	1:1	250.0	169.0	155.0
7	**Gabapentin**	**RS-mandelic acid**	**1:1**	**161.0**	**134.0**	**125.0**
	Gabapentin	**S-mandelic acid**	**1:1**	**161.0**	**130.0**	**129.0**
	Gabapentin	**R-mandelic acid**	**1:1**	**161.0**	**130.0**	**129.0**
8	Gabapentin	DL-Tartaric acid	1:1	161.0	205.0	157.0
	Gabapentin	L-Tartaric acid	1:1	161.0	169.0	132.0
	Gabapentin	D-Tartaric acid	1:1	161.0	169.0	132.0
9	**Amoxapine**	**DL-Tartaric Acid**	**1:1**	**183.1**	**205.0**	**147.1**
	Amoxapine	**D-Tartaric Acid**	**1:1**	**183.1**	**169.0**	**147.2**
10	(R)-Flurbiprofen	DL-Proline	1:1	108.0	207.8	146.9
	(R)-Flurbiprofen	L-Proline	1:1	108.0	226.6	144.9
	(R)-Flurbiprofen	D-Proline	1:1	108.0	226.6	143.6
11	**(R)-Flurbiprofen**	**DL-Proline**	**2:1**	**108.0**	**207.8**	**147.6**
	(R)-Flurbiprofen	**L-Proline**	**2:1**	**108.0**	**226.6**	**156.5**
	(R)-Flurbiprofen	**D-Proline**	**2:1**	**108.0**	**226.6**	**152.1**
12	(RS)-Flurbiprofen	L-Proline	1:1	114.0	226.6	149.7 (P)
	(RS)-Flurbiprofen	L-Proline	1:1	114.0	226.6	188.3 (P)
	(RS)-Flurbiprofen	L-Proline	1:1	114.0	226.6	151.6 (P)
	(R)-Flurbiprofen	L-Proline	1:1	108.0	226.6	144.9
13	(RS)-Flurbiprofen	D-Proline	1:1	114.0	226.6	185.4 (P)
	(RS)-Flurbiprofen	D-Proline	1:1	114.0	226.6	142.6 (P)
	(R)-Flurbiprofen	D-Proline	1:1	108.0	226.6	143.6
14	(RS)-Flurbiprofen	L-Proline	2:1	114.0	226.6	160.4
	(R)-Flurbiprofen	L-Proline	2:1	108.0	226.6	156.5
15	(RS)-Flurbiprofen	D-Proline	2:1	114.0	226.6	154.0

	(R)-Flurbiprofen	D-Proline	2:1	108.0	226.6	152.1
16	(RS)-Naproxen	4,4'-bipyridine	2:1	153.0	111.8	135.0
	(S)-Naproxen	4,4'-bipyridine	2:1	155.0	111.8	119.0
17	(RS)-Naproxen	Piperazine	2:1	153.0	108.0	218.0
	(S)-Naproxen	Piperazine	2:1	155.0	108.0	213.0
18	(RS)-Naproxen	DL-Proline	1:1	153.0	207.8	193.8 (P)
	(RS)-Naproxen	DL-Proline	1:1	153.0	207.8	152.0 (P)
	(RS)-Naproxen	L-Proline	2:2	153.0	226.6	160.0
	(RS)-Naproxen	L-Proline	1:1	153.0	226.6	162.0 (P)
	(RS)-Naproxen	L-Proline	1:1	153.0	226.6	159.0 (P)
19	**(RS)-Naproxen**	**DL-Proline**	**2:4**	**153.0**	**207.8**	**169.0**
	(S)-Naproxen	**DL-Proline**	**1:2**	**155.0**	**207.8**	**182.0**
20	**(RS)-Naproxen**	**L-Proline**	**2:2**	**153.0**	**226.6**	**160.0**
	(RS)-Naproxen	**L-Proline**	**1:1**	**153.0**	**226.6**	**162.0 (P)**
	(RS)-Naproxen	**L-Proline**	**1:1**	**153.0**	**226.6**	**159.0 (P)**
	(S)-Naproxen	**L-Proline**	**1:1**	**155.0**	**226.6**	**184.0**
1	(S)-mandelic acid	R-Proline amide	1:1	132.6	92.7	191.8
	(R)-mandelic acid	R-Proline amide	1:1	132.6	92.7	153.3
2	(RS)-Flurbiprofen	D-Proline	1:1	114.0	226.6	142.6
	(RS)-Flurbiprofen	D-Proline	1:1	114.0	226.6	185.4
	(RS)-Flurbiprofen	L-Proline	1:1	114.0	226.6	149.7
	(RS)-Flurbiprofen	L-Proline	1:1	114.0	226.6	188.3
	(RS)-Flurbiprofen	L-Proline	1:1	114.0	226.6	151.6
3	(RS)-Flurbiprofen	L-Proline	2:1	114.0	226.6	160.4
	(RS)-Flurbiprofen	D-Proline	2:1	114.0	226.6	154.0
4	(S)-Naproxen	L-Proline	1:1	155.0	226.6	184.0
	(S)-Naproxen	D-Proline	1:1	155.0	226.6	155.0

[a](P) is polymorphic forms;

Table S5 The number of API-based co-crystals having a melting point below (l), between (b) and above (h) the melting points of the individual compounds included in its

№	API	$T_{fus}(CF) < T_{fus}(API)$							$T_{fus}(API) < T_{fus}(CF)$							Total						
		N	l	b	h	l [%]	b [%]	h[%]	N	l	b	h	l [%]	b[%]	h[%]	N	l	b	h	l[%]	b[%]	h[%]
1	Nicotinamide	13	5	8	0	38.5	61.5	0.0	77	20	54	3	26.0	70.1	3.9	90	25	62	3	27.8	68.9	3.3
2	4,4'-bipyridine	11	0	2	9	0.0	18.2	81.8	64	3	43	18	4.7	67.2	28.1	75	3	45	27	4.0	60.0	36.0
3	Succinic acid	45	17	23	5	37.8	51.1	11.1	26	11	15	0	42.3	57.7	0.0	71	28	38	5	39.4	53.5	7.0
4	Isonicotinamide	31	5	16	10	16.1	51.6	32.3	40	15	20	5	37.5	50.0	12.5	71	20	36	15	28.2	50.7	21.1
5	Carbamazepine	41	18	23	0	43.9	56.1	0.0	19	15	4	0	78.9	21.1	0.0	60	33	27	0	55.0	45.0	0.0
6	2-OH-BA	26	14	8	4	53.8	30.8	15.4	32	12	18	2	37.5	56.3	6.3	58	26	26	6	44.8	44.8	10.3
7	D- or L-Proline	36	5	31	0	13.9	86.1	0.0	18	11	7	0	61.1	38.9	0.0	54	16	38	0	29.6	70.4	0.0
8	Fumaric Acid	54	25	29	0	46.3	53.7	0.0	0	0	0	0	0.0	0.0	0.0	54	25	29	0	46.3	53.7	0.0
9	Saccharin	37	16	17	4	43.2	45.9	10.8	12	10	0	2	83.3	0.0	16.7	49	26	17	6	53.1	34.7	12.2
10	Isoniazid	19	12	5	2	63.2	26.3	10.5	30	19	9	2	63.3	30.0	6.7	49	31	14	4	63.3	28.6	8.2
11	4-OH-BA	37	17	18	2	45.9	48.6	5.4	9	4	4	1	44.4	44.4	11.1	46	21	22	3	45.7	47.8	6.5
12	Pyrazinamide	16	16	0	0	100.0	0.0	0.0	27	22	4	1	81.5	14.8	3.7	43	38	4	1	88.4	9.3	2.3
13	Theophylline	43	17	25	1	39.5	58.1	2.3	0	0	0	0	0.0	0.0	0.0	43	17	25	1	39.5	58.1	2.3
14	4-Aminobenzoic acid	18	11	7	0	61.1	38.9	0.0	24	14	9	1	58.3	37.5	4.2	42	25	16	1	59.5	38.1	2.4
15	Glutaric acid	***3***	***1***	***0***	***2***	***33.3***	***0.0***	***66.7***	37	7	26	4	18.9	70.3	10.8	40	8	26	6	20.0	65.0	15.0
16	1,4-I, 4F-Benz	25	5	13	7	20.0	52.0	28.0	14	3	4	7	21.4	28.6	50.0	39	8	17	14	20.5	43.6	35.9
17	Oxalic Acid	25	5	13	7	20.0	52.0	28.0	14	6	4	4	42.9	28.6	28.6	39	11	17	11	28.2	43.6	28.2
18	Caffeine	27	20	7.0	0.0	74.1	25.9	0.0	11	6	5	0	54.5	45.5	0.0	38	26	12	0	68.4	31.6	0.0
19	Adipic acid	11	5	4	2	45.5	36.4	18.2	26	8	13	5	30.8	50.0	19.2	37	13	17	7	35.1	45.9	18.9
20	Benzoic Acid	***5***	***2***	***1***	***2***	***40.0***	***20.0***	***40.0***	27	11	12	4	40.7	44.4	14.8	32	13	13	6	40.6	40.6	18.8

21	bipyeta	8	0	2	6	0.0	25.0	75.0	24	0	19	5	0.0	79.2	20.8	32	0	21	11	0.0	65.6	34.4
22	Quercetin	29	12	17	0	41.4	58.6	0.0	***2***	***2***	***0***	***0***	***100.0***	***0.0***	***0.0***	31	14	17	0	45.2	54.8	0.0
23	Bipyete	11	1	5	5	9.1	45.5	45.5	18	3	11	4	16.7	61.1	22.2	29	4	16	9	13.8	55.2	31.0
24	Sulfadimidine	17	0	13	4	0.0	76.5	23.5	12	4	6	2	33.3	50.0	16.7	29	4	19	6	13.8	65.5	20.7
25	D- or L-Tartaric Acid	***6***	***3***	***0***	***3***	***50.0***	***0.0***	***50.0***	22	14	7	1	63.6	31.8	4.5	28	17	7	4	60.7	25.0	14.3
26	4-Aminosalicylic acid	14	1	8	5	7.1	57.1	35.7	12	0	6	6	0.0	50.0	50.0	27	5	16	6	18.5	59.3	22.2
27	3-OH-BA	22	12	10	0	54.5	45.5	0.0	***5***	***4***	***1***	***0***	***80.0***	***20.0***	***0.0***	27	16	11	0	59.3	40.7	0.0
28	Urea	***3***	***0***	***1***	***2***	***0.0***	***33.3***	***66.7***	23	0	20	3	0.0	87.0	13.0	26	0	21	5	0.0	80.8	19.2

[a] l – low; b – between; h – higher;

3-OH-BA – 3-hydroxybenzoic acid;

2-OH-BA – 2-hydroxybenzoic acid;

1,4-I,4F-Benz – 1,4-diiodotetrafluorobenzene;

Bipyeta – 1,2-bis-(4-pyridyl)ethane;

Bipyete -1,2-bis(4-pyridyl)ethylene;

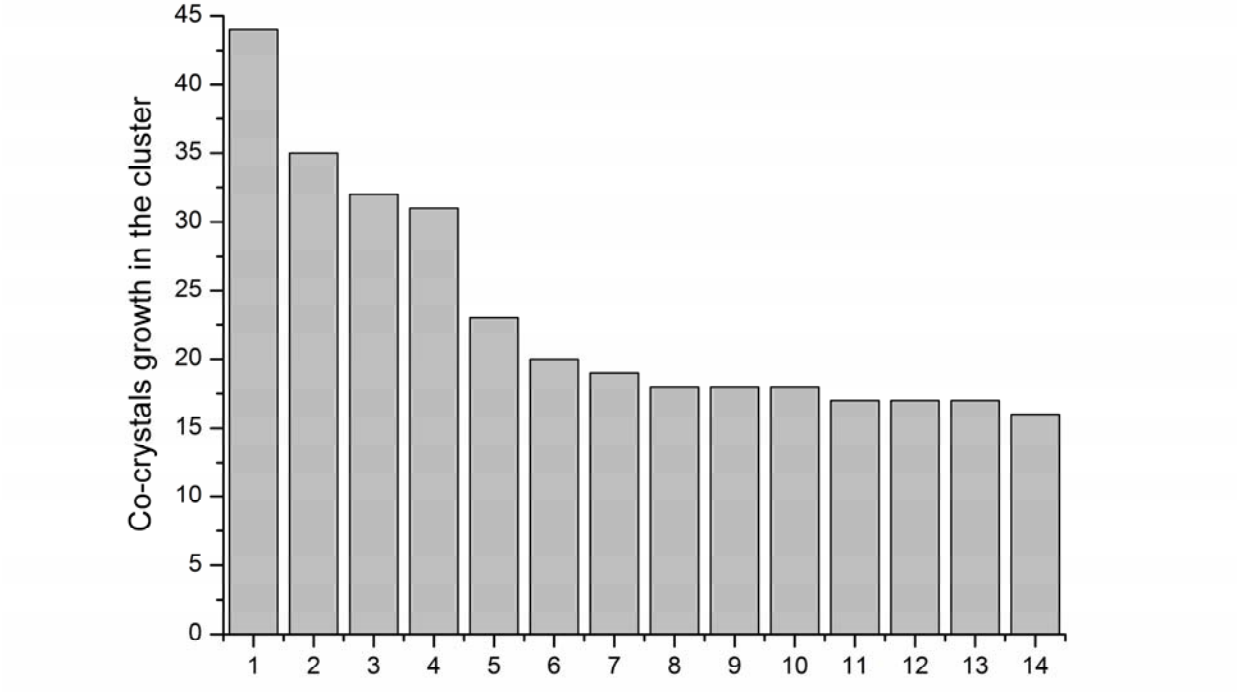

Figure S1 Co-crystals growth in the clusters. The numbering OY-axis corresponds to co-crystals based on: 1 - D- or L-Proline, 2 - Isonicotinamide, 3 - Fumaric acid, 4 - Nicotinamide, 5 - 44BP, 6 - Salicylic acid, 7 - Isoniazid, 8 – Theophylline, 9 – Flurbiprofen, 10 - D- or L-Tartaric acid, 11 – CBZ, 12 – Pyrazinamide, 13 - 4-Aminobenzoic acid, 14 - CL20.