SUPPORTING INFORMATION

Thermodynamic characteristics of cocrystal formation and melting points for rational design of pharmaceutical two-component systems

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CONTENT:

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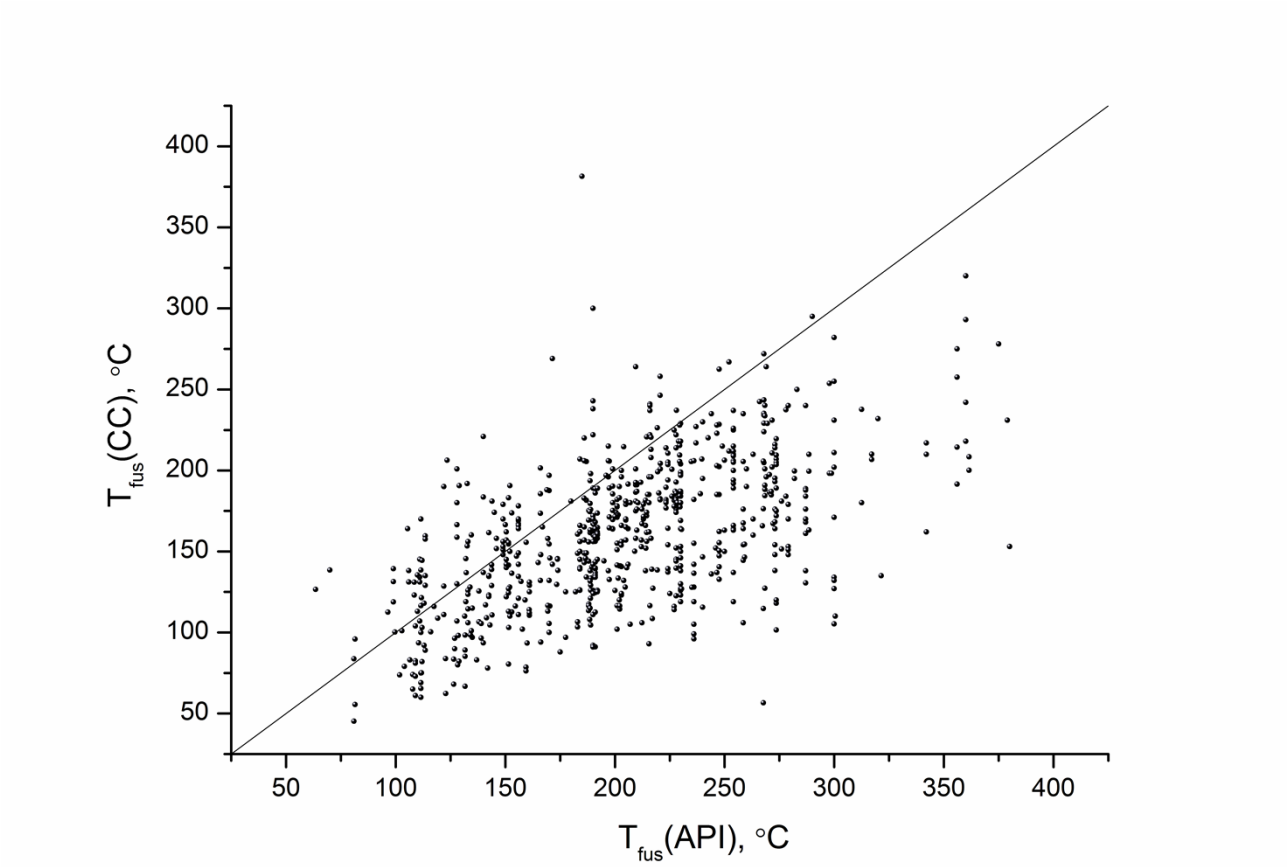


Figure 1SI. The experimental data of the analyzed database in co-ordinates $T_{fus}(CC)$ versus $T_{fus}(API)$. Black line corresponds to bisector.

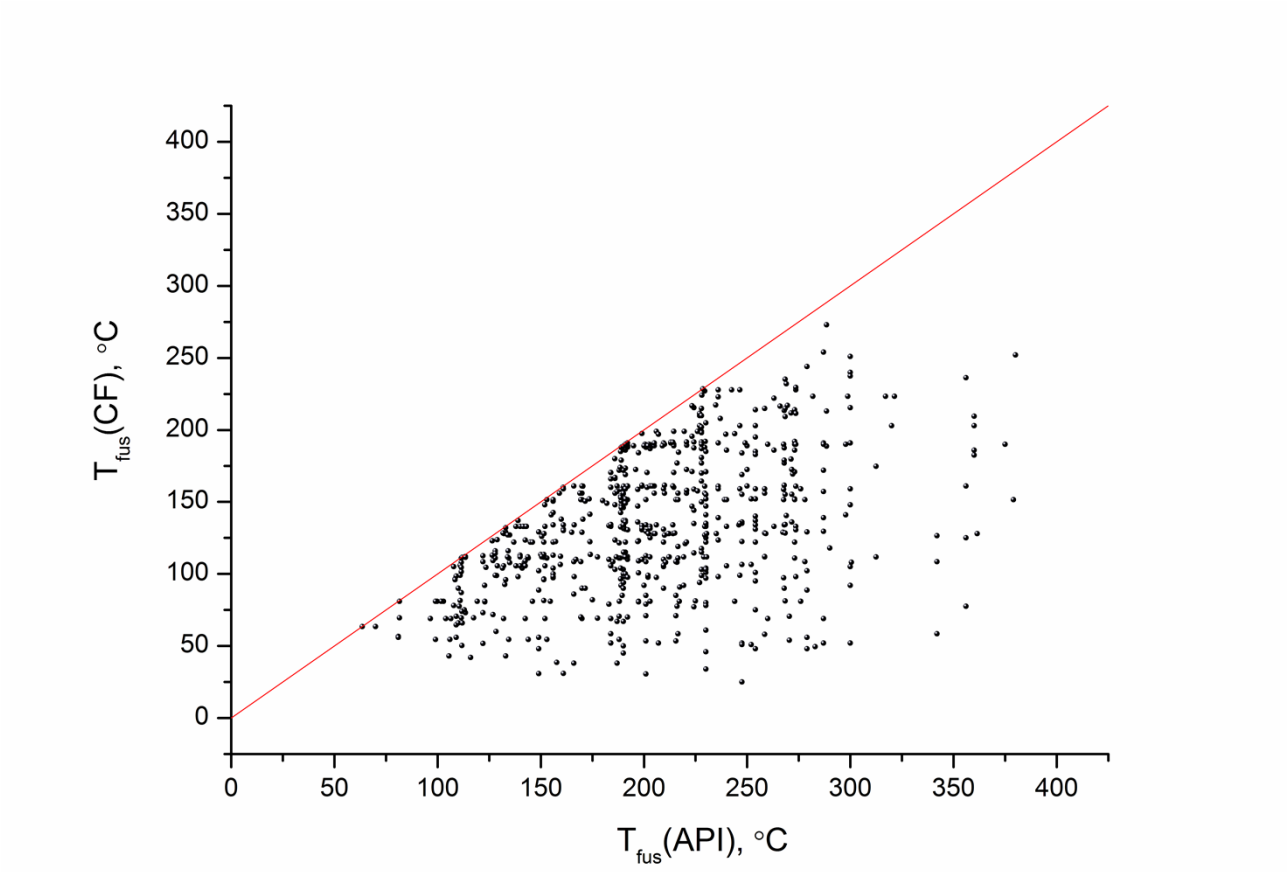


Figure 2SI. The experimental data of the analyzed database in co-ordinates $T_{fus}(CF)$ versus $T_{fus}(API)$. Red line corresponds to bisector.

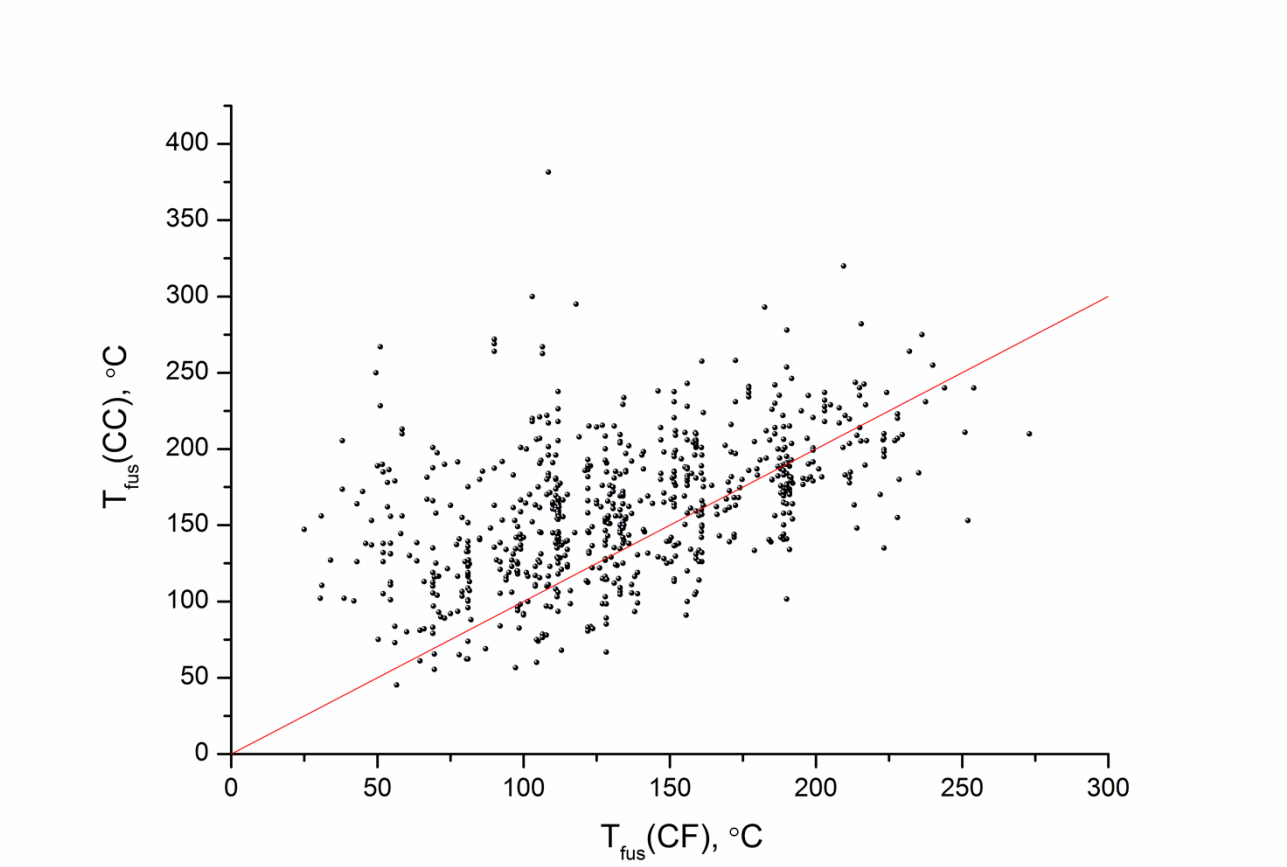


Figure 3SI. The experimental data of the analyzed database in co-ordinates $T_{fus}(CC)$ versus $T_{fus}(CF)$. Red line corresponds to bisector.

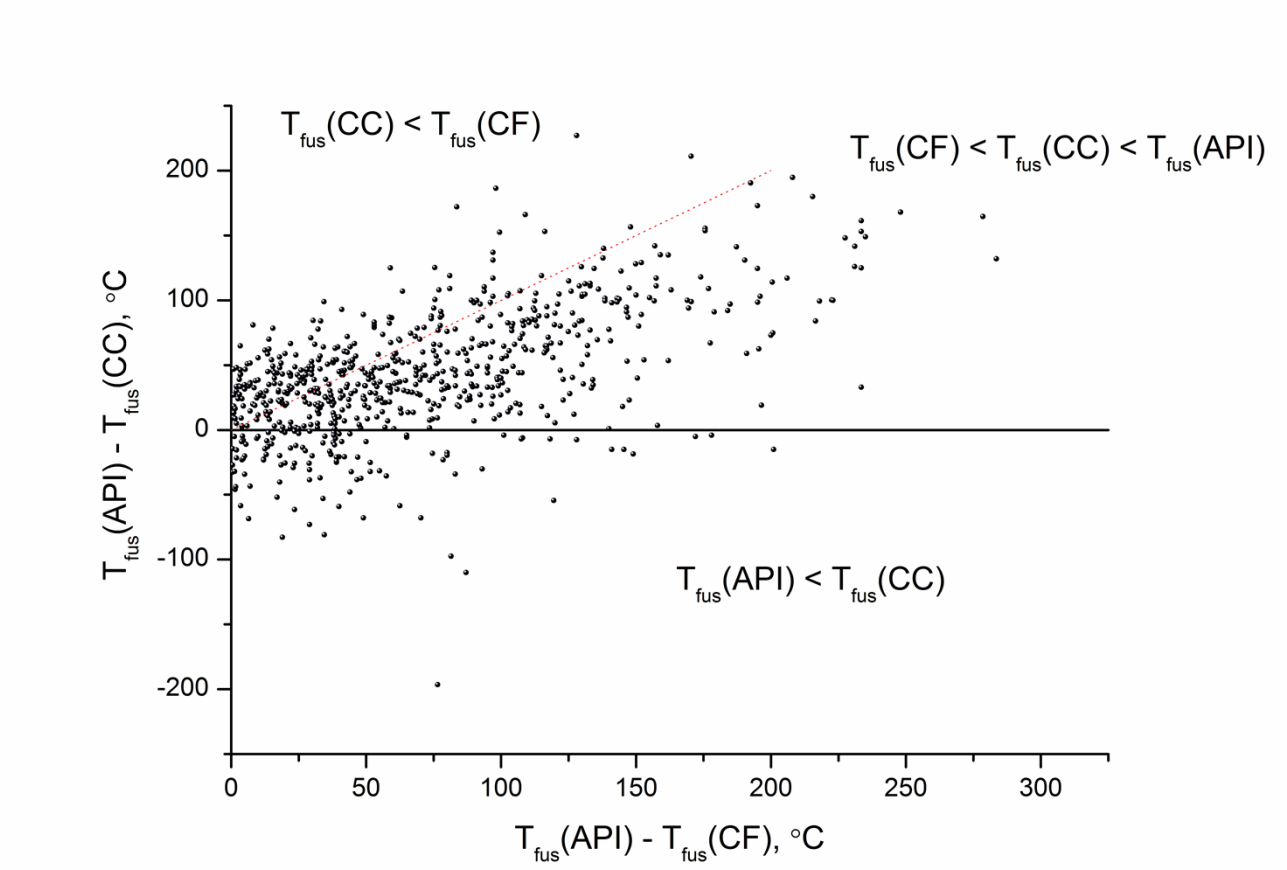


Figure 4SI. The experimental data of the analyzed database in co-ordinates ($T_{fus}(API)$ - $T_{fus}(CC)$) versus ($T_{fus}(API)$ - $T_{fus}(CF)$). Red line corresponds to bisector.

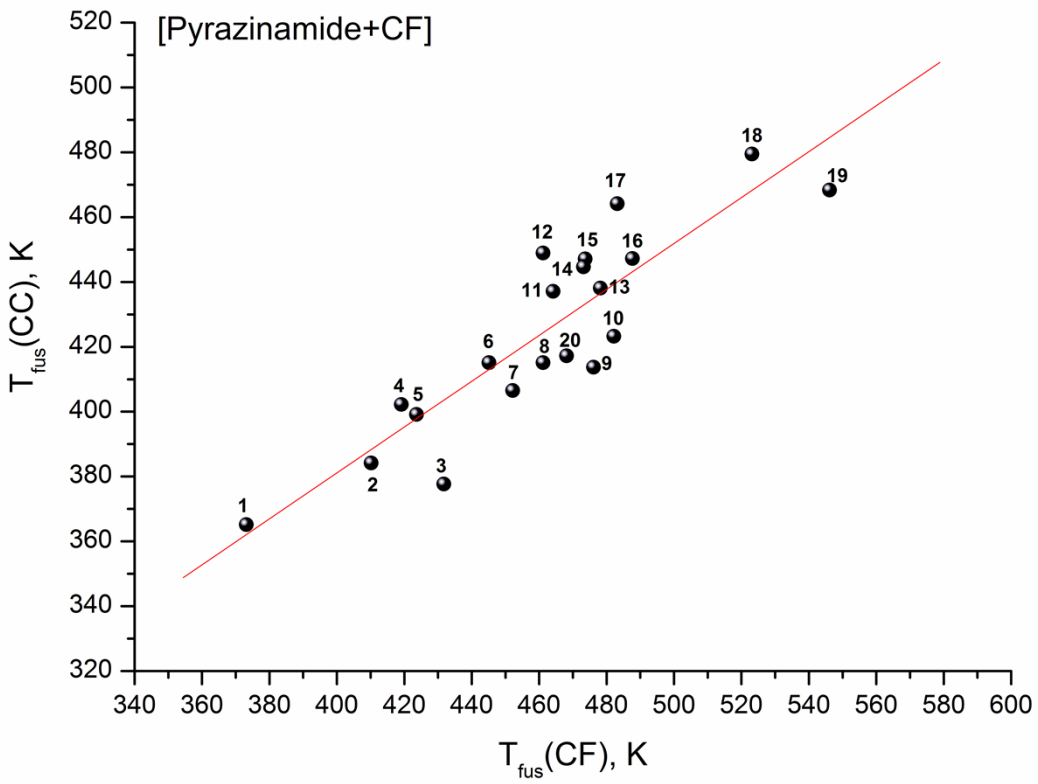


Figure 5SI. Correlation dependence (equation (1)) for potential coformers (CF) used at [Pyrazinamide+CF] cocrystals design: 1 – glutaric acid (1:1); 2 – malonic acid (1:1); 3 – salicylic acid (1:1); 4 – 2-NH_2-benzoic acid (1:1); 5 – 4-NH_2- salicylic acid (1:1); 6 – Isoniazid (1:1); 7 – 3-NH_2-benzoic acid (1:1); 8 – succinic acid (1:1); 9 – 3-OH-benzoic acid (1:1); 10 – vanilic acid; 11 – succinic acid (2:1); 12 – 4-NH_2-benzoic acid (1:1); 13 – 2,5-OH-benzoic acid (1:1); 14 – 4-NO_2-benzamide (1:1); 15 – 3,4-OH-benzoic acid (1:1); 16 – 4-OH-benzoic acid (1:1); 17 – temozolomide (1:1); 18 – gallic acid (1:1); 19 – Hydrochlorothiazide (1:1); 20 – 1-OH-2-COOH-Naph (1:1).

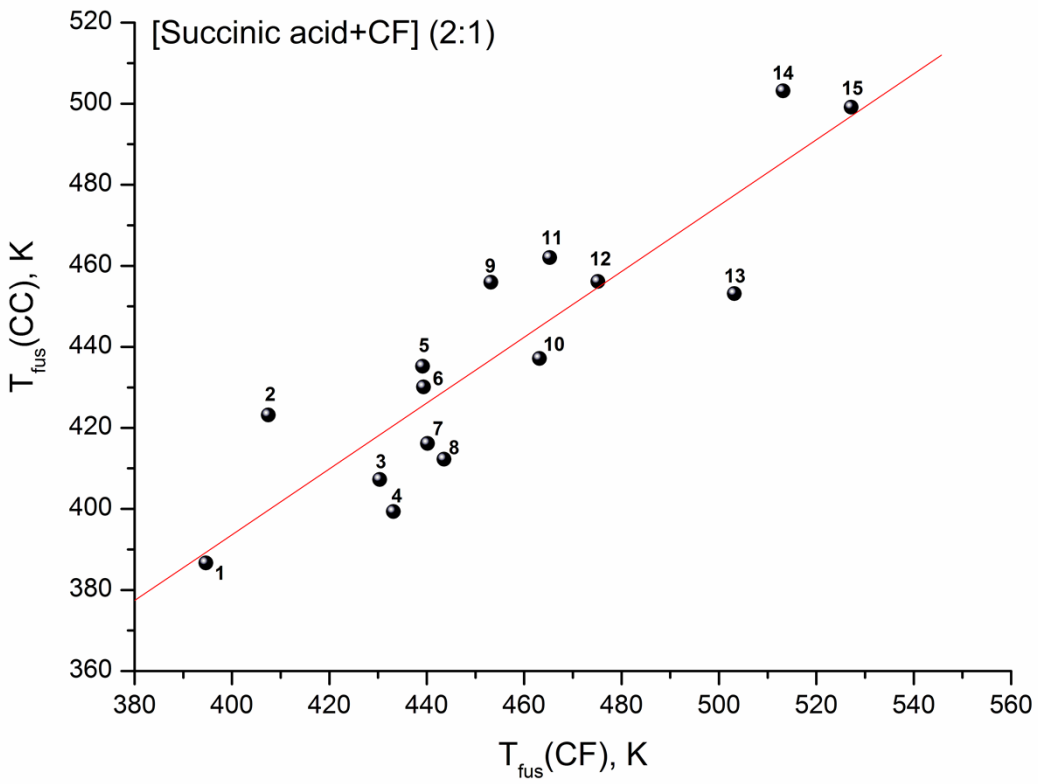


Figure 6SI. Correlation dependence (equation (1)) for potential coformers (CF) used at [Succinic acid +CF] (2:1) cocrystals design: 1 – diphenylcyclopropenone; 2 – urea; 3 – fluoxetine hydrochloride; 4 – N'-(Propan-2-ylidene)isonicotinohydrazide; 5 – itraconazole (form I); 6 – itraconazole (form II); 7 – Pfizer 1; 8 – isonicotinic acid hydrazide; 9 – salbutamol; 10 – pyrazinamide; 11 – carbamazepine; 12 – nitazoxanide; 13 – AMG517; 14 – meloxicam (form I); 15 – meloxicam (form II).

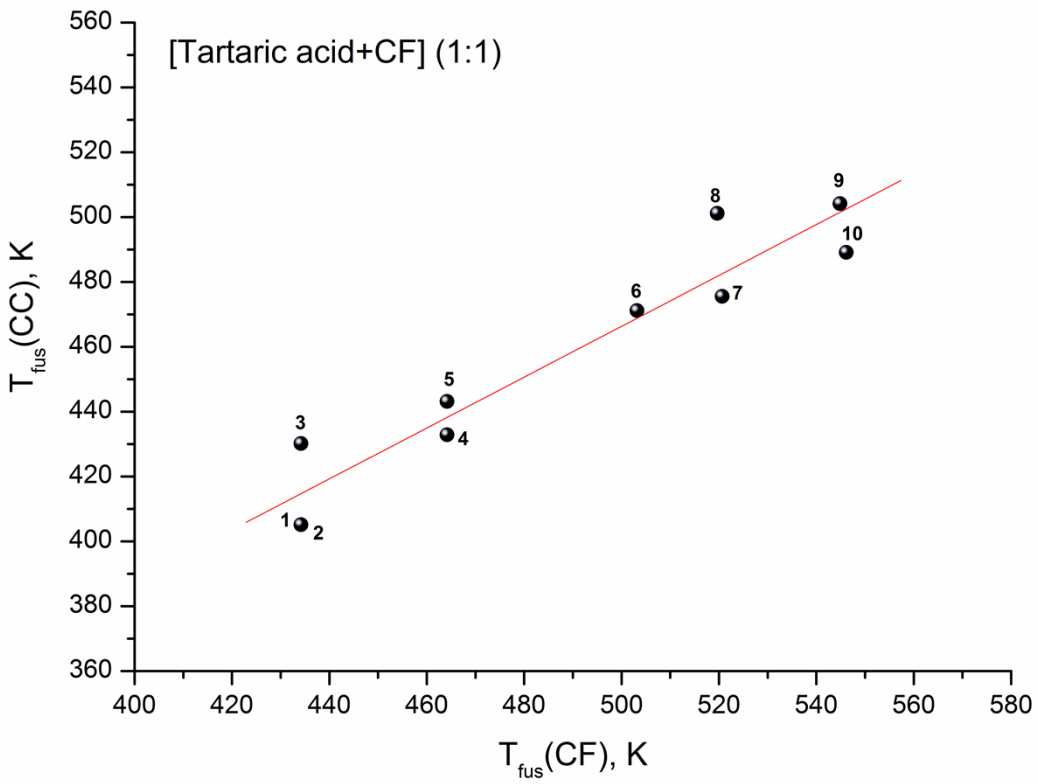
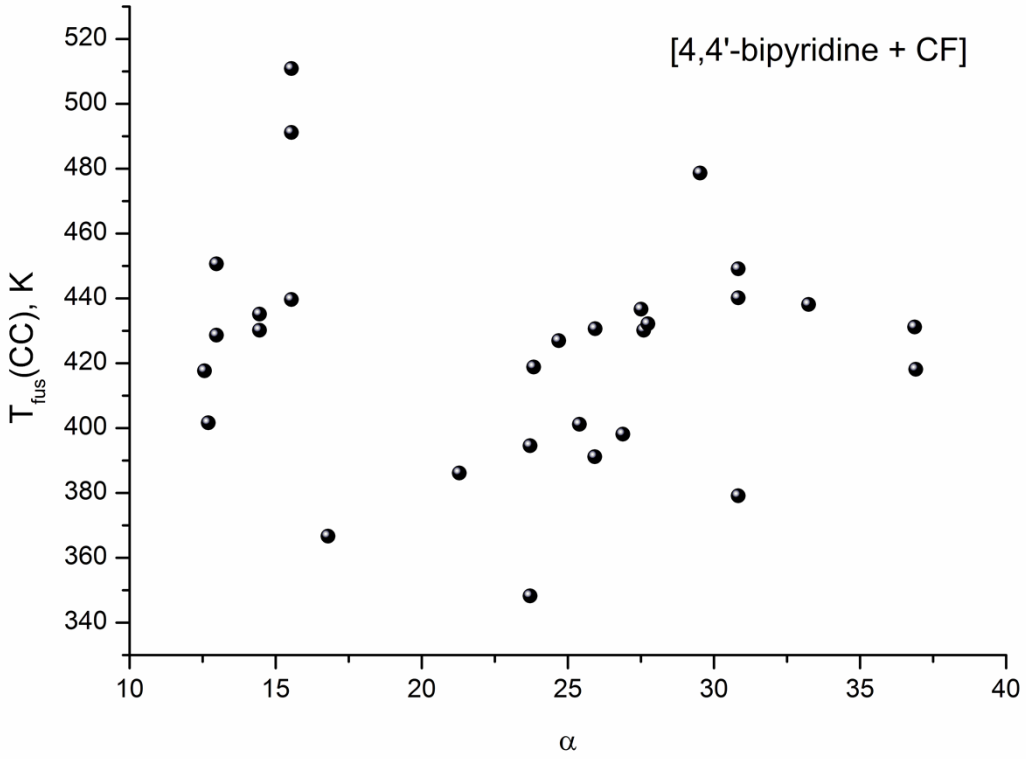
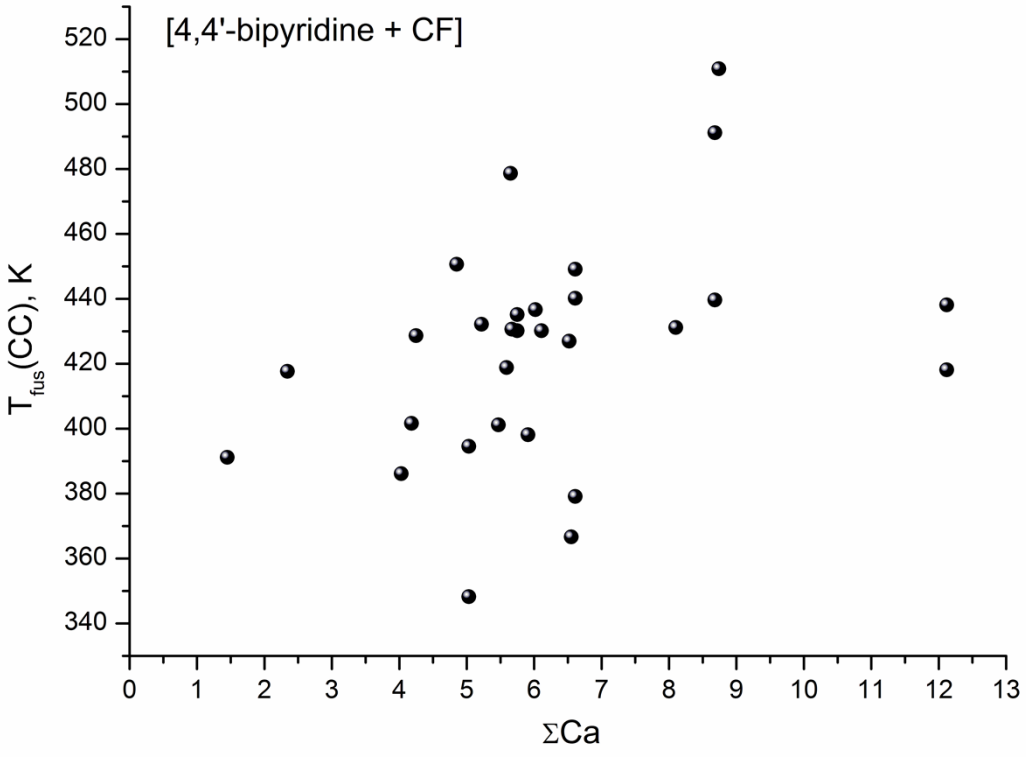


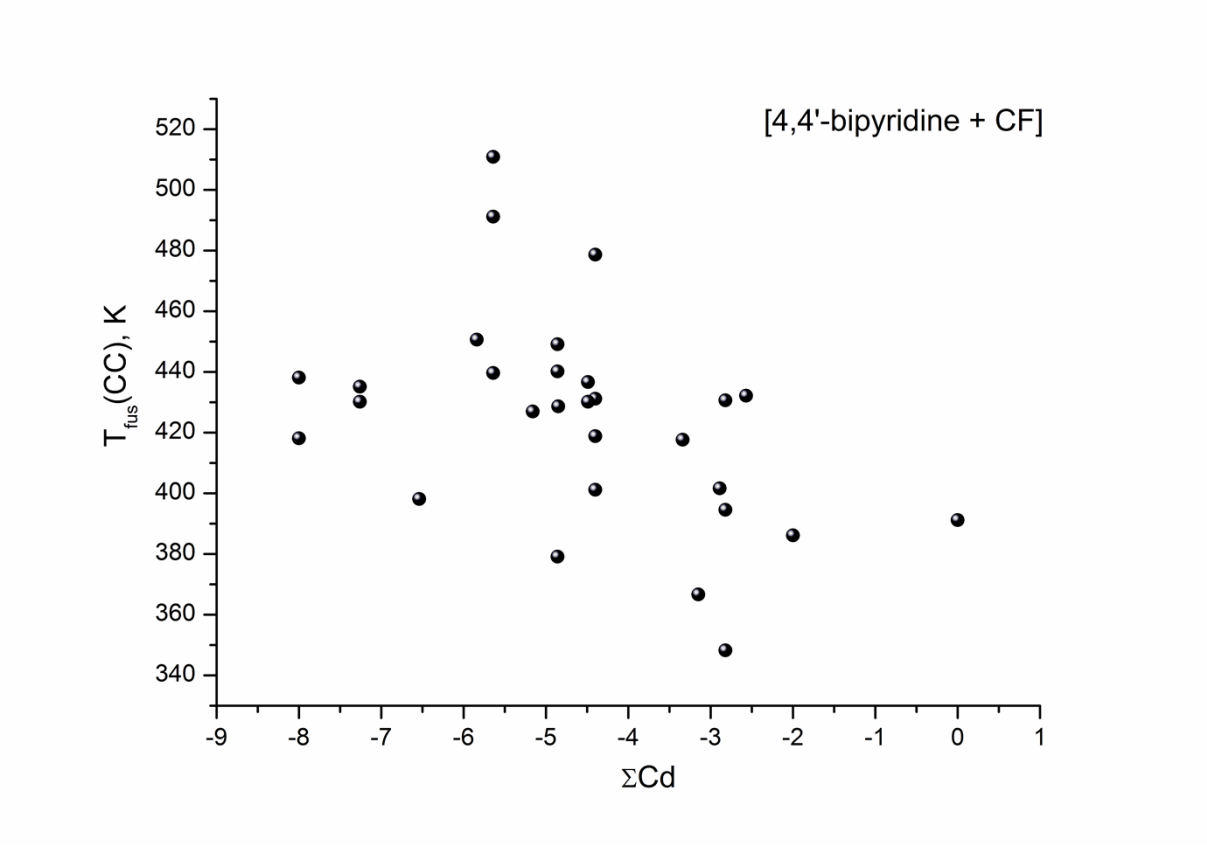
Figure 7SI. Correlation dependence (equation (1)) for potential coformers (CF) used at [Tartaric acid +CF] (1:1) cocrystals design: 1 – [Tartaric acid (D)+gabapentin]; 2 – [Tartaric acid (L)+gabapentin]; 3 – [Tartaric acid (DL)+gabapentin]; 4 – [Tartaric acid (L)+carbamazepine]; 5 – [Tartaric acid (DL)+carbamazepine]; 6 – [Tartaric acid (L)+AMG517]; 7 – [Tartaric acid (L)+STL(+)]; 8 – [Tartaric acid (DL)+nevirapine]; 9 – [Tartaric acid (DL)+ciprofloxacin]; 10 – [Tartaric acid (L)+minoxidil].


[4,4'-bipyridine + CF]
T_{fus}(CC), K
520
500
480
460
440
420
400
380
360
340
10
15
20
25
30
35
40
α

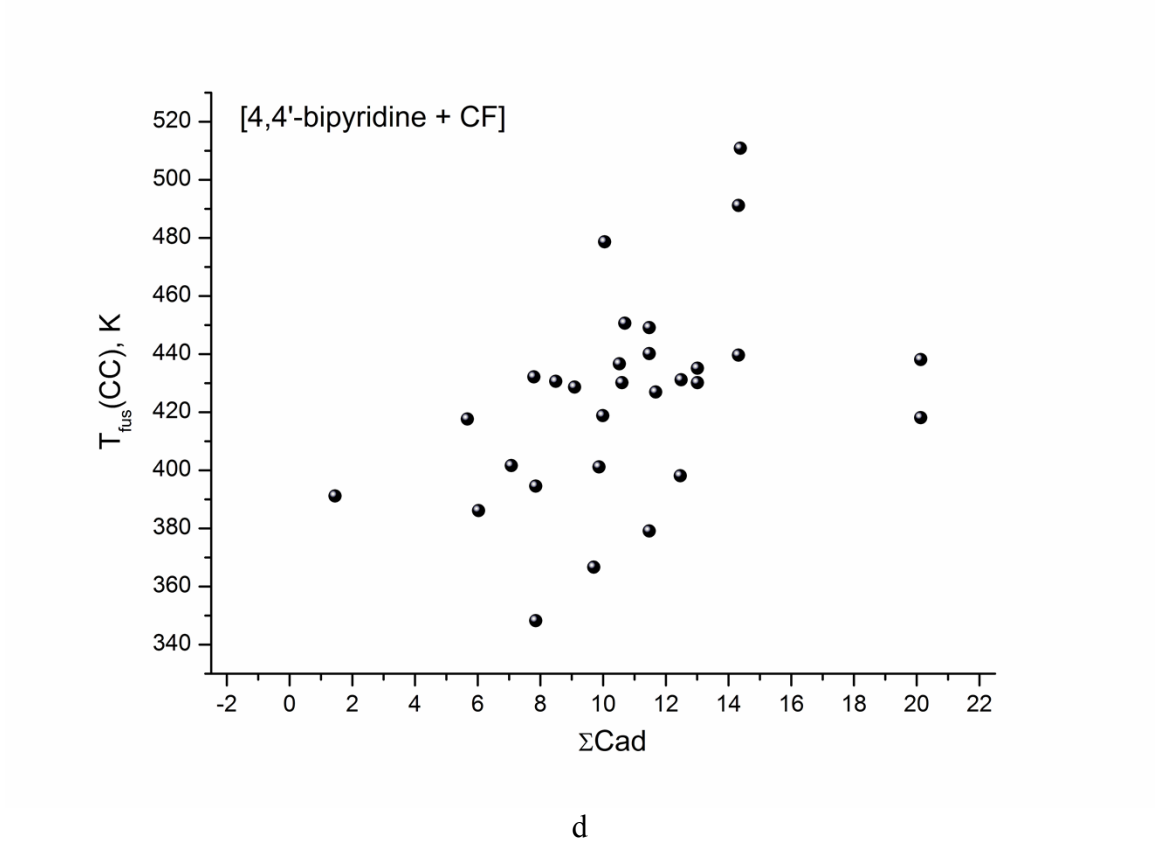
a


[4,4'-bipyridine + CF]
T_{fus}(CC), K
520
500
480
460
440
420
400
380
360
340
0
1
2
3
4
5
6
7
8
9
10
11
12
13
ΣCa

b



c



d

Figure 8SI. Experimental data of the melting points of 4,4'-bipyridine cocrystals versus HYBOT's physicochemical descriptors of the second components (coformers) (α - molecular polarizability; ΣC_a - the sum of H-bond acceptor factors; ΣC_d - the sum of H-bond donor factors; ΣC_{ad} - the sum of H-bond donor and acceptor factors).

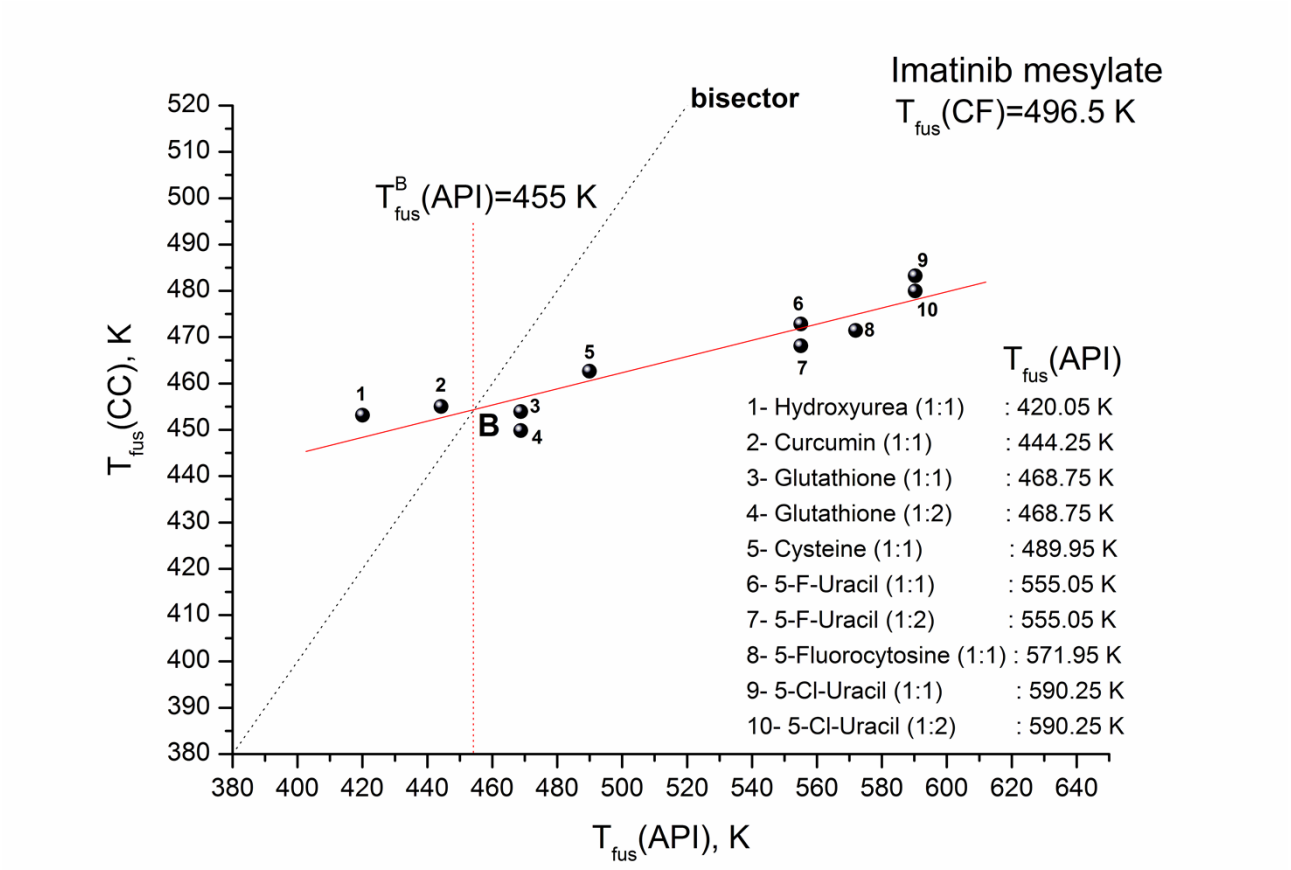


Figure 9SI. Correlation dependence (equation (1)) for potential API used at [API + Imatinib mesylate] cocrystals design.