Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

for

Prediction of Molecular Packing Characteristics of Two-Component Crystals

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Table S1. Estimated values of the free volumes, V_{free}^{HXR}, and the unit cell volumes, V_{cell}^{HXR}, for the some cocrystals of 4-hydroxy-benzoic acid described in literature without solving crystal structure[a]

N	CF1	CF2	Stoich	$V^{vdw}(CF1)$ [Å^3]	$V^{vdw}(CF2)$ [Å^3]	C^{HXR}	D^{HXR}	$\beta^{HXR}(CF2)$ [%]	$\beta^{HXR}(CC)$ [%]	V_{free}^{HXR} [Å^3]	V_{cell}^{HXR} [Å^3]	$T_{fus}(CC)$ [°C]
1	4-OH-BA	Meloxicam	1:1[c]	118.81	274.59	-12.27	0.682	35.5	11.9	46.84	440.24	207.5
2	4-OH-BA	Tenoxicam	1:1[d]	118.81	256.31	-12.27	0.682	36.5	12.6	47.35	422.47	205.2
3	4-OH-BA	Nitrofurantoin	1:1[e]	118.81	177.58	-12.27	0.682	35.6	12.0	35.59	331.98	243.6
4	4-OH-BA	4-N(Me)$_2$-Py[b]	1:1[f]	118.81	124.20	-12.27	0.682	38.3	13.9	33.66	276.67	190.0
5	4-OH-BA	Progesterone	1:1[g]	118.81	318.94	-12.27	0.682	44.8	18.3	80.04	517.79	141.3
6	4-OH-BA	Lesinurad	1:1[h]	118.81	292.03	-12.27	0.682	45.0	18.4	75.70	486.55	159.9

[a] $V^{vdw}(CF1)$, $V^{vdw}(CF2)$ are van der Waals volumes of coformers 1 and 2, correspondingly; C^{HXR} and D^{HXR} are correlation coefficients of equation (4) for the high temperature X-Ray experiments;

[b] 4-N(Me)$_2$-Py is dimethylamino pyridine;

[c] Cheney et al. CGD, 2010, 4401. 10.1021/cg100514g

[d] Patel et al. IJP, 2012, 685. 10.1016/j.ijpharm.2012.07.034;

[e] Vangala et al. CrystEngComm, 2011, 759. 10.1039/c0ce00772b;

[f] Lou et al. J Mol Struc., 2015, 516. 10.1016/j.molstruc.2015.07.008;

[g] Samipillai et al, J. Crystal Growth, 2019, 270. 10.1016/j.jcrysgro.2018.10.050;

[h] S.V. Narasayya et al. / Materials Today: Proceedings 14 (2019) 532–544.

Table S2. Estimated values of the free volumes, V_{free}^{LXR}, and the unit cell volumes, V_{cell}^{LXR}, for the some cocrystals of Carbamazepine described in literature without solving crystal structure[a]

N	CF1	CF2	Stoich	$V^{vdw}(CF1)$ [Å^3]	$V^{vdw}(CF2)$ [Å^3]	C^{LXR}	D^{LXR}	$\beta^{LXR}(CF2)$ [%]	$\beta^{LXR}(CC)$ [%]	V_{free}^{LXR} [Å^3]	V_{cell}^{LXR} [Å^3]	$T_{fus}(CC)$ [°C]
1	CBZ	Oxalic Acid	1:1[b]	206.43	66.71	25.05	0.438	15.05	31.64	86.43	359.57	157.7
2	CBZ	Glycolic Acid	1:1[b]	206.43	64.18	25.05	0.438	30.70	38.50	104.18	374.79	139.3
3	CBZ	L-Tartaric Acid	1:1[b]	206.43	117.26	25.05	0.438	18.40	33.11	107.17	430.86	91.1
4	CBZ	Trimesic acid	1:1[c]	206.43	165.00	25.05	0.438	15.32	31.76	117.97	489.40	278.0
5	CBZ	Urea	1:1[d]	206.43	53.45	25.05	0.438	36.39	40.99	106.52	366.40	169.0

[a] $V^{vdw}(CF1)$, $V^{vdw}(CF2)$ are van der Waals volumes of coformers 1 and 2, correspondingly; C^{LXR} and D^{LXR} are correlation coefficients of equation (4) for the low temperature X-Ray experiments;

[b] Childs et al. CrystEngComm, 2008, 856. 10.1039/b715396a;

[c] Fleischman et al. CGD, 2003, 919. 10.1021/cg034035x;

[d] Lu et al. CrystEngComm, 2008, 665. 10.1039/b801713c;

Table S3. Estimated values of the free volumes, V_{free}^{HXR}, and the unit cell volumes, V_{cell}^{HXR}, for the some cocrystals of Carbamazepine described in literature without solving crystal structure[a]

N	CF1	CF2	Stoich	$V^{vdw}(CF1)$ [Å^3]	$V^{vdw}(CF2)$ [Å^3]	C^{HXR}	D^{HXR}	$\beta^{HXR}(CF2)$ [%]	$\beta^{HXR}(CC)$ [%]	V_{free}^{HXR} [Å^3]	V_{cell}^{HXR} [Å^3]	$T_{fus}(CC)$ [°C]
1	CBZ	Oxalic Acid	1:1[b]	206.43	66.71	27.24	0.406	16.32	33.87	92.50	365.64	157.7
2	CBZ	Glycolic Acid	1:1[b]	206.43	64.18	27.24	0.406	30.70	39.70	107.44	378.05	139.3
3	CBZ	L-Tartaric Acid	1:1[b]	206.43	117.26	27.24	0.406	20.90	35.73	115.64	439.33	91.1
4	CBZ	Trimesic acid	1:1[c]	206.43	165.00	27.24	0.406	20.80	35.68	132.54	503.97	278.0
5	CBZ	Urea	1:1[d]	206.43	53.45	27.24	0.406	38.25	42.77	111.15	371.03	169.0

[a] $V^{vdw}(CF1)$, $V^{vdw}(CF2)$ are van der Waals volumes of coformers 1 and 2, correspondingly; C^{HXR} and D^{HXR} are correlation coefficients of equation (4) for the high temperature X-Ray experiments;

[b] Childs et al. CrystEngComm, 2008, 856. 10.1039/b715396a;

[c] Fleischman et al. CGD, 2003, 919. 10.1021/cg034035x;

[d] Lu et al. CrystEngComm, 2008, 665. 10.1039/b801713c;

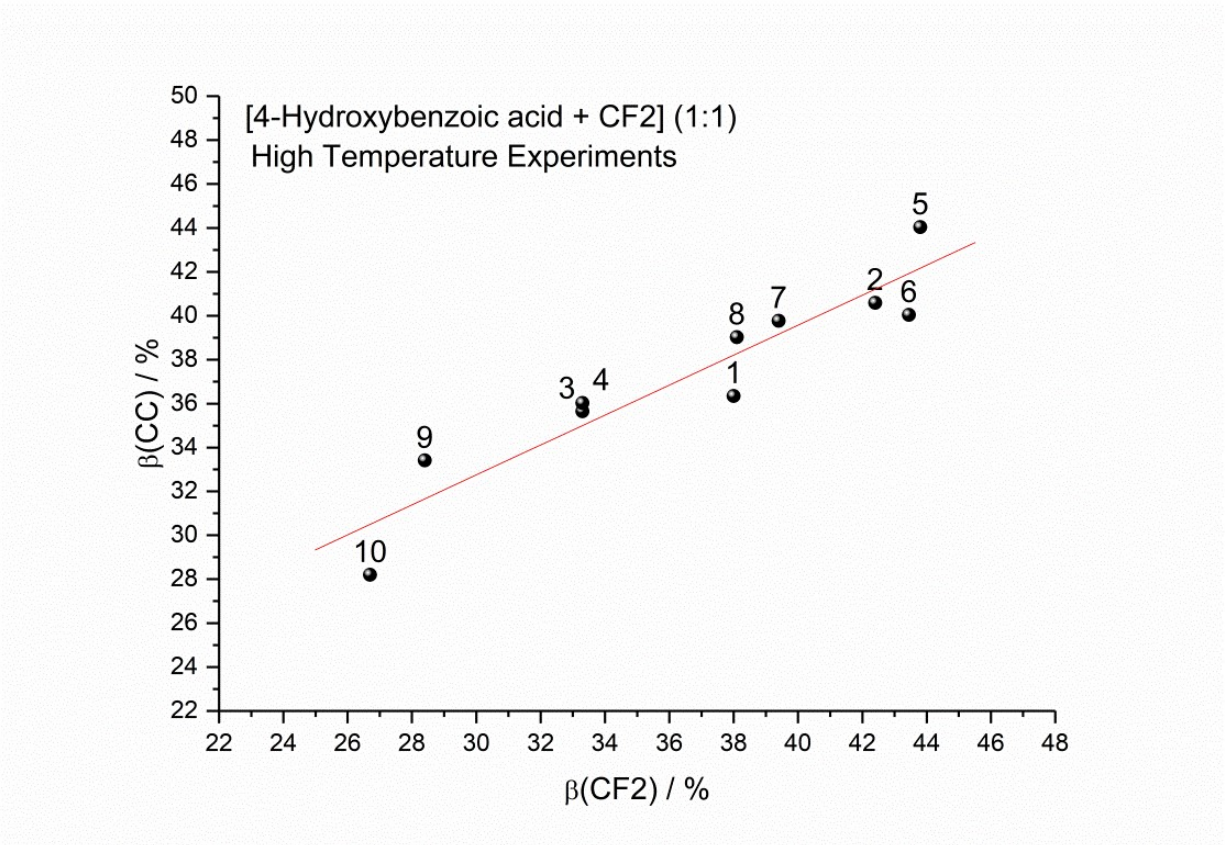

Figure S1. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [4-hydroxybenzoic acid+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- nicotinamide, 2- voriconazole, 3- pyrazinamide (cocrystal form I), 4- pyrazinamide (cocrystal form II), 5- nefiracetam, 6- abiraterone acetate, 7- fluconazole, 8- paliperidone, 9- acefylline, 10- malonic acid

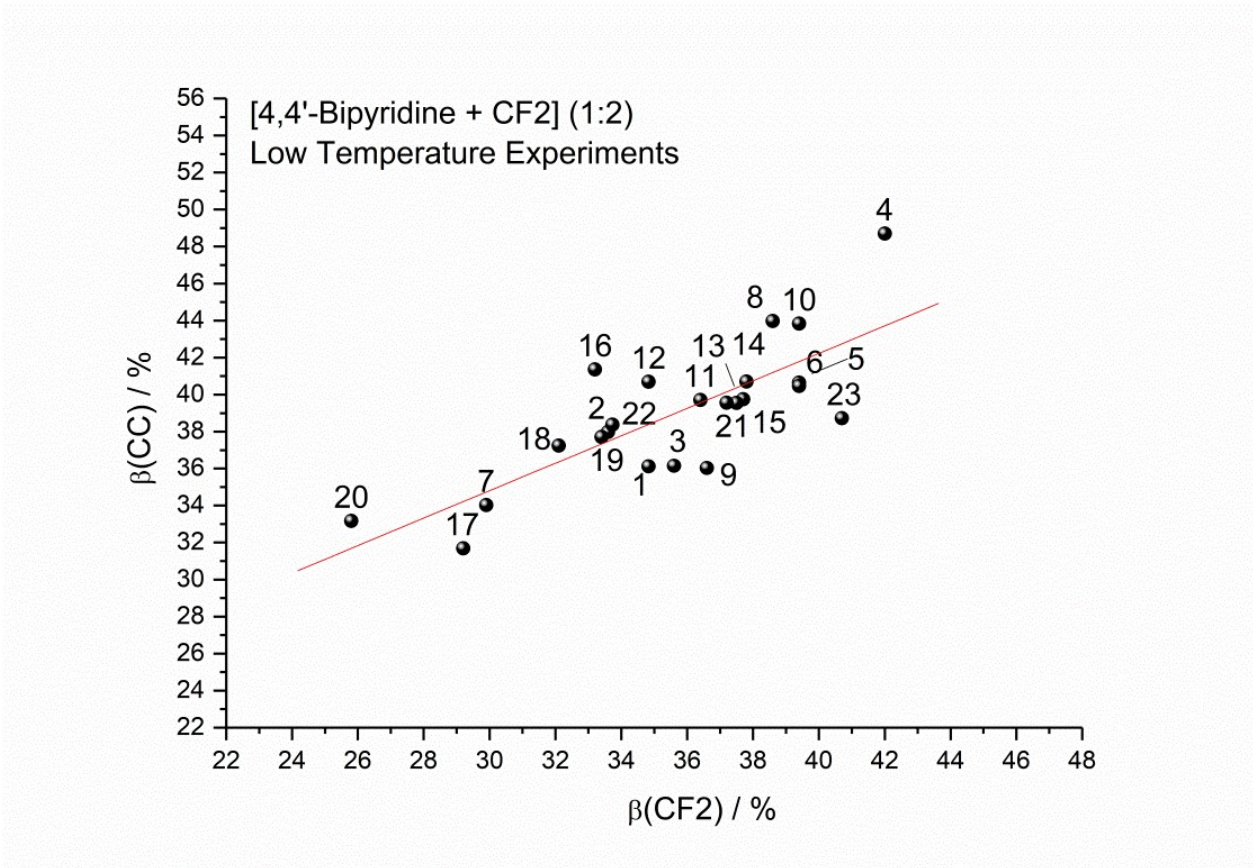

Figure S2. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [4,4′-bipyridine+CF2] (1:2) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- flufenamic acid (cocrystal form I), 2- tolfenamic acid, 3- mefenamic acid, 4- carbamazepine, 5- (RS)-ibuprofen (cocrystal form I), 6- (S)-ibuprofen, 7- salicylic acid, 8- thiophanate-methyl, 9- flurbiprofen, 10- (RS)-ibuprofen (cocrystal form II), 11- felodipine, 12- flufenamic acid (cocrystal form II), 13- (S)-naproxen, 14- (RS)-naproxen, 15- N-oxaprozin, 16- acetylsalicylic acid, 17- emodin, 18- furosemide, 19- nimesulide, 20- 4-hydroxybenzoic acid, 21- 3,5-dibromophenol, 22- p-toluic acid, 23- (RS)-2-phenylbutyric acid

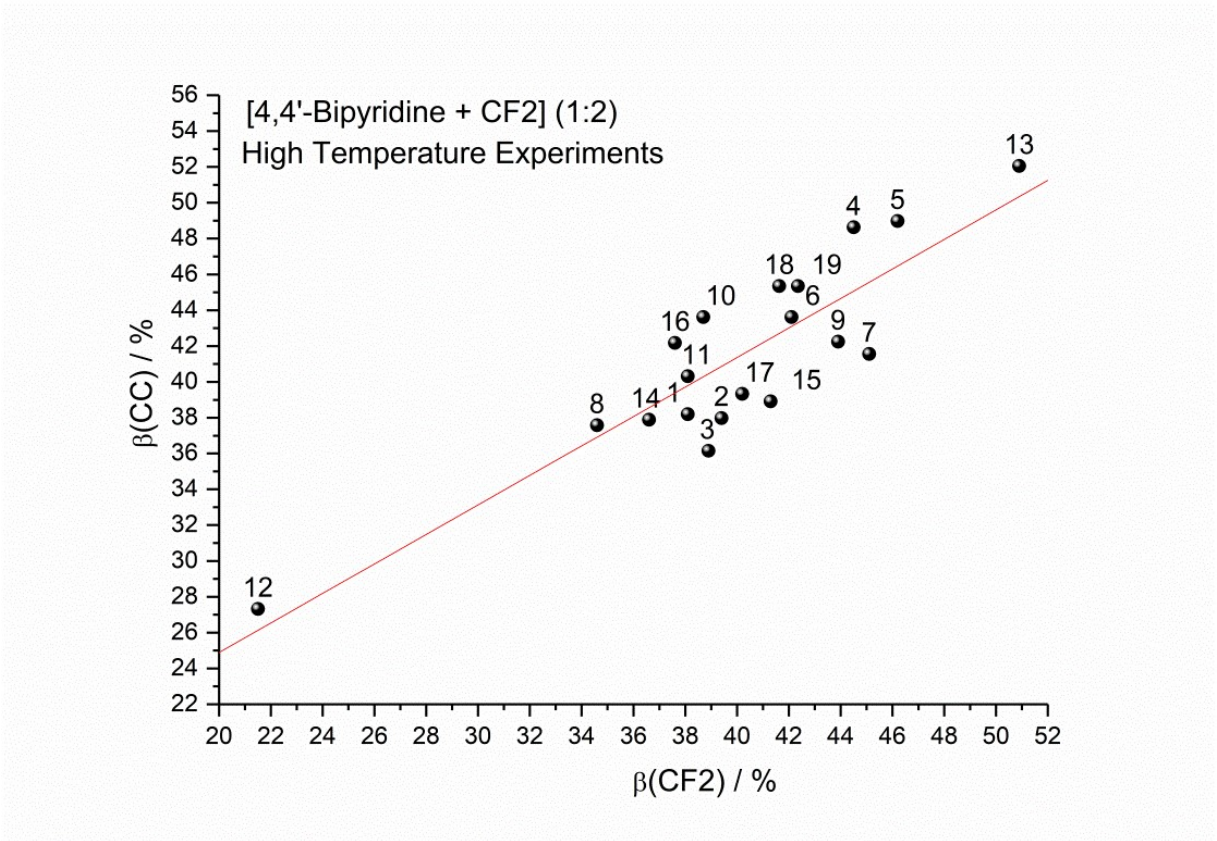

Figure S3. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [4,4′-bipyridine+CF2] (1:2) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- N-phenylanthranilic acid (cocrystal form I), 2- tolfenamic acid, 3- mefenamic acid, 4- haloprogin, 5- iodopropynyl butylcarbamate, 6- carprofen, 7- ibuprofen, 8- salicylic acid, 9- meclofenamic acid, 10- acetylsalicylic acid, 11- N-phenylanthranilic acid (cocrystal form II), 12- quinolinic acid, 13- 2,6-diisopropylphenol, 14- diflunisal, 15- N-bromophthalimide, 16- 3-chloro-2-nitrobenzoic acid, 17- zaltoprofen, 18- azilsartan, 19- diclofenac

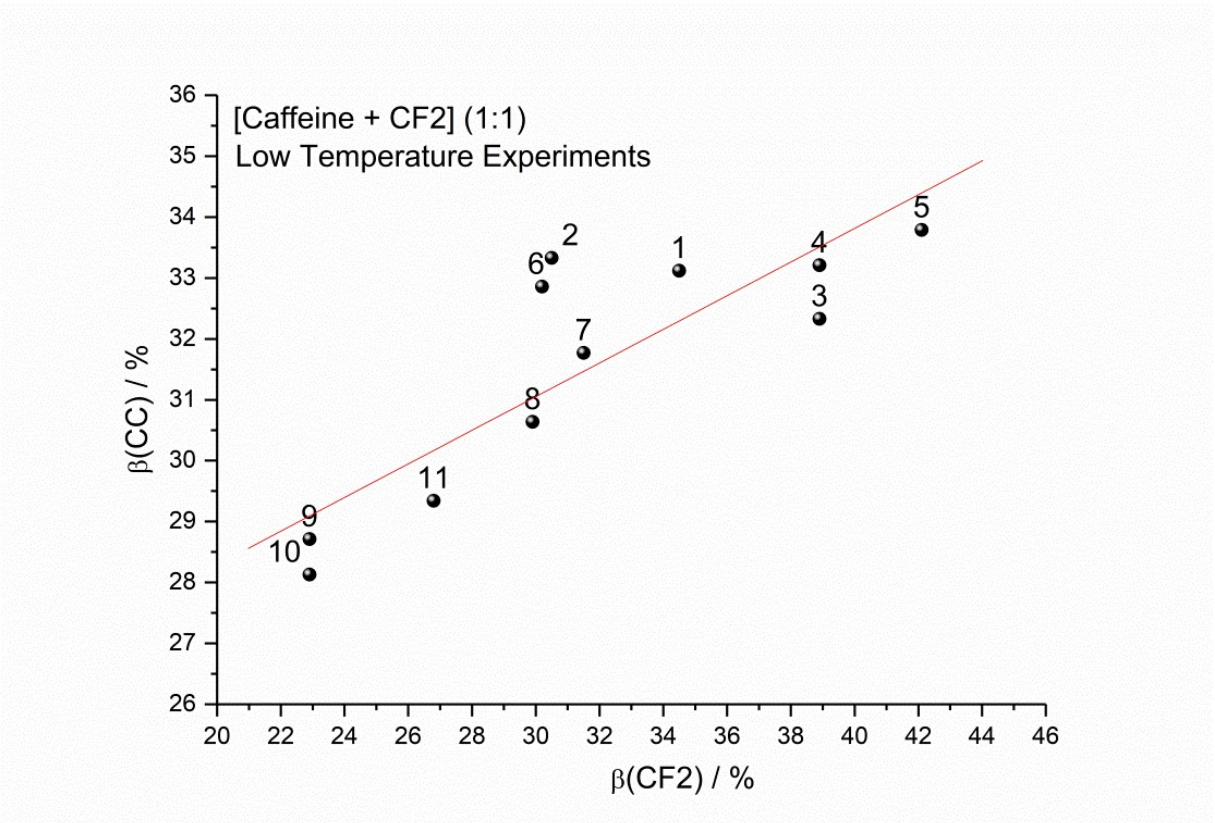

Figure S4. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Caffeine+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- furosemide, 2- niclosamide, 3- pterostilbene (cocrystal form I), 4- pterostilbene (cocrystal form II), 5- zonisamide, 6- maleic acid, 7- glutaric acid, 8- salicylic acid, 9- citric acid (cocrystal form I), 10- citric acid (cocrystal form II), 11- isophthalic acid

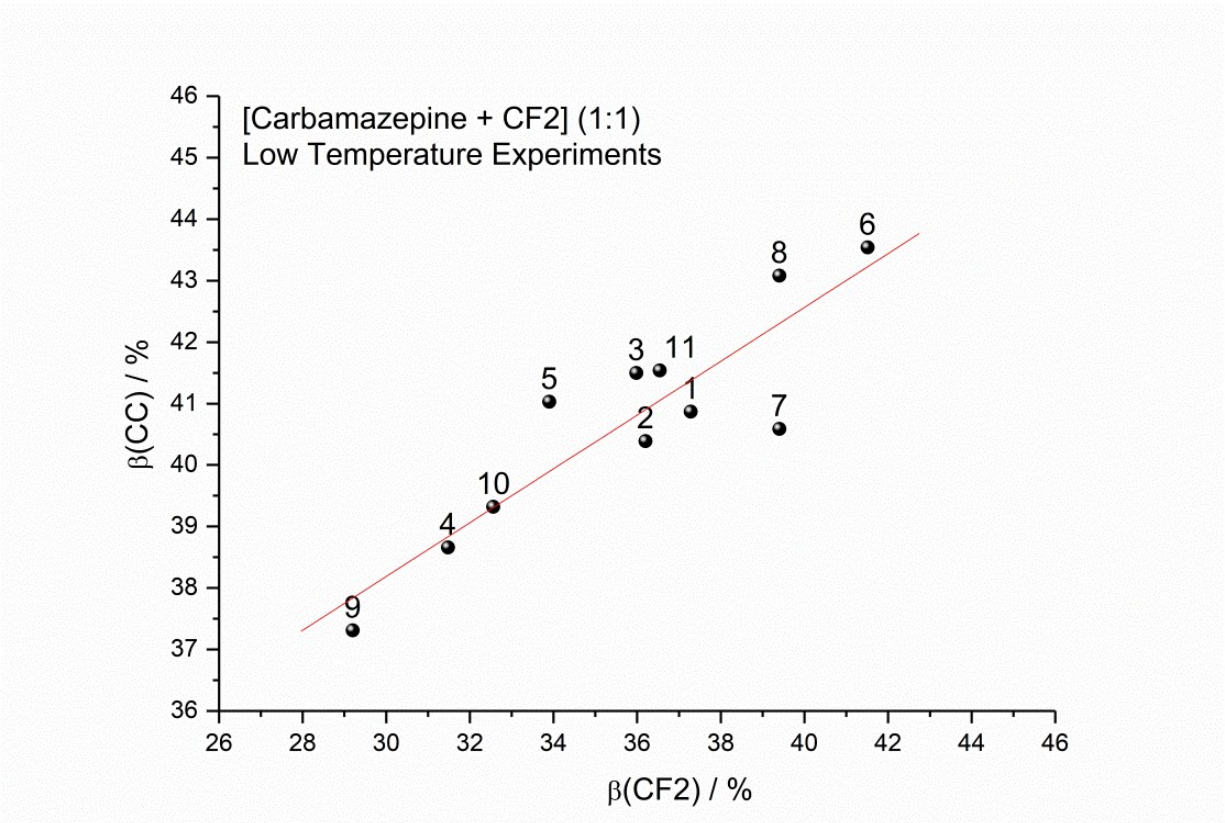

Figure S5. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Carbamazepine+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- benzoic acid, 2- 1-hydroxy-2-naphthoic acid, 3- nicotinamide, 4- glutaric acid, 5- salicylic acid, 6- 4-hydroxybenzamide, 7- saccharin (cocrystal form I), 8- saccharin (cocrystal form II), 9- emodin, 10- benzamide, 11- isonicotinamide

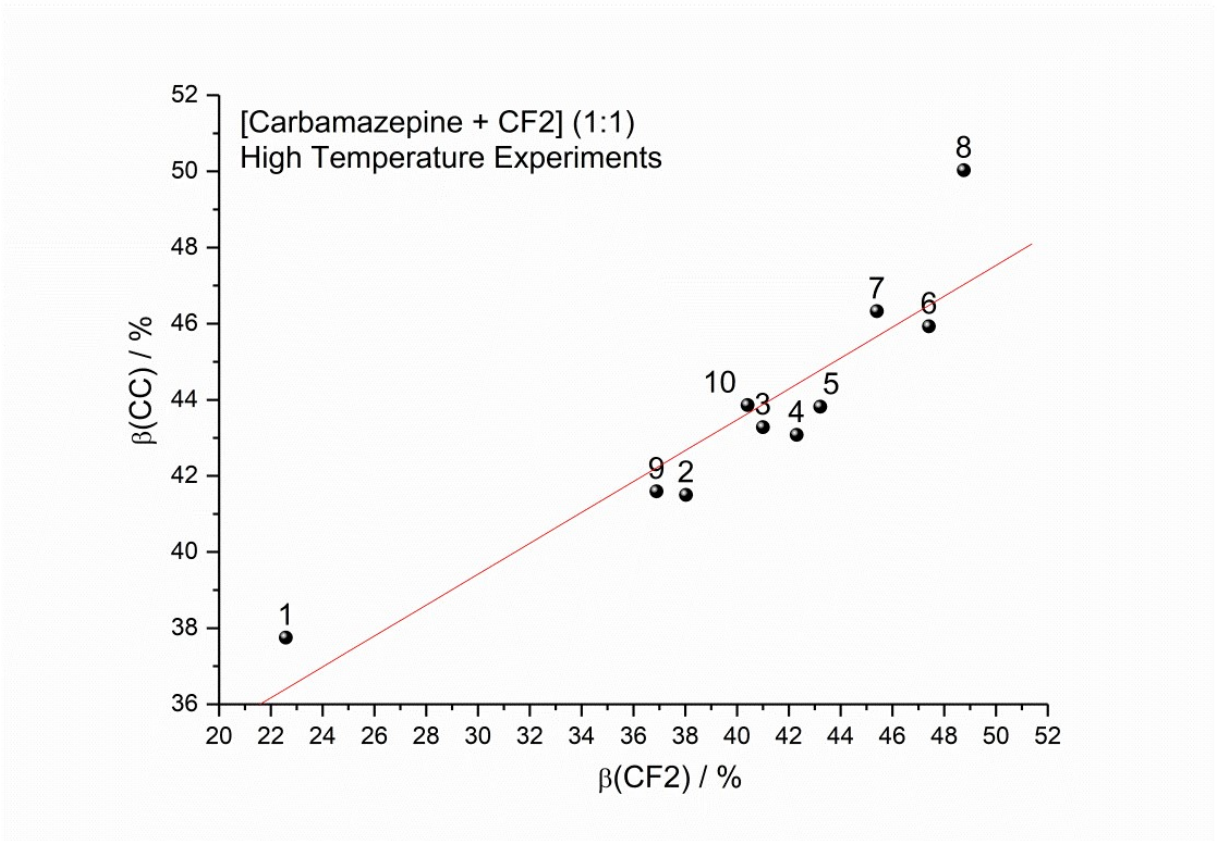

Figure S6. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Carbamazepine+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- DL-tartaric Acid, 2- nicotinamide, 3- cinnamic acid, 4- saccharin, 5- indomethacin, 6- 7-hydroxyflavanone, 7- naringenin, 8- paeonol, 9- 2,6-dihydroxybenzoic acid, 10- isonicotinamide

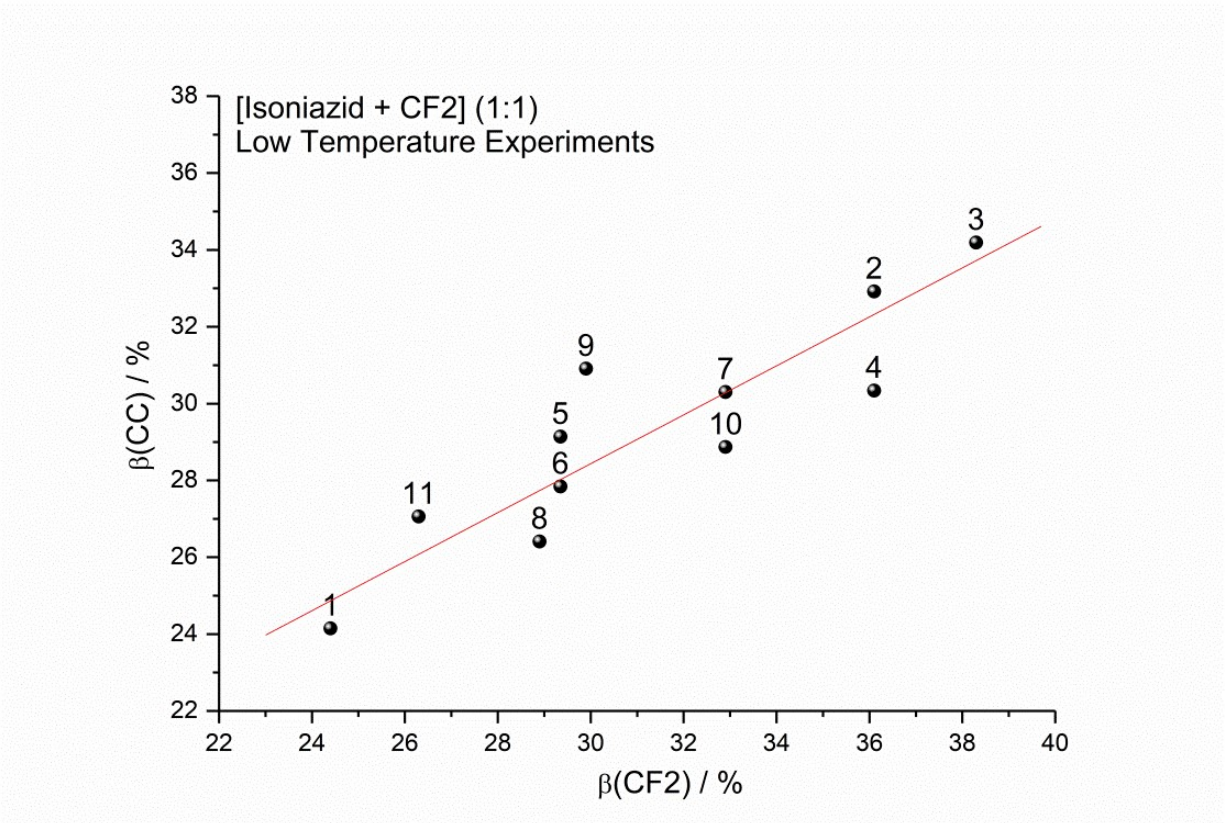

Figure S7. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Isoniazid+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- gallic acid, 2- cinnamic acid (cocrystal form I), 3- benzoic acid, 4- cinnamic acid (cocrystal form II), 5- caffeic acid (cocrystal form I), 6- caffeic acid (cocrystal form II), 7- pimelic acid, 8- 2,4-dihydroxybenzoic acid, 9- salicylic acid, 10- 4-hydroxycinnamic acid, 11- 2,5-dihydroxybenzoic acid

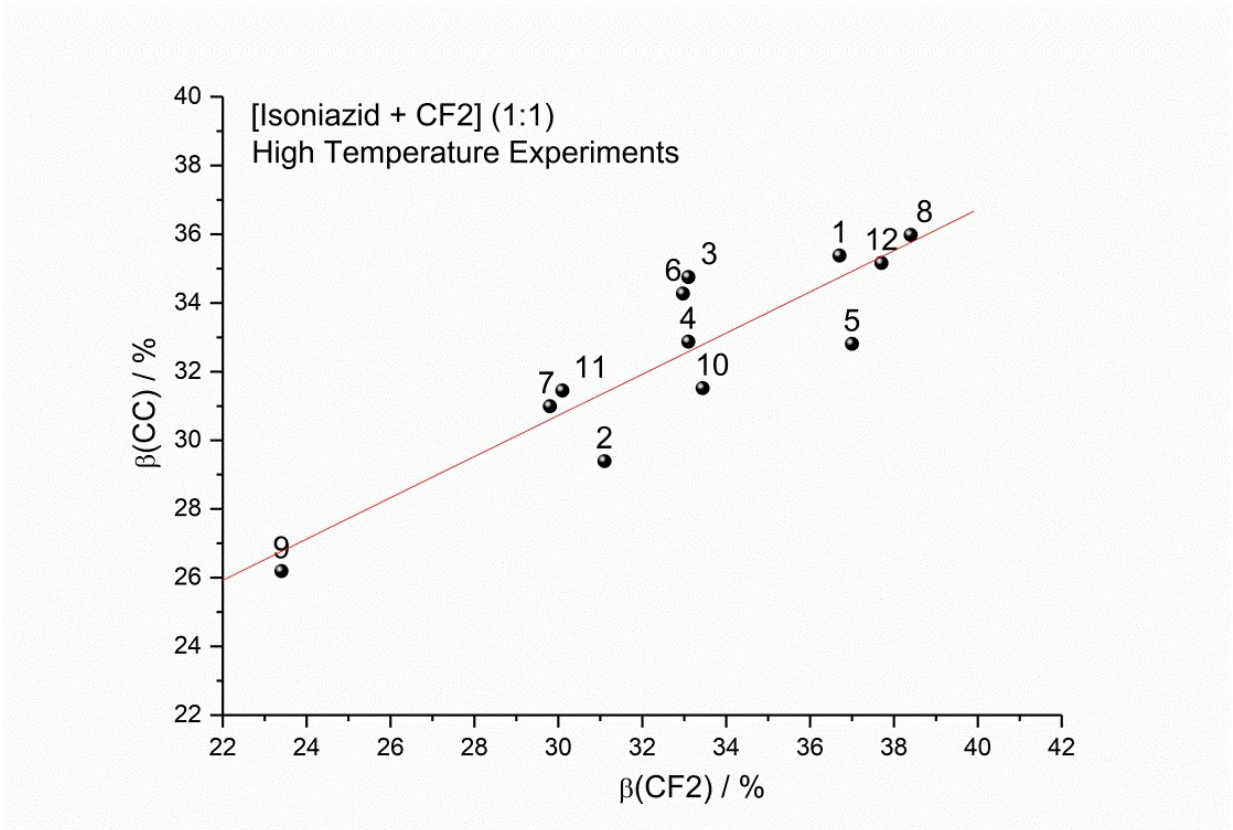

Figure S8. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Isoniazid+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- 2,3-dihydroxybenzoic acid, 2- 3,5-dihydroxybenzoic acid, 3- vanillic acid (cocrystal form I), 4-vanillic acid (cocrystal form II), 5- ferulic acid, 6- resorcinol, 7- 4-nitrobenzoic acid, 8- 4-cyanobenzoic acid, 9- gallic acid, 10- picric acid, 11- resveratrol, 12- 4-aminosalicylic acid

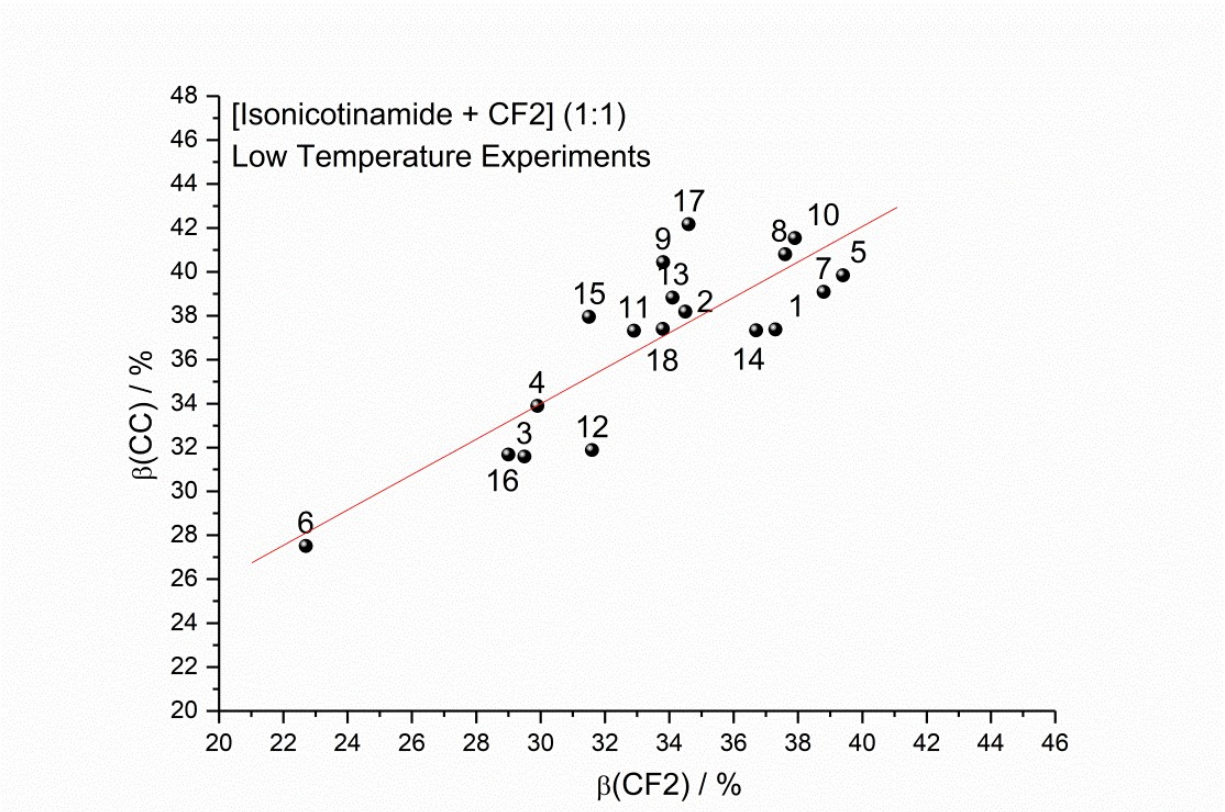

Figure S9. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Isonicotinamide+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- benzoic acid, 2- furosemide, 3- pyrazinoic acid, 4- salicylic acid, 5- (RS)-Ibuprofen, 6- quercetin, 7- etodolac, 8- progesterone, 9- vanillin, 10- carbamazepine, 11- pimelic acid, 12- suberic acid, 13- azelaic acid, 14- adipic acid, 15- glutaric acid, 16- 3,5-dinitrobenzoic acid, 17- succinamic acid, 18- (S)-mandelic acid

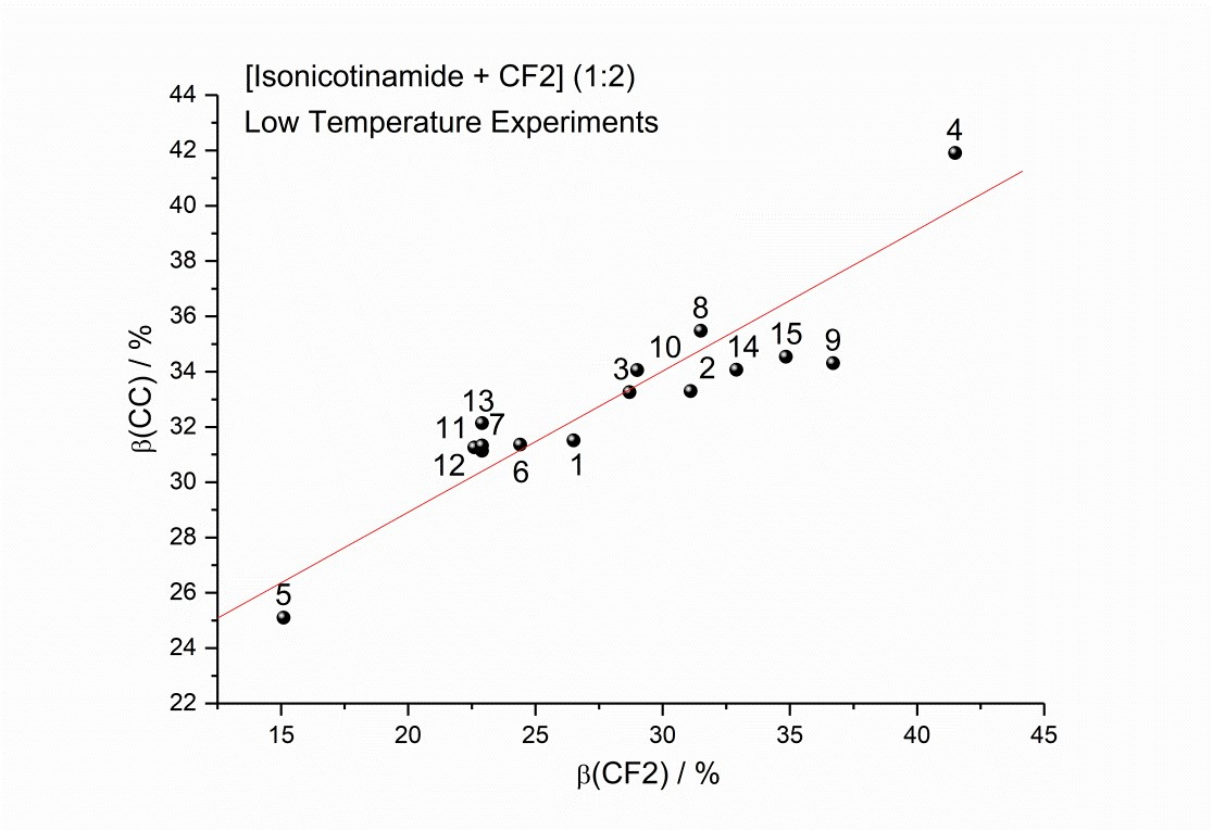

Figure S10. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Isonicotinamide+CF2] (1:2) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- L-tartaric acid, 2- genistein, 3- dihydrocaffeic acid, 4- naringenin, 5- oxalic acid, 6- malonic acid, 7- succinic acid, 8- glutaric acid, 9- adipic acid, 10- 3,5-dinitrobenzoic acid, 11- citric acid (cocrystal form I), 12- citric acid (cocrystal form II), 13- citric acid (cocrystal form III), 14- pimelic acid, 15- sebacic acid

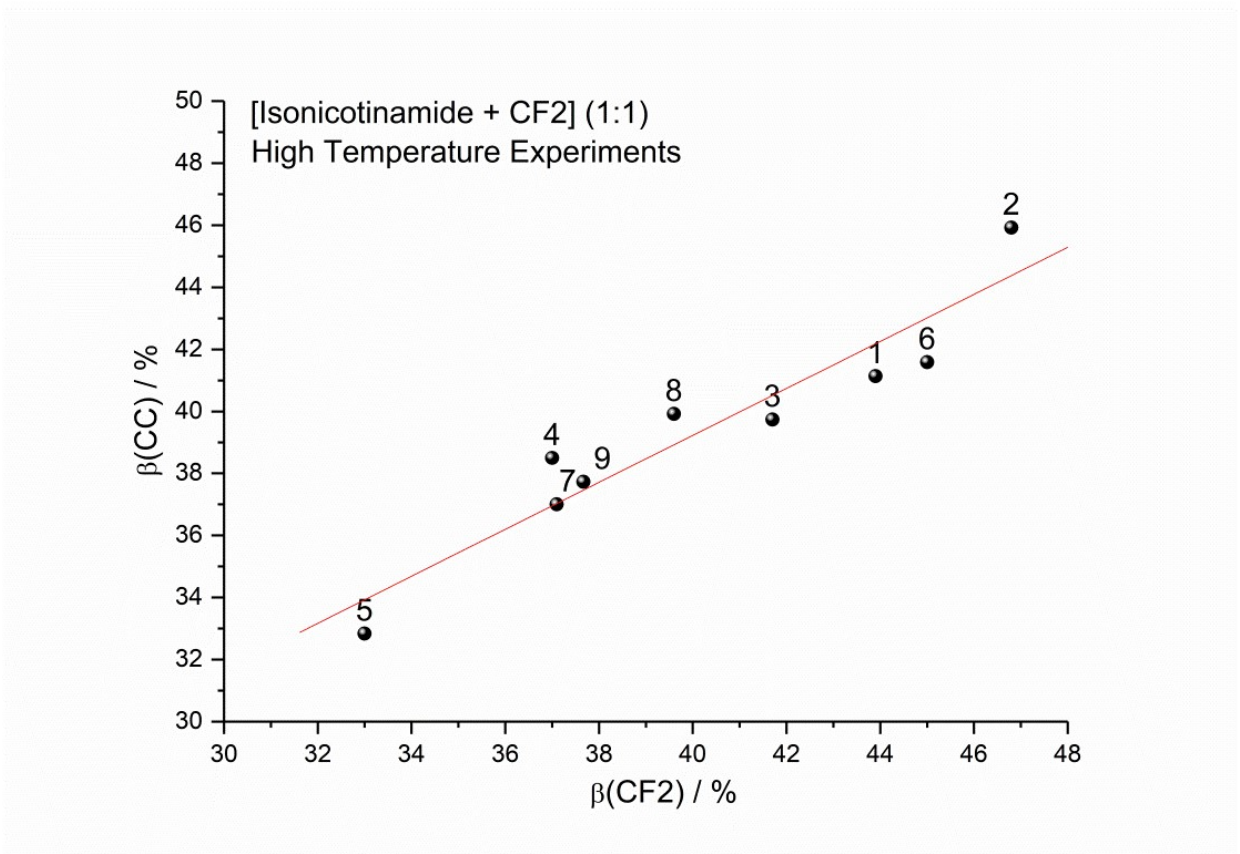

Figure S11. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Isonicotinamide+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- meclofenamic acid, 2- Agomelatine, 3- (S)-naproxen, 4- ferulic acid, 5- theophylline, 6- febuxostat, 7- entacapone, 8- zileuton, 9- glutaric acid

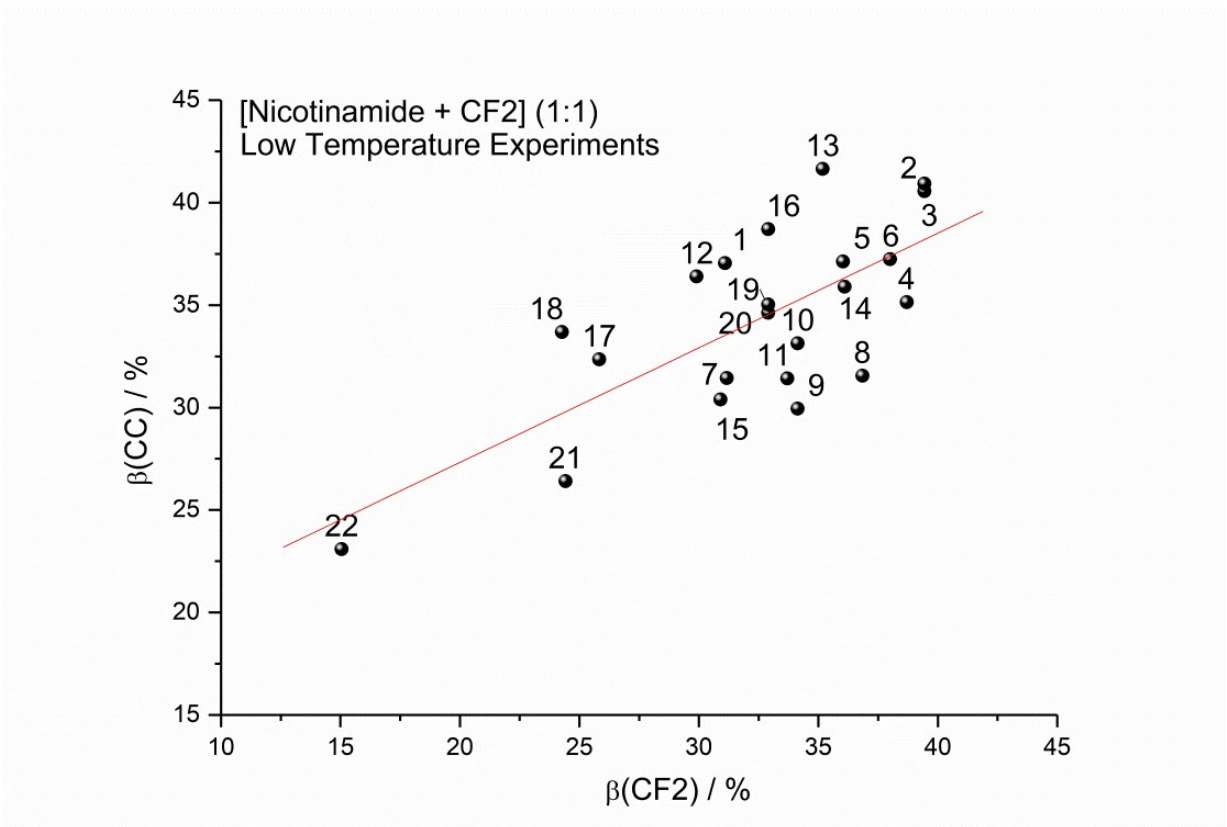

Figure S12. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Nicotinamide+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- acetazolamide, 2- (RS)-ibuprofen, 3- (S)-ibuprofen, 4- flurbiprofen, 5- flufenamic acid, 6- carbamazepine, 7- baicalein, 8- ethylparaben, 9- 4-coumaric acid (cocrystal form I), 10- 4-coumaric acid (cocrystal form II), 11- hydrochlorothiazide, 12- salicylic acid, 13- diethylstilbestrol, 14- trans-cinnamic acid, 15- vanillin, 16- pimelic acid, 17- 4-hydroxybenzoic acid, 18- fumaric acid, 19- (R)-mandelic acid (cocrystal form I), 20- (R)-mandelic acid (cocrystal form II), 21- malonic acid, 22- oxalic acid

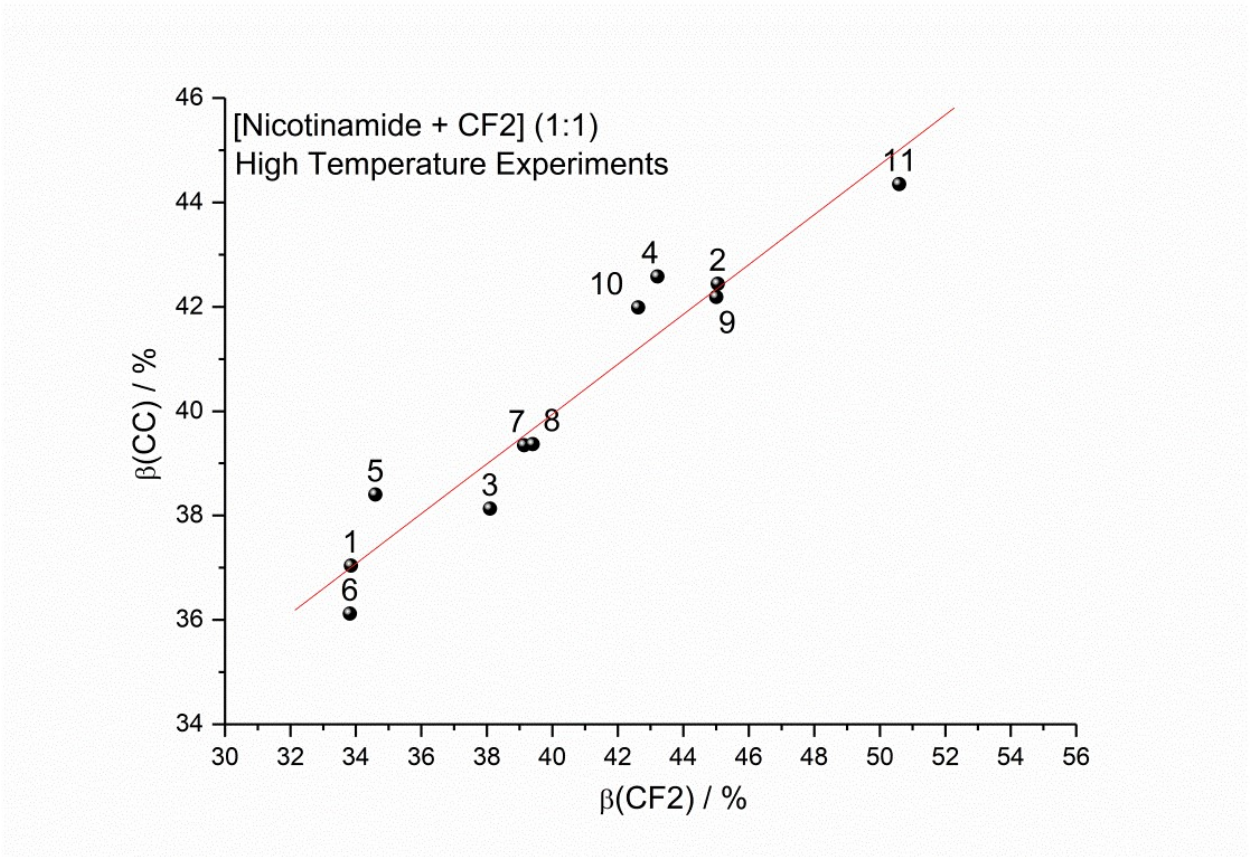

Figure S13. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Nicotinamide+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- furosemide (cocrystal form I), 2- febuxostat, 3- furosemide (cocrystal form II), 4- indomethacin, 5- salicylic acid, 6- sinapic acid, 7- acemetacin, 8- metaxalone, 9- lesinurad, 10- zaltoprofen, 11- lorazepam

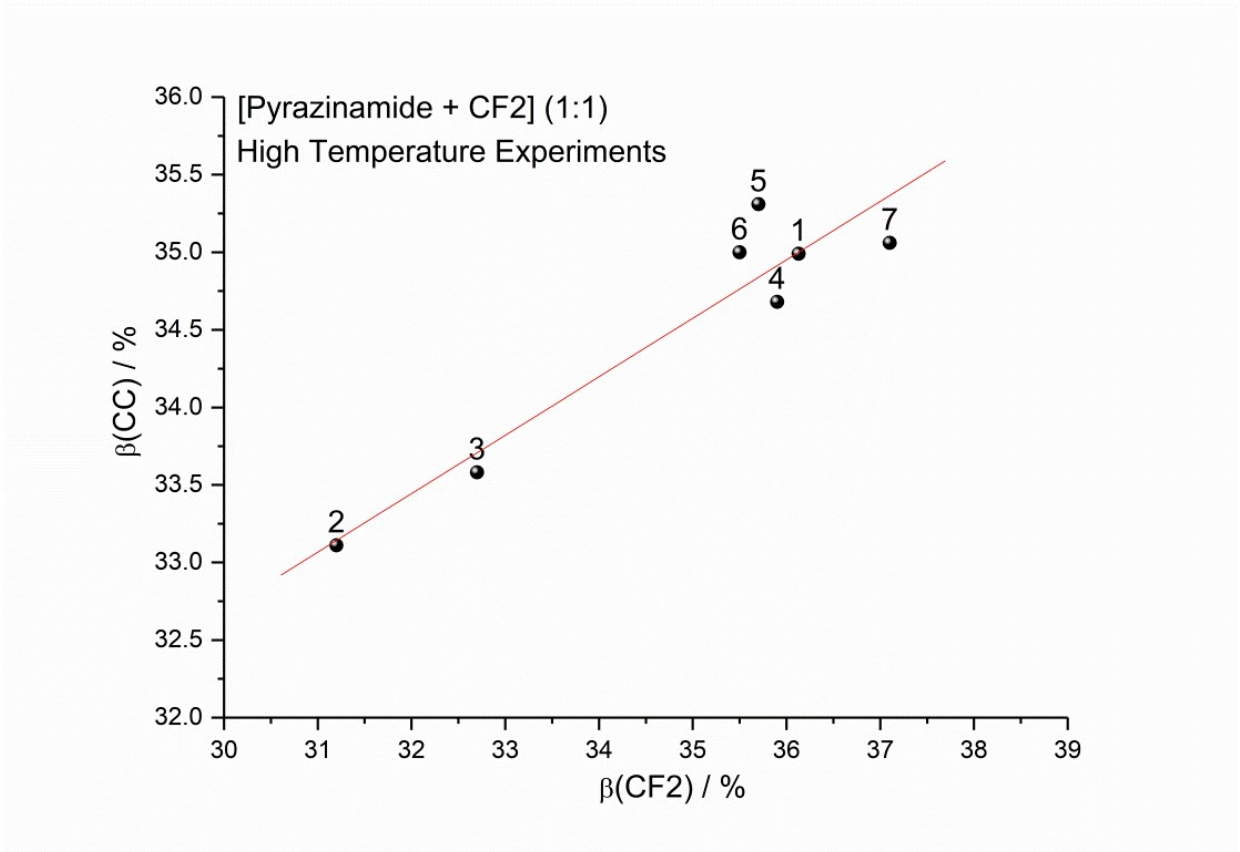

Figure S14. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Pyrazinamide+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- p-aminobenzoic acid, 2- malonic acid, 3- 3,4-dihydroxybenzoic acid, 4- methylmalonic acid, 5- hydrochlorothiazide, 6- theophylline, 7- entacapone

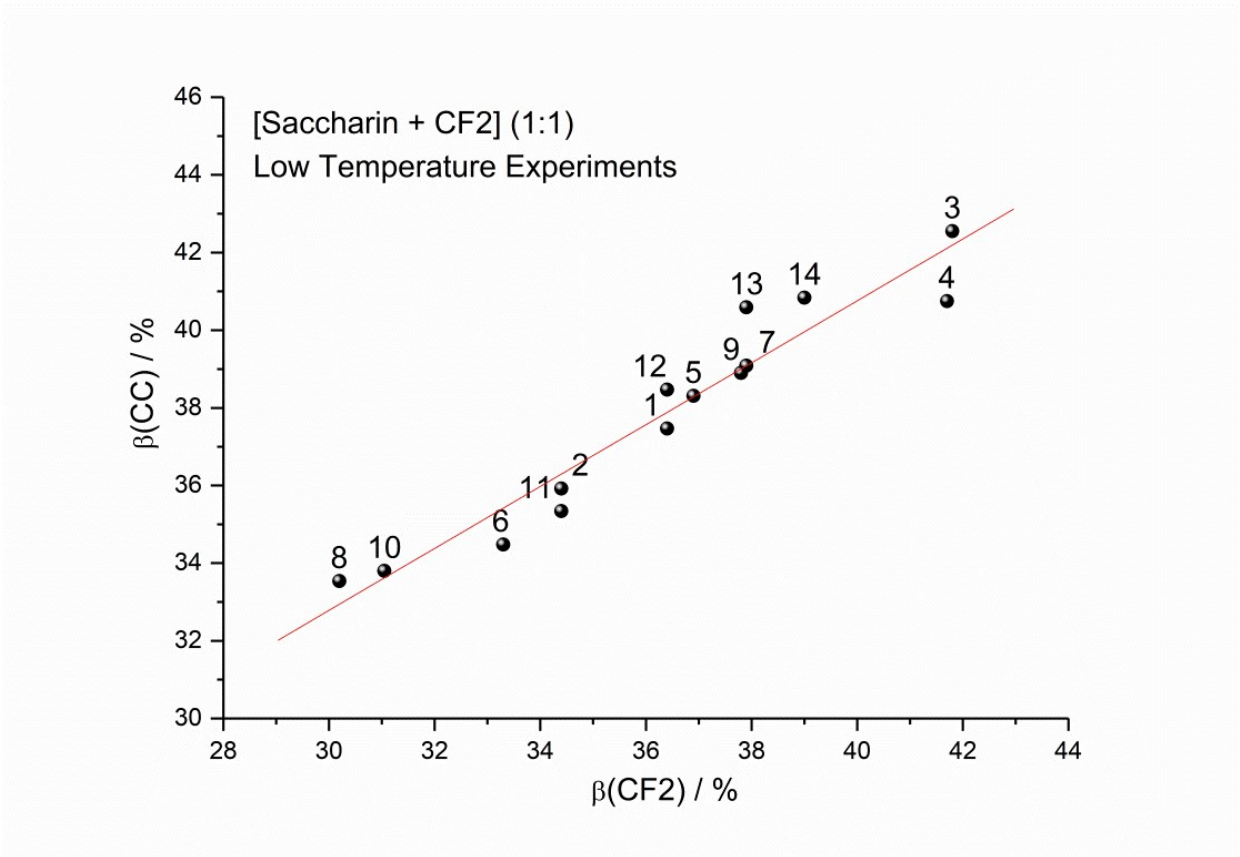

Figure S15. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Saccharin+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- dihydrocarbamazepine, 2- cyheptamide, 3- quinine, 4- sertraline, 5- venlafaxine, 6- piroxicam, 7- carbamazepine (cocrystal form I), 8- theophylline, 9- indomethacin, 10- vanillin isoniazid, 11- 2-ethoxybenzamide, 12- apatinib, 13- carbamazepine (cocrystal form II), 14- abiraterone acetate (cocrystal form II)

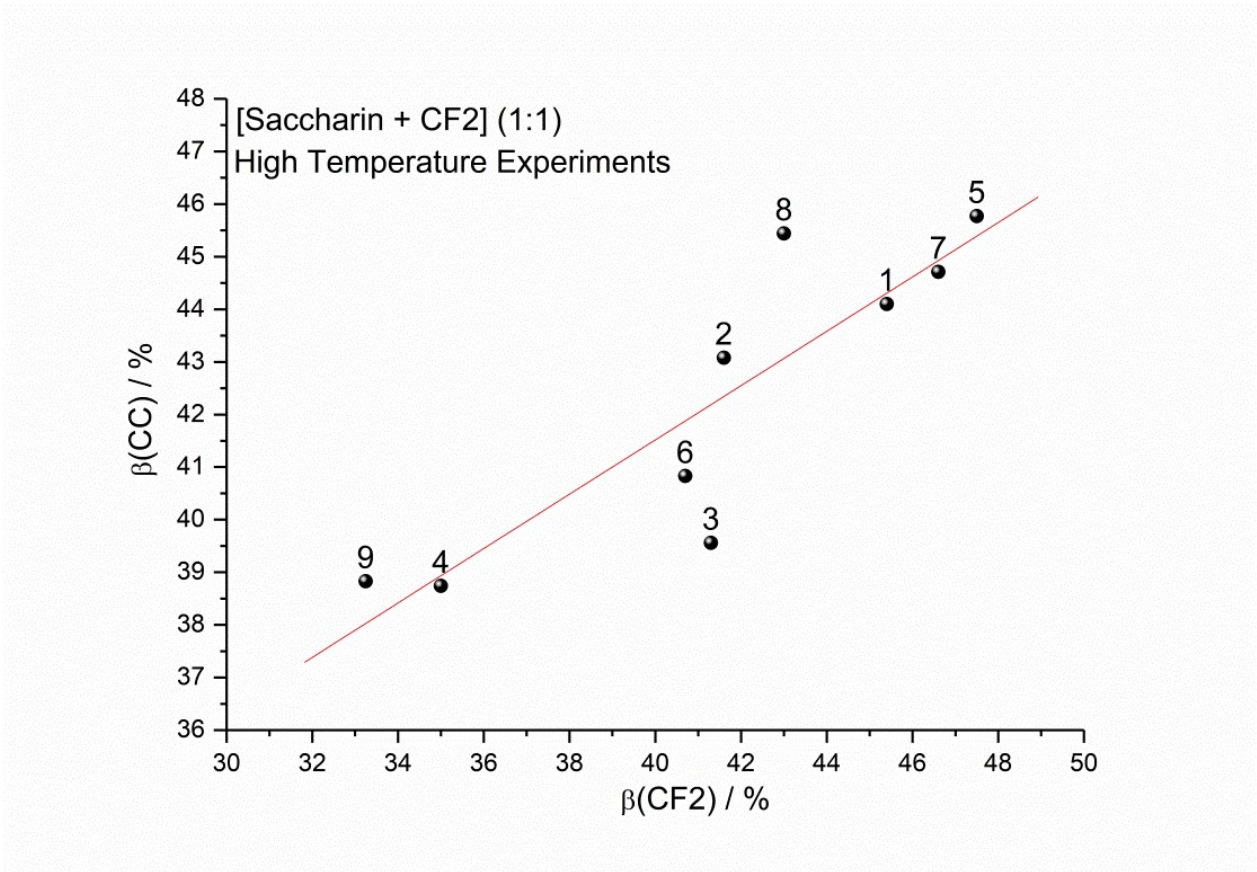

Figure S16. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Saccharin+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- sertraline, 2- carbamazepine, 3- megestrol acetate, 4- ciprofloxacin, 5- clofazimine, 6- antipyrine, 7- aminophenazone, 8- spironolactone, 9- emtricitabine

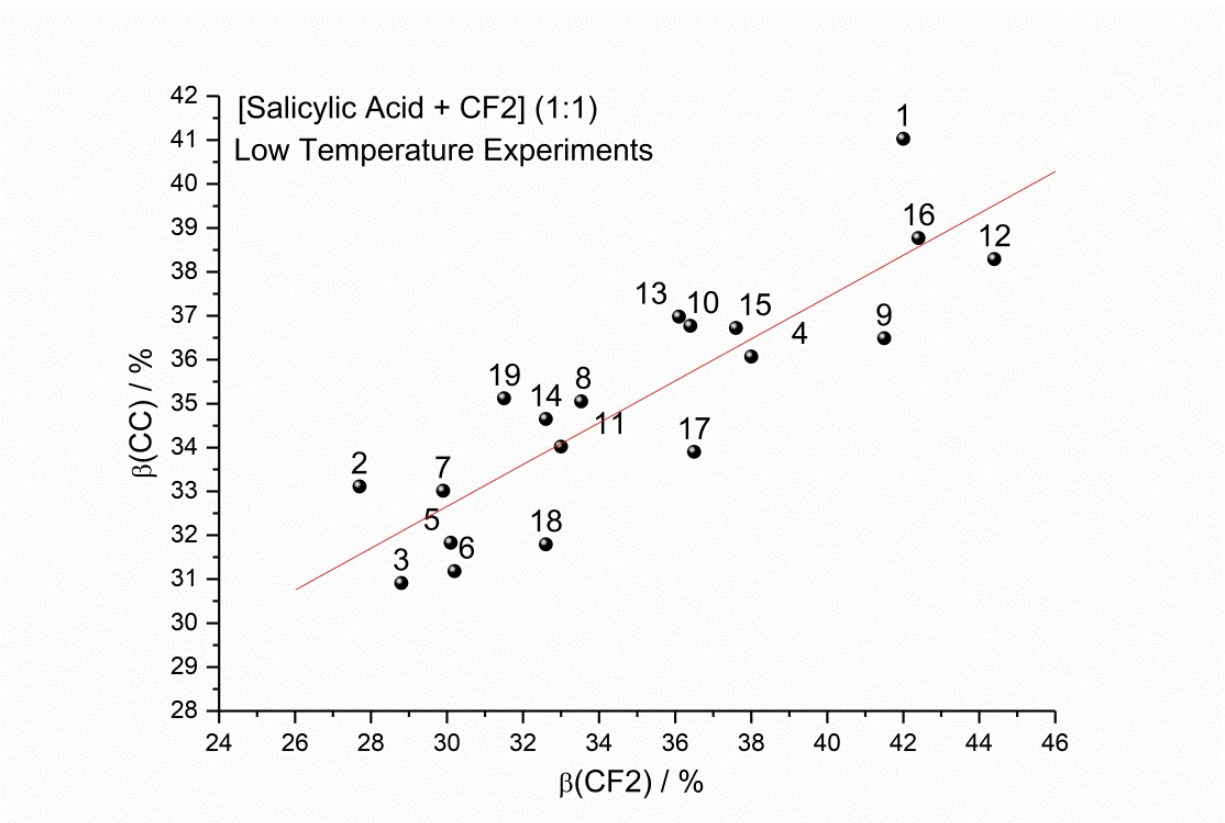

Figure S17. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Salicylic acid+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- carbamazepine, 2- nicotinic acid, 3- isoniazid, 4- N'-(propan-2-ylidene)isonicotinohydrazide, 5- caffeine, 6- theophylline, 7- gabapentin, 8- 4-dimethylaminopyridine, 9- 4-hydroxybenzamide, 10- apatinib, 11- theobromine, 12- 11-Azaartemisinin, 13- benznidazole, 14- tinidazole, 15- progesterone, 16- nicotinamide, 17- isonicotinamide, 18- benzamide, 19- 3-nitrobenzamide

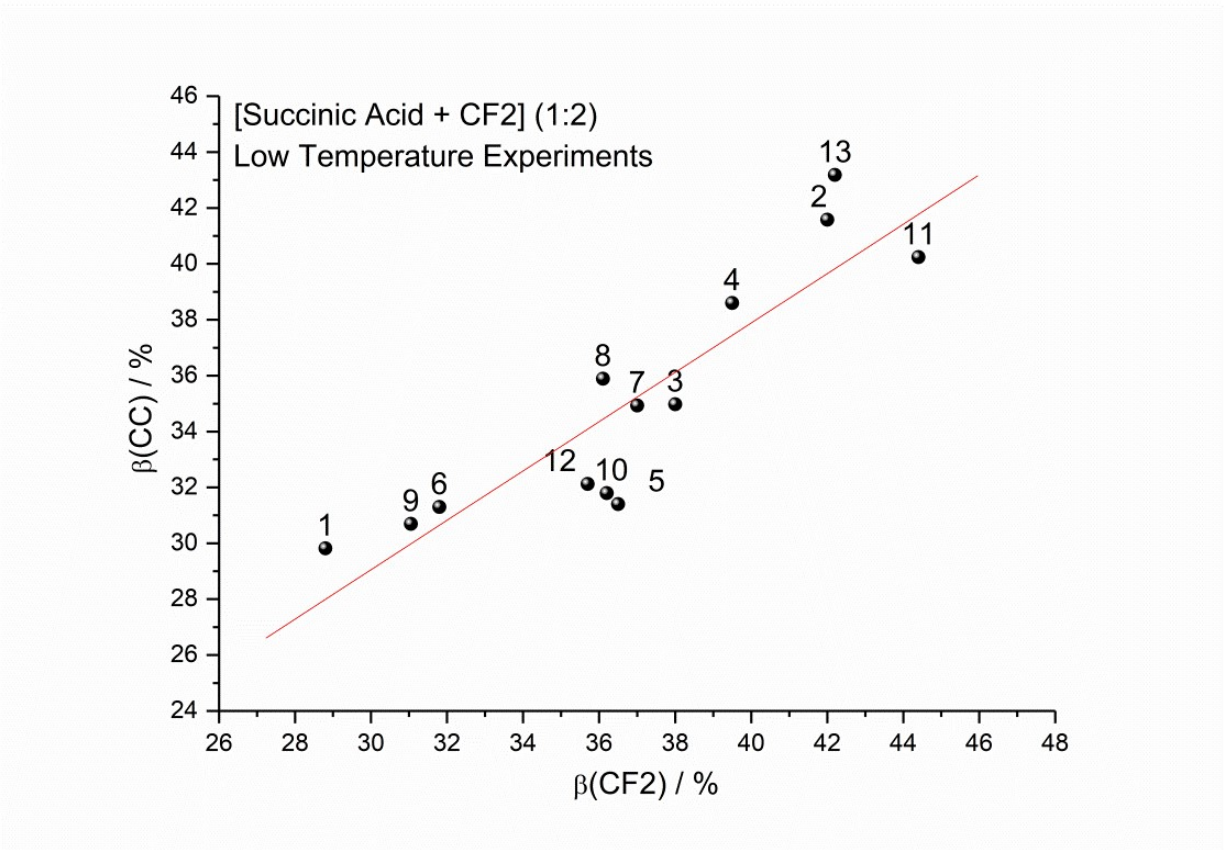

Figure S18. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Succinic acid+CF2] (1:2) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- isoniazid, 2- carbamazepine, 3- N'-(propan-2-ylidene)isonicotinohydrazide, 4- itraconazole, 5- isonicotinamide, 6- meloxicam, 7- 4-bromobenzamide, 8- piroxicam, 9- 4-aminobenzamide, 10- 4-hydroxybenzamide, 11- 11-Azaartemisinin, 12- piperine, 13- baricitinib

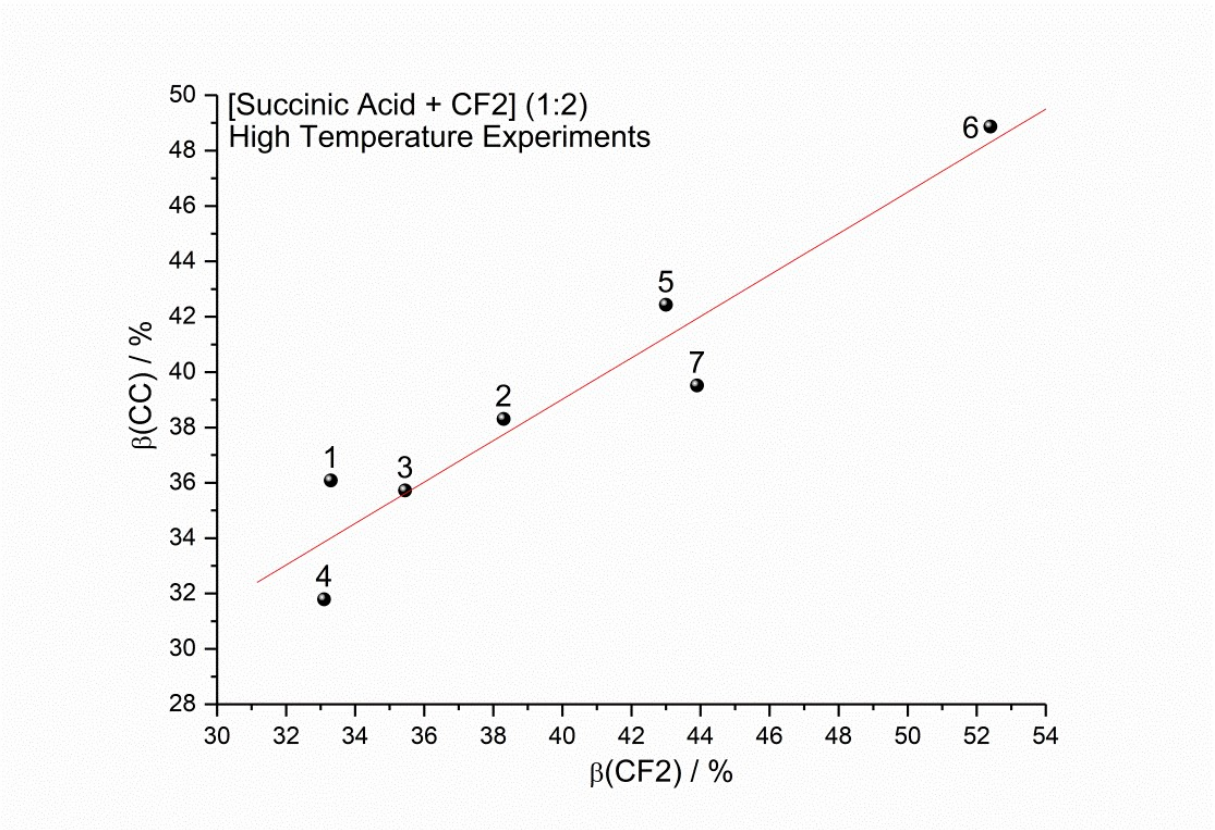

Figure S19. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Succinic acid+CF2] (1:2) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- pyrazinamide, 2- urea, 3- meloxicam, 4- isoniazid, 5- itraconazole, 6- adefovir dipivoxil, 7- 9-ethyladenine

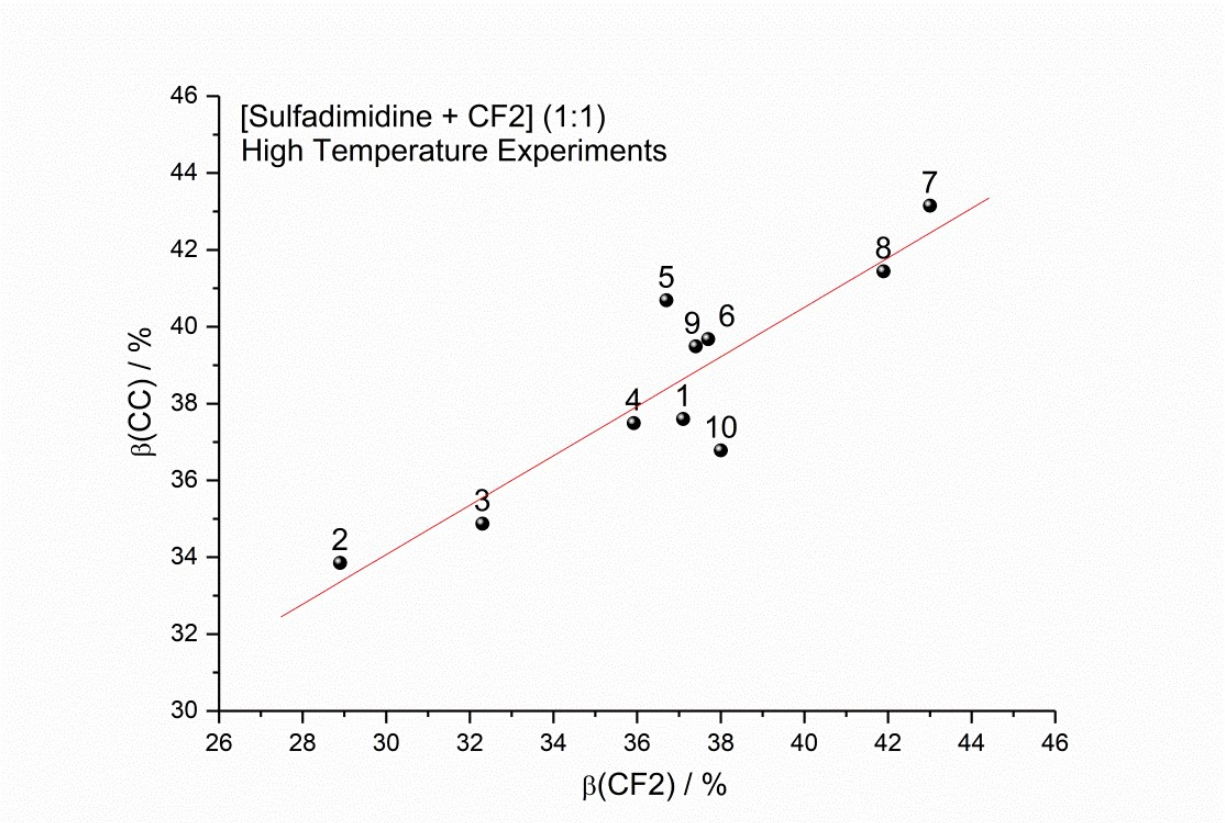

Figure S20. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Sulfatimidine+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- 2-aminobenzoic acid, 2- 4-hydroxybenzoic acid, 3- 2,4-dihydroxybenzoic acid, 4- benzamide, 5- picolinamide, 6- 4-aminosalicylic acid, 7- flufenamic acid (form I), 8- niflumic acid, 9- 4-aminobenzoic acid, 10- nicotinamide

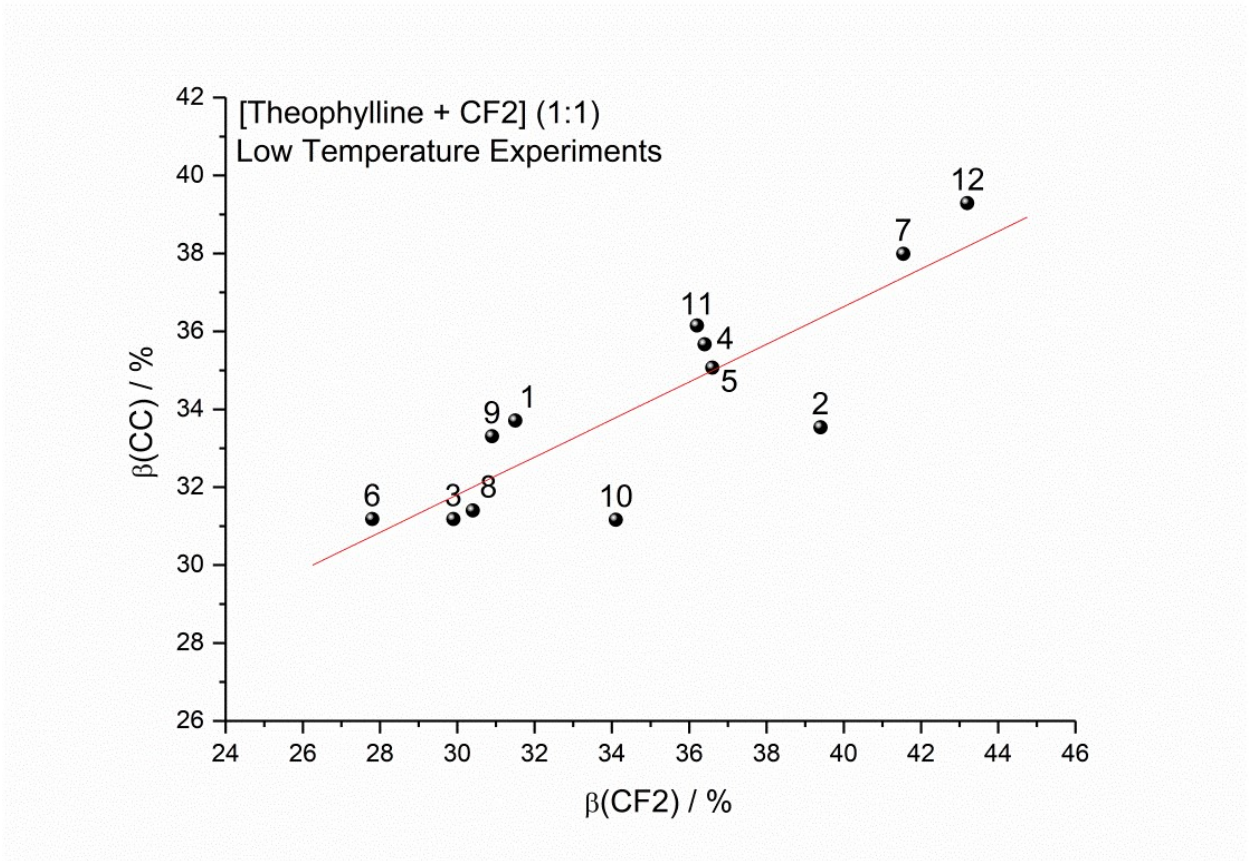

Figure S21. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Theophylline+CF2] (1:1) two-component crystals obtained from low temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- glutaric acid, 2- saccharin, 3- salicylic acid, 4- urea, 5- benzamide, 6- pyrazinamide, 7- benzoic acid, 8- 4-aminobenzoic acid, 9- paracetamol, 10- p-coumaric acid, 11- diclofenac, 12- pyrimethamine

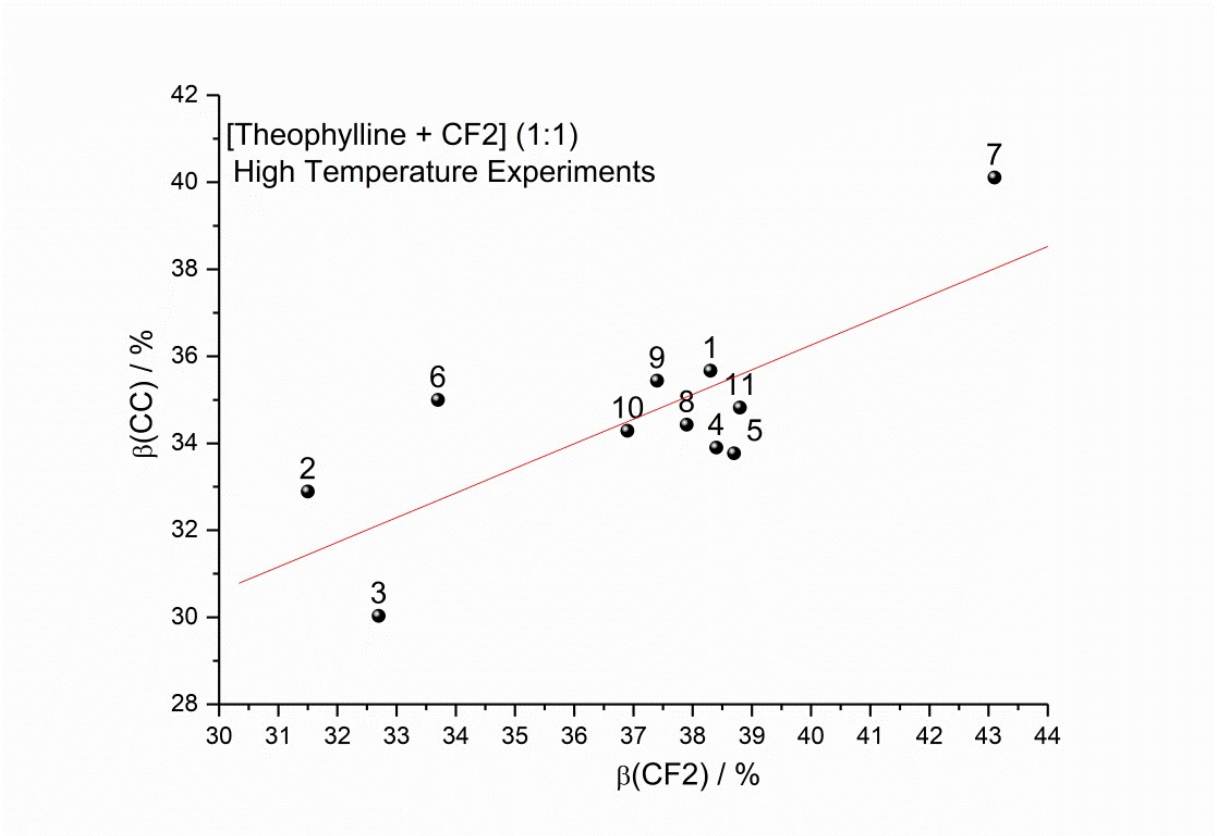

Figure S22. Correlation between the $\beta(CC)$ and $\beta(CF2)$ parameters for the cluster of the [Theophylline+CF2] (1:1) two-component crystals obtained from high temperature X-Ray experiments. The numbers correspond to the following coformers (CF2): 1- urea, 2- 3,5-dihydroxybenzoic acid, 3- 3,4-dihydroxybenzoic acid, 4- cinnamic acid, 5- benzamide, 6-pyrazinamide, 7- benzoic acid, 8- acetylsalicylic acid, 9- 4-aminobenzoic acid, 10- 3-aminobenzoic acid, 11- paracetamol