Supplementary Materials:

The following supporting information can be downloaded at: www.mdpi.com/xxx/s1.

Cocrystal Screening List

Table S1: List of the potential coformers and results of grinding experiments: **P** indicates diffractograms showing a mixture of the parent compounds, **X** denotes the diffractograms where new peaks were observed suggesting the identification of a new (salt) cocrystal or a new salt (8), **A** refers to the experiments that led to an amorphous phase (5).

CCFs tested	Results
(D)-(+)-Camphoric acid	P
(D)-Phenylglycinamide	A
(D, L)-3-Phenyllactic acid	P
(D, L)-Aspartic acid	P
(D, L)-Histidine	P
(D, L)-Tryptophan	P
(DL)-Mandelic acid	P
(L)-3-Phenyllactic acid	P
(L)-Aspartic acid	P
(L)-Histidine	P
(L)-Malic acid	P
(L)-Phenylalanine	P
(L)-Phenylglycine	P
(L)-Proline	A
(L)-Tryptophan	P
(L)-Tyrosine	P
(R)-(-)-2-Phenylglycine methyl ester hydrochloride	P
(R)-Mandelic acid	P
(R, S)-1-(4-Bromophenyl)ethylamine	A
(R, S)-2-Phenylbutyric acid	P
(R, S)-Diphylline	P
(R, S)-Ibuprofen	P
(S)-2-Pyrrolidone-5-carboxylic acid	P
(S)-Ibuprofen	P
1-Hydroxy-2-naphtoic acid	P
2,2-Dimethylsuccinic acid	P
2,3-Dihydroxybenzoic acid	P
2,4-Dihydroxybenzoic acid	P
2,5-Dihydroxybenzoic acid	P
2-Amino-6-chloropurine	P
3,4-Dihydroxybenzoic acid	P
3,5-Dihydroxybenzoic acid	P
4-Aminobenzoic acid	P
4-Aminobenzoic acid	P
4-Hydroxybenzoic acid	P
4-Nitrobenzamide	X
4-Nitrobenzoic acid	P
5-(Hydroxymethyl)uracil	P

5-Aminouracil	P
5-Carboxy-2-thiouracil	A
5-Methyl-2-thiouracil	P
5-Methyl-2-thiouracil	P
5-Propyl-2-thiouracil	P
6-(Chloromethyl)uracil	P
6-Aminouracil	P
6-Chlorouracil	P
Adenine	X
Caffeine	X
Carbamazepine	X
Citraconic acid	P
Citric acid	P
Dithiouracil	P
Ethyl 7-theophyllineacetate	P
Fumaric acid	P
Hippuric acid	P
Hypoxanthine	X
Indoprofen	P
Isonicotinamide	X
Menadione	P
Methylsuccinic acid	P
Nicotinamide	X
Orotic acid anhydrous	P
Oxalic acid	P
Oxcarbazepine	P
Pyrazinamide	P
Theobromine	P
Theophylline	X
Theophylline-7-acetic acid	P
Thymine	P
Trans-4-hydroxy-L-proline	A
Trans-cinnamic acid	P
Uric acid	P
Xanthine	P

X-ray Powder Diffraction Data

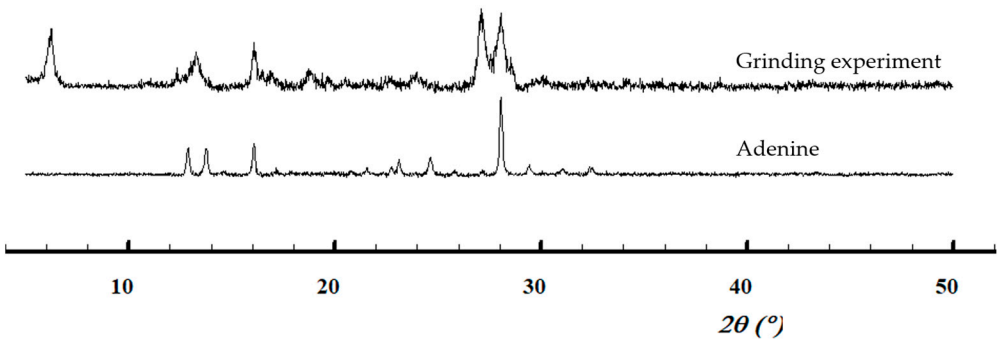

Figure S1: Normalised experimental diffraction patterns of the ground powder of Pyruvic Acid and Adenine (1:1 ratio) and of Adenine.

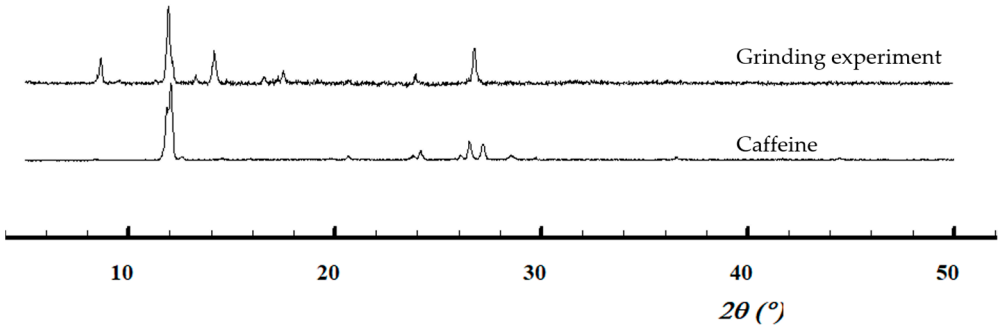

Figure S2: Normalised experimental diffraction patterns of the ground powder of Pyruvic Acid and Caffeine (1:4 ratio) and of Caffeine.

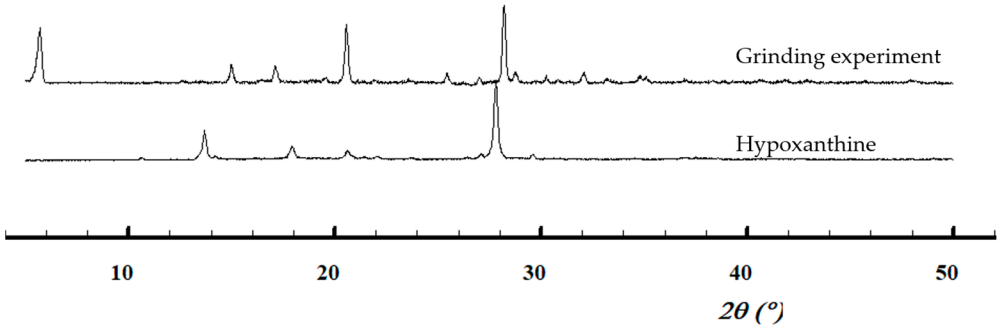

Figure S3: Normalised experimental diffraction patterns of the ground powder of Pyruvic Acid and Hypoxanthine (1:4 ratio) and of Hypoxanthine.

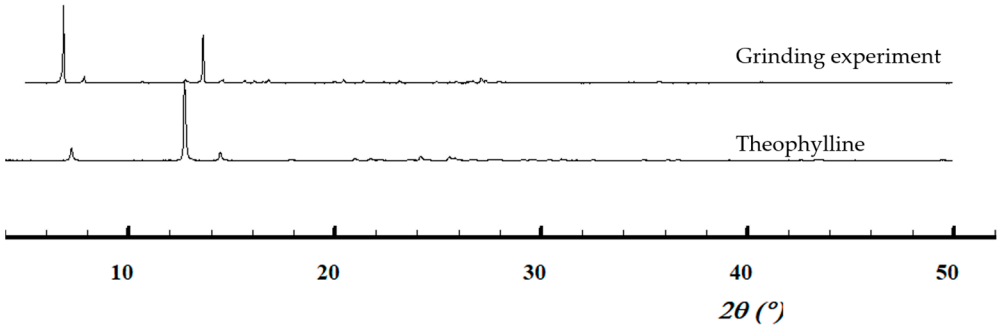

Figure S4: Normalised experimental diffraction patterns of the ground powder of Pyruvic Acid and Theophylline (1:4 ratio) and of Theophylline.

Single-Crystal X-ray Diffraction Data

Table S2. Crystal data and structure refinement for the 1:1 Pyruvic acid-4-Nitrobenzamide cocrystal.

Identification code	1:1 Pyruvic acid-4-Nitrobenzamide Cocrystal
Empirical formula	$C_7H_6N_2O_3$, $C_3H_4O_3$
Formula weight	254.20
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 5.3463(5) Å
	b = 19.6423(14) Å
	c = 10.8234(7) Å
	α= 90°
	β= 90.316(7)°
	γ= 90°
Volume	1136.59(16) Å^3
Z	4
Density (calculated)	1.486 mg/m^3
Absorption coefficient	0.125 mm^{-1}
F_{000}	528
Crystal size	0.35 x 0.05 x 0.05 mm^3
Theta range for data collection	3.637 to 25.018°
Index ranges	-6 ≤ h ≤ 6, -23 ≤ k ≤ 23, 0 ≤ l ≤ 12
Reflections collected	1988
Independent reflections	1988 [R_{int} = 0]*
Completeness to theta = 25.018°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.62615
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1988 / 0 / 166
Goodness-of-fit on F^2	1.070
Final R indices [$I > 2\sigma_I$]	R_1 = 0.0465, wR_2 = 0.1156
R indices (all data)	R_1 = 0.0744, wR_2 = 0.1292
Extinction coefficient	n/a
Largest diff. peak and hole	0.164 and -0.166 e.Å^{-3}

*twinned structure refined against HKLF5 formatted reflections

Table S3. Crystal data and structure refinement for 1:1 Pyruvic Acid-Carbamazepine cocrystal.

Identification code	1:1 Pyruvic Acid-Carbamazepine
Empirical formula	$C_{15}H_{12}N_2O$, $C_3H_4O_3$
Formula weight	324.33
Temperature	297(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 5.3912(6) Å
	b = 16.6752(15) Å
	c = 18.2383(18) Å
	α= 90°
	β= 97.324(10)°
	γ = 90°
Volume	1626.2(3) Å^3
Z	4
Density (calculated)	1.325 mg/m^3
Absorption coefficient	0.095 mm^{-1}
F_{000}	680
Crystal size	0.40 x 0.04 x 0.04 mm^3
Theta range for data collection	3.323 to 25.240°
Index ranges	-6 ≤ h ≤ 6, -20 ≤ k ≤ 20, -21 ≤ l ≤ 21
Reflections collected	9499
Independent reflections	2897 [R_{int} = 0.0623]
Completeness to theta = 25.240°	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.57011
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2897 / 109 / 274
Goodness-of-fit on F^2	1.172
Final R indices [I > 2σI]	R_1 = 0.0757, wR_2 = 0.1160
R indices (all data)	R_1 = 0.1343, wR_2 = 0.1330
Extinction coefficient	n/a
Largest diff. peak and hole	0.134 and -0.160 e.Å^{-3}

Table S4. Crystal data and structure refinement for 1:1 Pyruvic Acid-Isonicotinamide salt.

Identification code	1:1 Pyruvic Acid-Isonicotinamide
Empirical formula	$C_6H_7N_2O$, $C_3H_3O_3$
Formula weight	210.19
Temperature	297(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 3.8349(6) Å
	b = 33.160(5) Å
	c = 7.6010(11) Å
	α= 90°
	β= 97.015(13)°
	γ = 90°
Volume	959.4(3) $Å^3$
Z	4
Density (calculated)	1.455 mg/m^3
Absorption coefficient	0.116 mm^{-1}
F_{000}	440
Crystal size	0.30 x 0.05 x 0.04 mm^3
Theta range for data collection	2.769 to 25.240°
Index ranges	$-4 \le h \le 4$, $-39 \le k \le 38$, $-9 \le l \le 9$
Reflections collected	5789
Independent reflections	1742 [R_{int} = 0.0614]
Completeness to theta = 25.240°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.61875
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1742 / 0 / 137
Goodness-of-fit on F^2	1.092
Final R indices [$I > 2\sigma_I$]	R_1 = 0.0904, wR_2 = 0.2090
R indices (all data)	R_1 = 0.1115, wR_2 = 0.2215
Extinction coefficient	n/a
Largest diff. peak and hole	0.343 and -0.316 e.$Å^{-3}$

Table S5. Crystal data and structure refinement for 2:3 Pyruvic Acid-Nicotinamide salt cocrystal.

Identification code	2:3 Pyruvic Acid-Nicotinamide
Empirical formula	$2(C_6H_7N_2O),2(C_3H_3O_3), C_3H_4O_3$
Formula weight	508.44
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 3.82010(12) Å
	b = 33.2921(9) Å
	c = 9.5234(2) Å
	α= 90°
	β= 98.606(3)°
	γ= 90°
Volume	1197.54(6) $Å^3$
Z	2
Density (calculated)	1.410 mg/m^3
Absorption coefficient	0.116 mm^{-1}
F_{000}	532
Crystal size	0.23 x 0.15 x 0.10 mm^3
Theta range for data collection	2.837 to 26.214°
Index ranges	-4 ≤ h ≤ 4, -41 ≤ k ≤ 37, -11 ≤ l ≤ 11
Reflections collected	8571
Independent reflections	2357 [R_{int} = 0.0166]
Completeness to theta = 25.242°	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.86352
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2357 / 58 / 192
Goodness-of-fit on F^2	1.098
Final R indices [I > 2σI]	R_1 = 0.0482, wR_2 = 0.1360
R indices (all data)	R_1 = 0.0516, wR_2 = 0.1384
Extinction coefficient	n/a
Largest diff. peak and hole	0.233 and -0.198 e.$Å^{-3}$

Proton Nuclear Magnetic Resonance (^{1}H NMR) Data

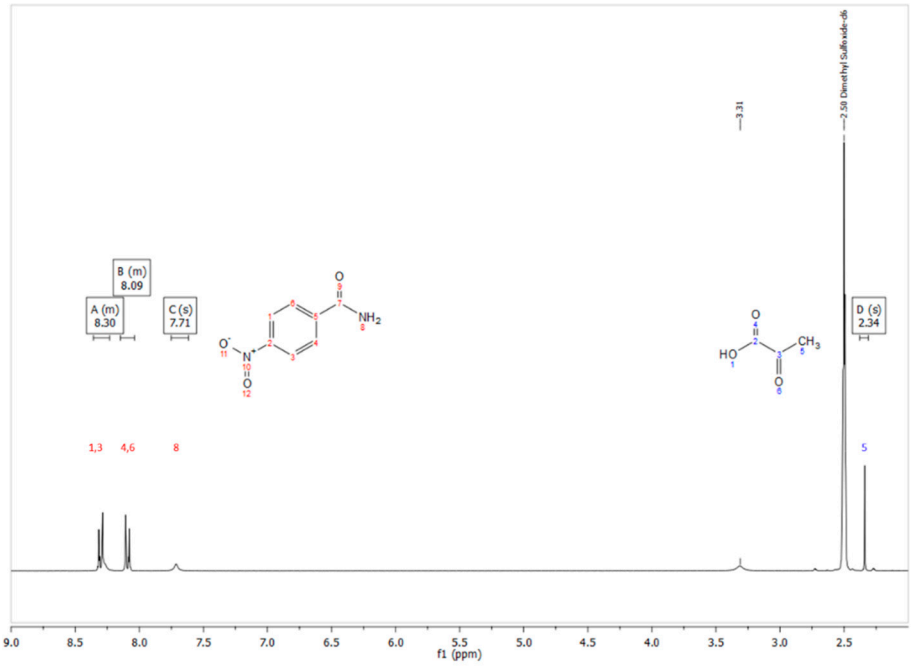

Figure S5: Proton NMR spectrum of 4-Nitrobenzamide-Pyruvic acid 1:1 cocrystal. The numbers corresponding to the protons of 4-nitrobenzamide are coloured in red while the numbers corresponding to the protons of pyruvic acid are coloured in blue.^{1}H NMR (300 MHz, DMSO) δ 8.33 – 8.25 (m, 4H, -C$_{Ar}$H, 1,3), 8.16 – 8.04 (m, 4H, -C$_{Ar}$H, 4,6), 7.71 (bs, 2H, -NH$_2$, 8), 2.34 (s, 3H, -CH$_3$, 5). δ 3.31 residual water peak.

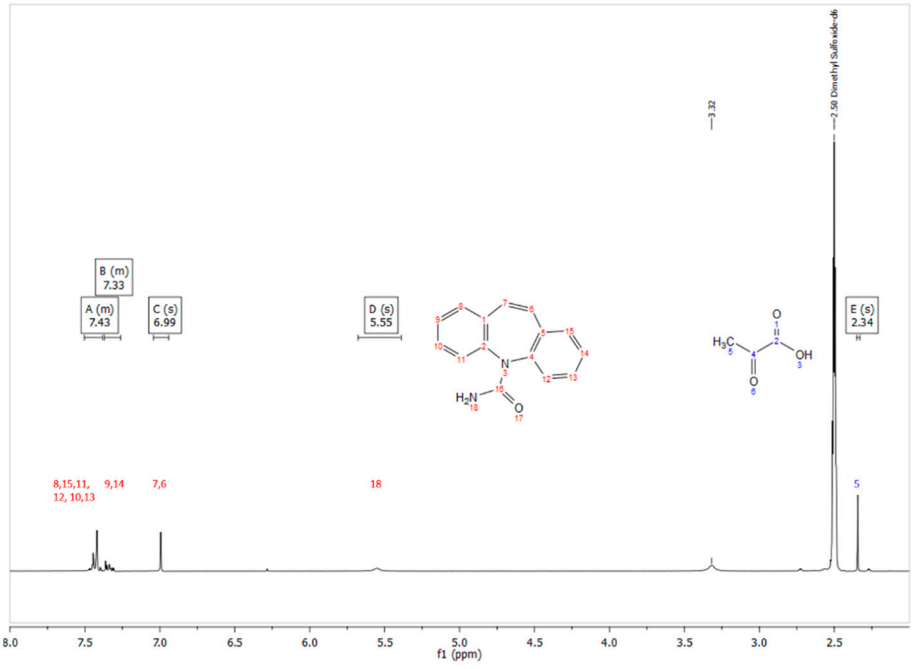

Figure S6: Proton NMR spectrum of Carbamazepine-Pyruvic acid 1:1 cocrystal. The numbers corresponding to the protons of carbamazepine are coloured in red while the numbers corresponding to the protons of pyruvic acid are coloured in blue.^{1}H NMR (300 MHz, DMSO) δ 7.50 – 7.38 (m, 6H, -C$_{Ar}$**H**, 8,10,11,12,13,15), 7.37 – 7.26 (m, 2H, C$_{Ar}$**H**, 9,14), 6.99 (s, 2H, -C$_{Ar}$**H**, 7,6), 5.55 (s, 2H, -N**H**$_2$, 18), 2.34 (s, 3H, -C**H**$_3$, 5). δ 3.31 residual water peak.

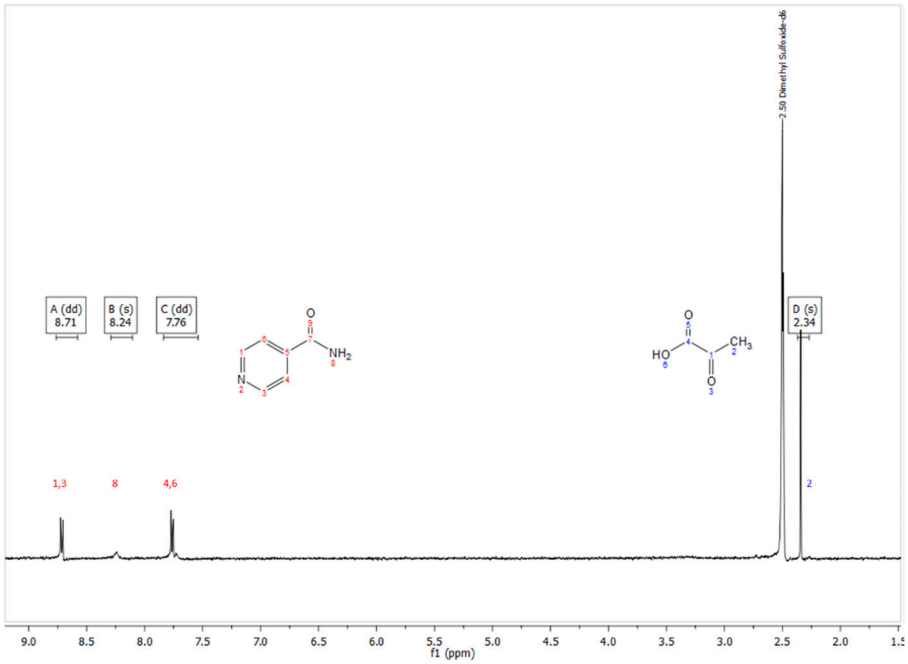

Figure S7: Proton NMR spectrum of Isonicotinamide-Pyruvic acid 1:1 salt. The numbers corresponding to the protons of isonicotinamide are coloured in red while the numbers corresponding to the protons of pyruvic acid are coloured in blue. ^{1}H NMR (300 MHz, DMSO) δ 8.71 (dd, J = 4.4, 1.6 Hz, 2H, C_{Ar}**H**, 1,3), 8.24 (s, 2H, -N**H**$_2$, 8), 7.76 (dd, J = 4.4, 1.7 Hz, 2H, C_{Ar}**H**, 4,6), 2.34 (s, 3H, -C**H**$_3$, 2).

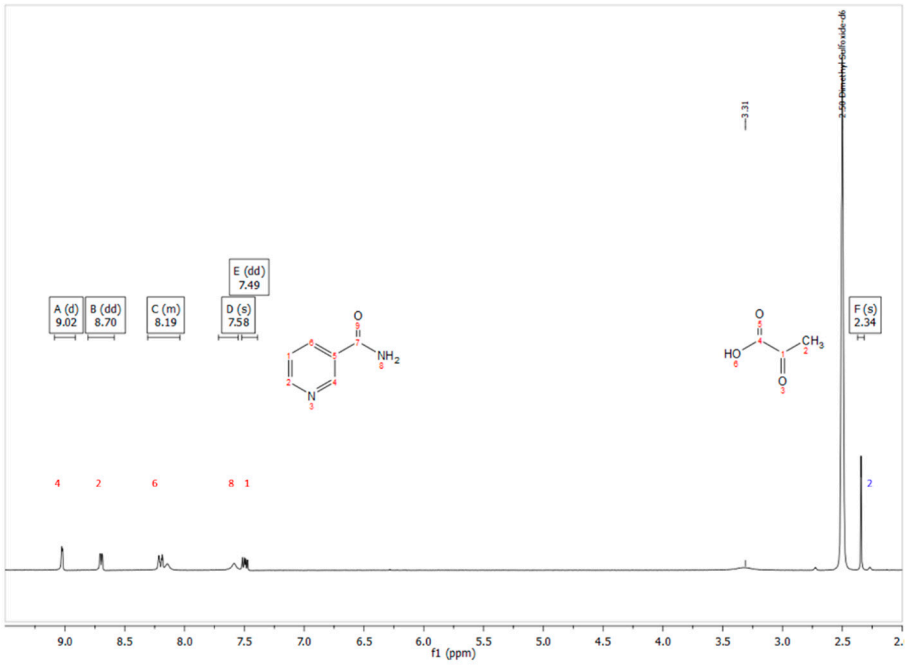

Figure S8: Proton NMR spectrum of Nicotinamide-Pyruvic acid 2:3 salt cocrystal. The numbers corresponding to the protons of nicotinamide are coloured in red while the numbers corresponding to the protons of pyruvic acid are coloured in blue.^{1}H NMR (300 MHz, DMSO) δ 9.02 (d, J = 1.8 Hz, 1H, C_{Ar}**H**, 4), 8.70 (dd, J = 4.8, 1.6 Hz, 1H, C_{Ar}**H**, 2), 8.31 – 8.04 (m, 1H, C_{Ar}**H**, 6), 7.58 (s, 1H, -N**H**$_2$, 8), 7.49 (dd, J = 7.9, 4.8 Hz, 1H, C_{Ar}**H**, 1), 2.34 (s, 5H, -C**H**$_3$, 2).

Thermogravimetric analysis (TGA)

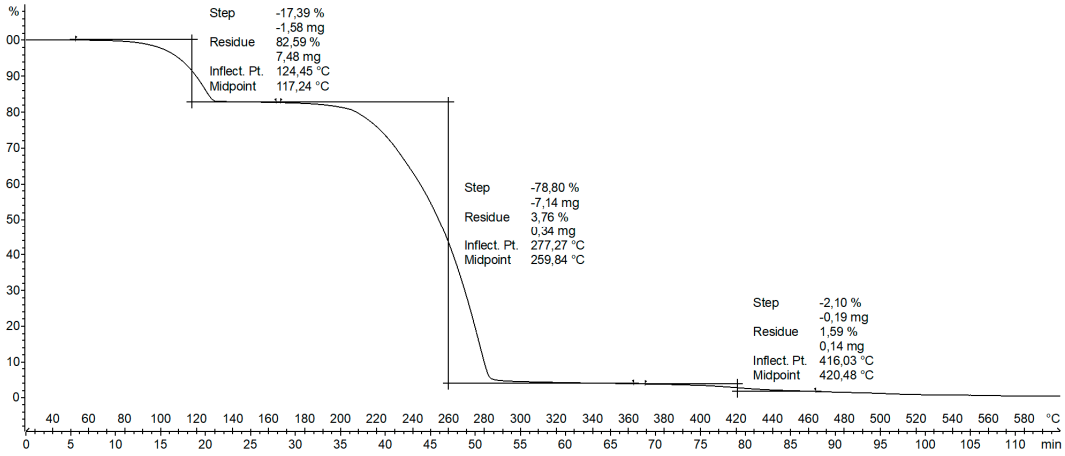

Figure S9: Thermogravimetric analysis of 4-Nitrobenzamide-Pyruvic acid 1:1 cocrystal obtained by slurry (1:1) in acetonitrile (initial sample mass: 9.06 mg), expressed in weight loss % as a function of temperature (°C) and time (min).

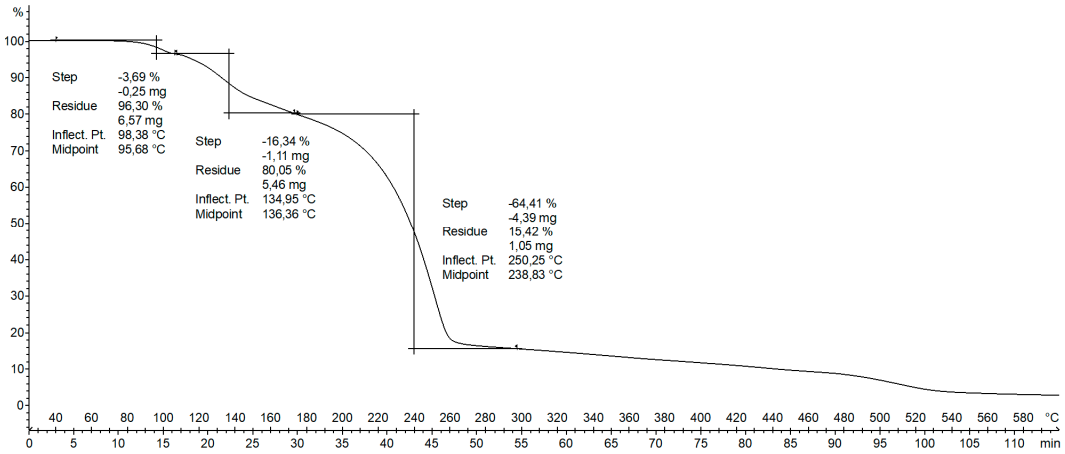

Figure S10: Thermogravimetric analysis of Carbamazepine-Pyruvic acid 1:1 cocrystal obtained by slurry (1:4) in acetonitrile (initial sample mass: 6.82 mg), expressed in weight loss % as a function of temperature (°C) and time (min).

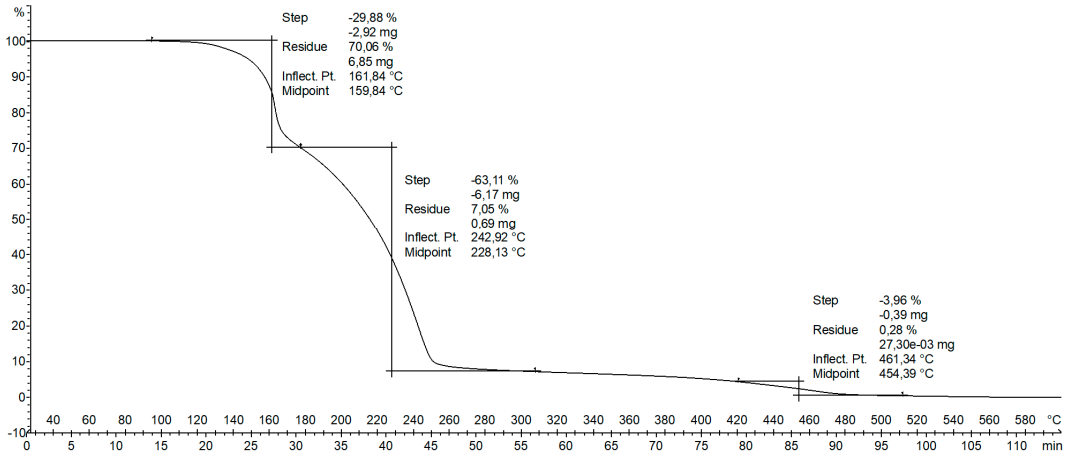

Figure S11: Thermogravimetric analysis of Isonicotinamide-Pyruvic acid 1:1 salt obtained by slurry (1:1) in acetonitrile (initial sample mass: 9.78 mg), expressed in weight loss % as a function of temperature (°C) and time (min).

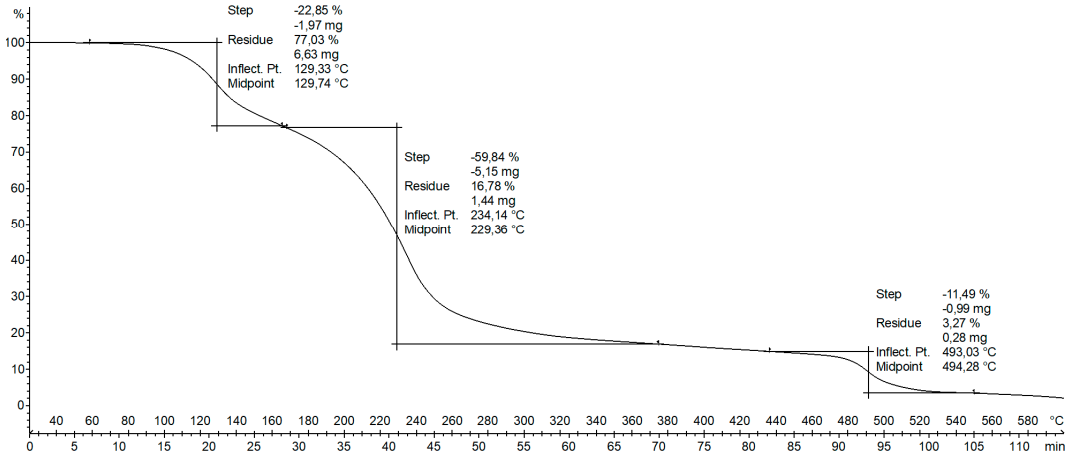

Figure S12: Thermogravimetric analysis of Nicotinamide-Pyruvic acid 2:3 salt cocrystal obtained by slurry (1:1) in ethyl acetate (initial sample mass: 8.61 mg), expressed in weight loss % as a function of temperature (°C) and time (min).

Differential Scanning Calorimetry (DSC) Analysis

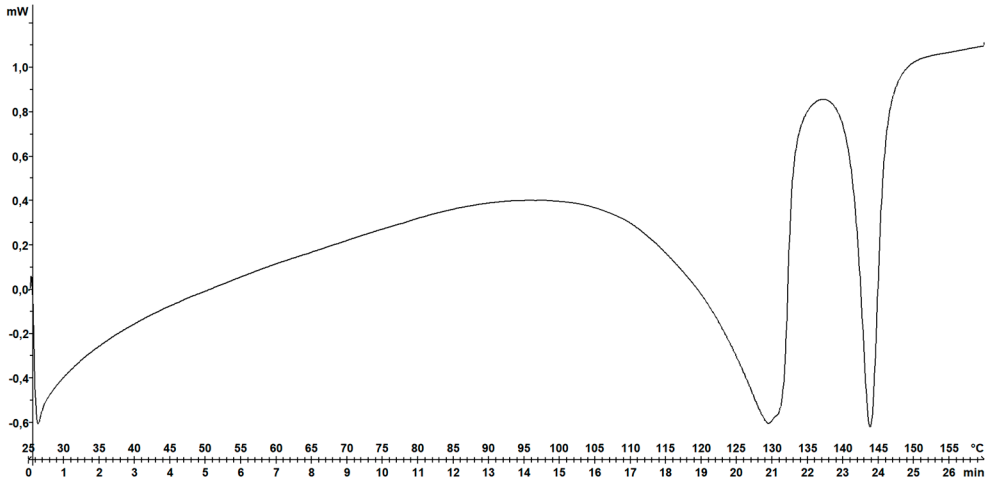

Figure S13: DSC analysis of the 4-Nitrobenzamide-Pyruvic acid 1:1 cocrystal obtained by slurry (1:1) in ethyl acetate, expressed in mW as a function of temperature (°C) and time (min).

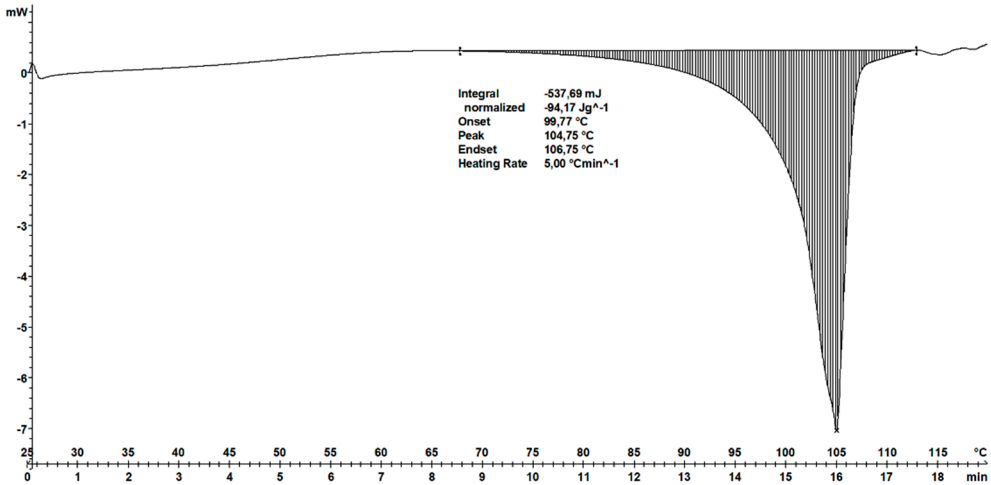

Figure S14: DSC analysis of the Carbamazepine-Pyruvic acid 1:1 cocrystal obtained by slurry (1:4) in ethyl acetate, expressed in mW as a function of temperature (°C) and time (min).

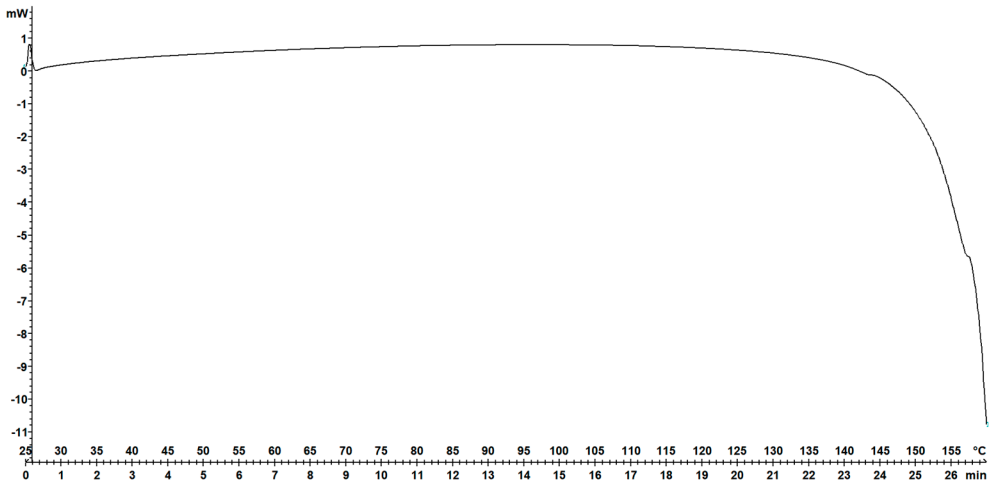

Figure S15: DSC analysis of the Isonicotinamide-Pyruvic acid 1:1 salt obtained by slurry (1:1) in acetonitrile, expressed in mW as a function of temperature (°C) and time (min).

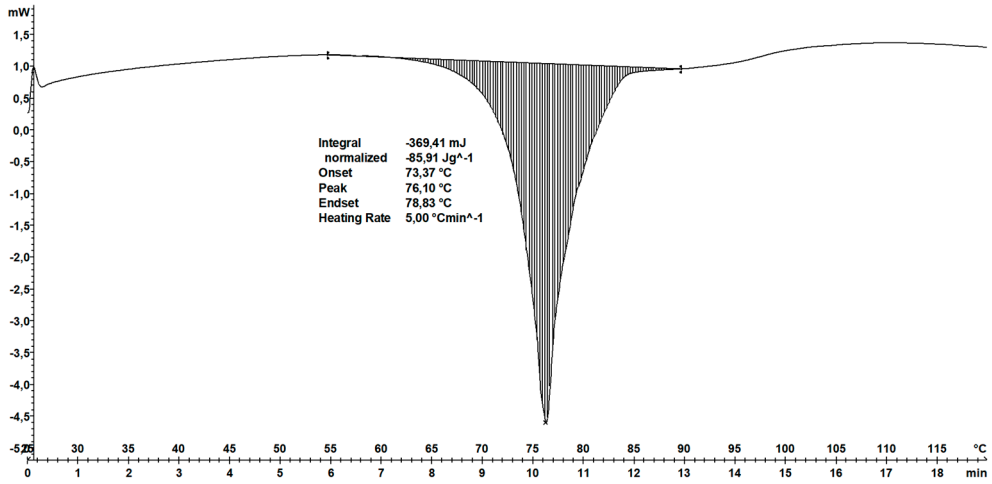

Figure S16: DSC analysis of the Nicotinamide-Pyruvic acid 2:3 salt cocrystal obtained by slurry (1:1) in ethyl acetate, expressed in mW as a function of temperature (°C) and time (min).

Example of combination of TGA and DSC Analysis

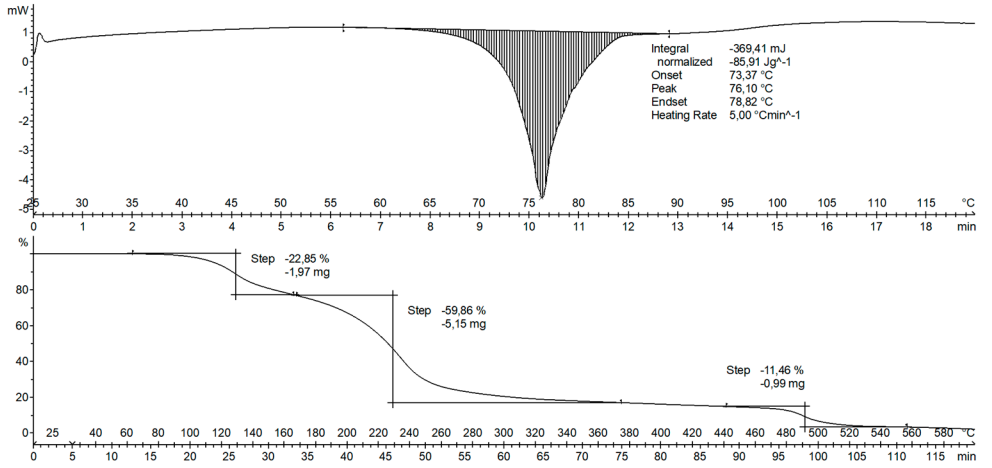

Figure S17: Combination of DSC analysis (expressed in mW as a function of temperature (°C) and time (min)) and TGA analysis (initial sample mass: 8.61 mg, expressed in weight loss % as a function of temperature (°C) and time (min)) of the Nicotinamide-Pyruvic acid 2:3 salt cocrystal obtained by slurry (1:1) in ethyl acetate.