

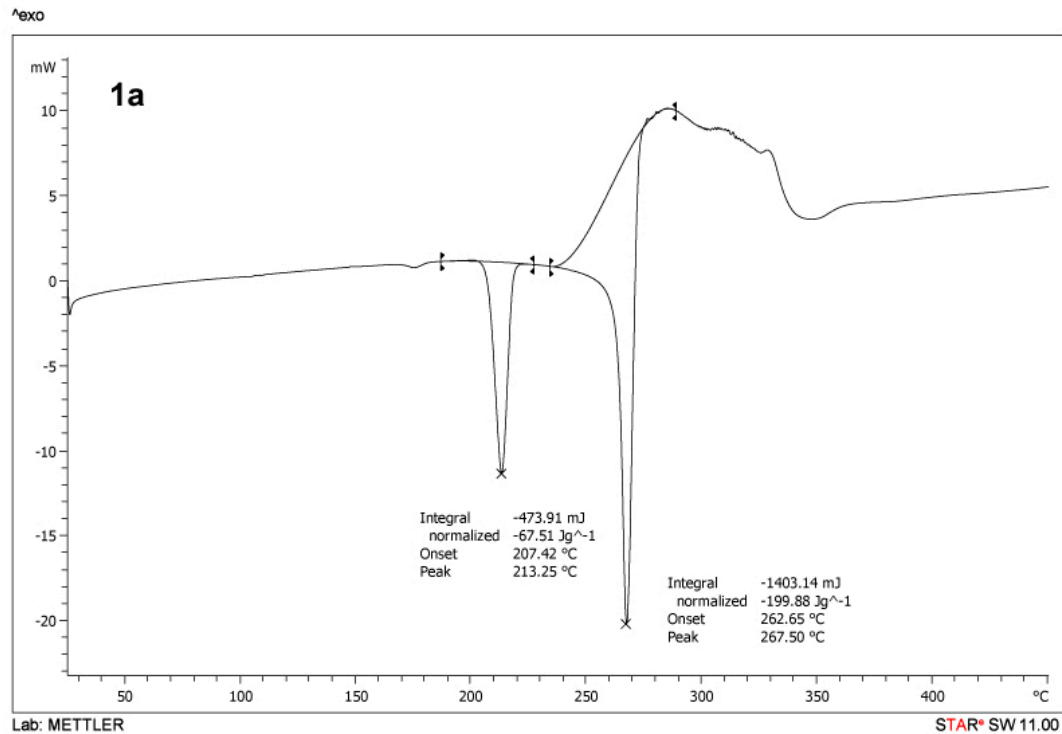
Table 1: Crystallographic data for the cocrystals **1a-1c**.

	1a	1b	1c
Formula	C ₁₃ H ₉ N: 2(C ₄ H ₃ F N ₂ O ₂)	C ₁₂ H ₈ N ₂ : 2(C ₄ H ₃ F N ₂ O ₂)	C ₁₂ H ₁₀ N ₂ : 4(C ₄ H ₃ F N ₂ O ₂)
Formula Wt.	439.38	440.37	702.56
Crystal habit	Blocks	Rectangular Blocks	Blocks
Crystal color	Yellow	Yellow	Yellow
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	6.794 (2)	5.803 (2)	5.913 (1)
<i>b</i> (Å)	7.229 (2)	7.626 (2)	22.137 (5)
<i>c</i> (Å)	9.568 (3)	10.456 (3)	12.418 (3)
α (deg)	82.08 (2)	83.07 (2)	90.00
β (deg)	86.10 (2)	79.37 (2)	117.85 (2)
γ (deg)	85.92 (2)	89.93 (2)	90.00
<i>V</i> (Å ³)	463.46 (2)	451.38 (2)	1437.1(3)
<i>Z</i>	1	1	2
<i>D</i> _{calc} (g cm ⁻³)	1.574	1.620	1.624
<i>T</i> (K)	180(2)	180(2)	180(2)
λ (Mo-K α)	0.71073	0.71073	0.71073
μ (mm ⁻¹)	0.126	0.131	0.139
2 θ range (deg)	64.08	50.54	60.12
Limiting indices	-10 ≤ <i>h</i> ≤ 10 -10 ≤ <i>k</i> ≤ 10 -14 ≤ <i>l</i> ≤ 14	-6 ≤ <i>h</i> ≤ 6 -9 ≤ <i>k</i> ≤ 9 -10 ≤ <i>l</i> ≤ 12	-8 ≤ <i>h</i> ≤ 8 -31 ≤ <i>k</i> ≤ 29 -17 ≤ <i>l</i> ≤ 17
<i>F</i> (000)	226	226	720
No. of Reflns. Measured	9294	4505	15157
No. Unique Reflns.	3206	1628	4197
No. of Reflns. Used	2604	1442	2907
No. of Parameters	146	145	226
GOF on <i>F</i> ²	1.047	1.072	1.061
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.0442	0.0344	0.0486
<i>wR</i> ₂	0.1194	0.0975	0.1208
Final diff. Fourier map (e ⁻ ·Å ⁻³) max, min	0.281, -0.276	0.218, -0.245	0.253, -0.251

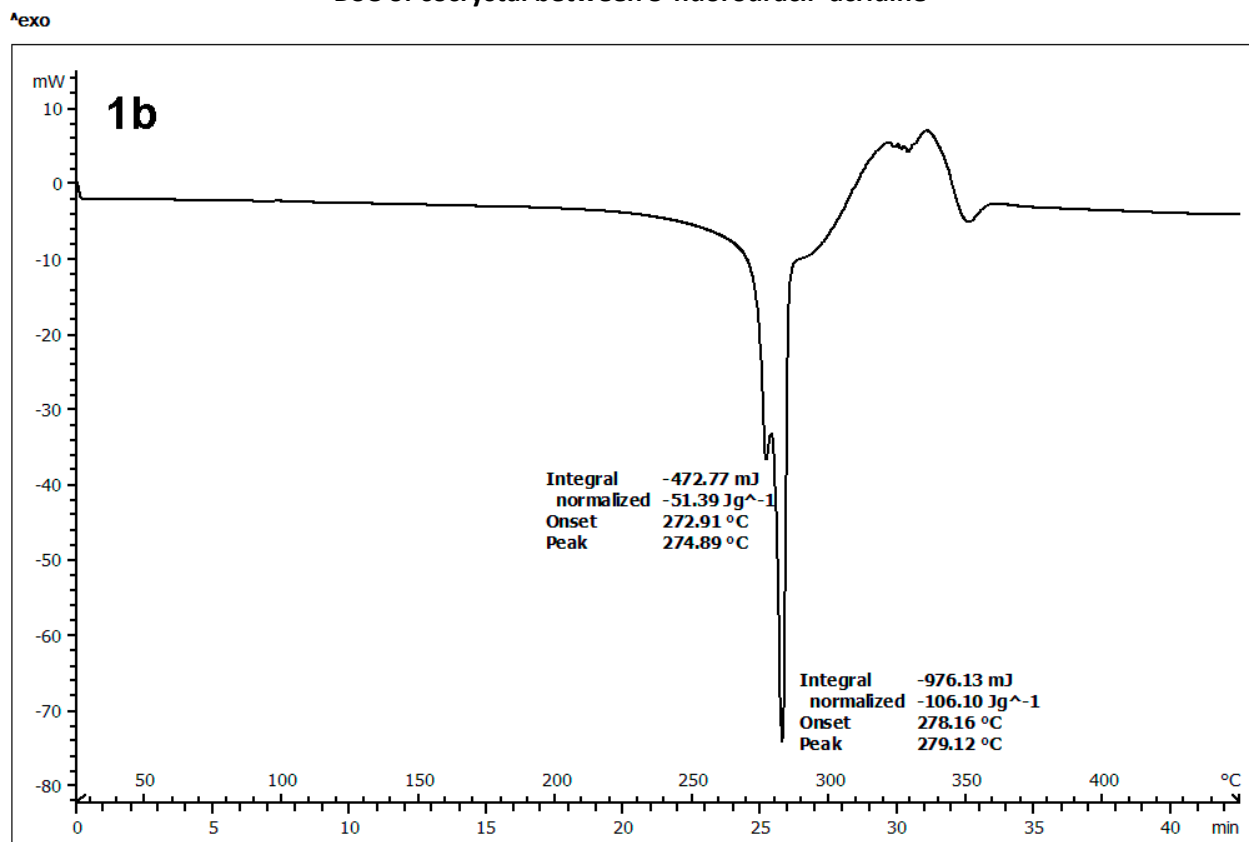
Table 2: Bond length and angles of the hydrogen bonds observed in the cocrystals **1a-1c**.

Hydrogen Bond, D-H...A	1a			1b			1c		
N-H...N							2.00	2.86	164
N-H...O	1.90	2.77	172	1.91	2.78	171	1.88	2.76	175
	2.03	2.86	157	1.97	2.84	167	2.04	2.89	163
							2.12	2.99	170
C-H...N	2.92	3.78	152	2.60	3.52	163			
C-H...O	2.48	3.38	157	2.45	3.39	172	2.22	3.01	140
	2.84	3.51	129				2.41	3.23	144
							2.42	3.19	137
							2.42	3.24	145
							2.60	3.30	131
C-H...F	2.50	3.45	176	2.41	3.32	160	2.64	3.50	150
	2.72	3.33	123	2.53	3.26	134			

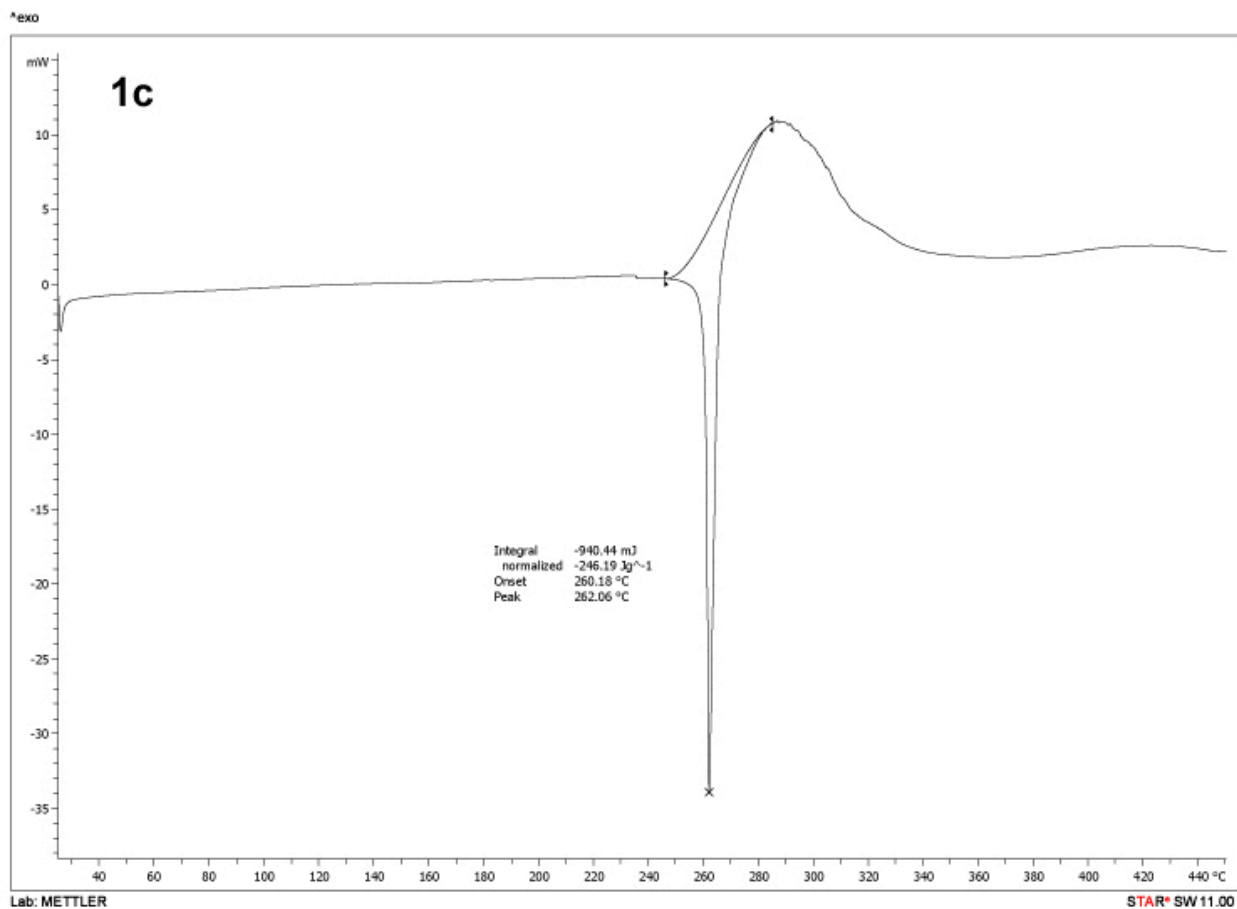
DSC:



DSC of cocrystal between 5-fluorouracil+acridine

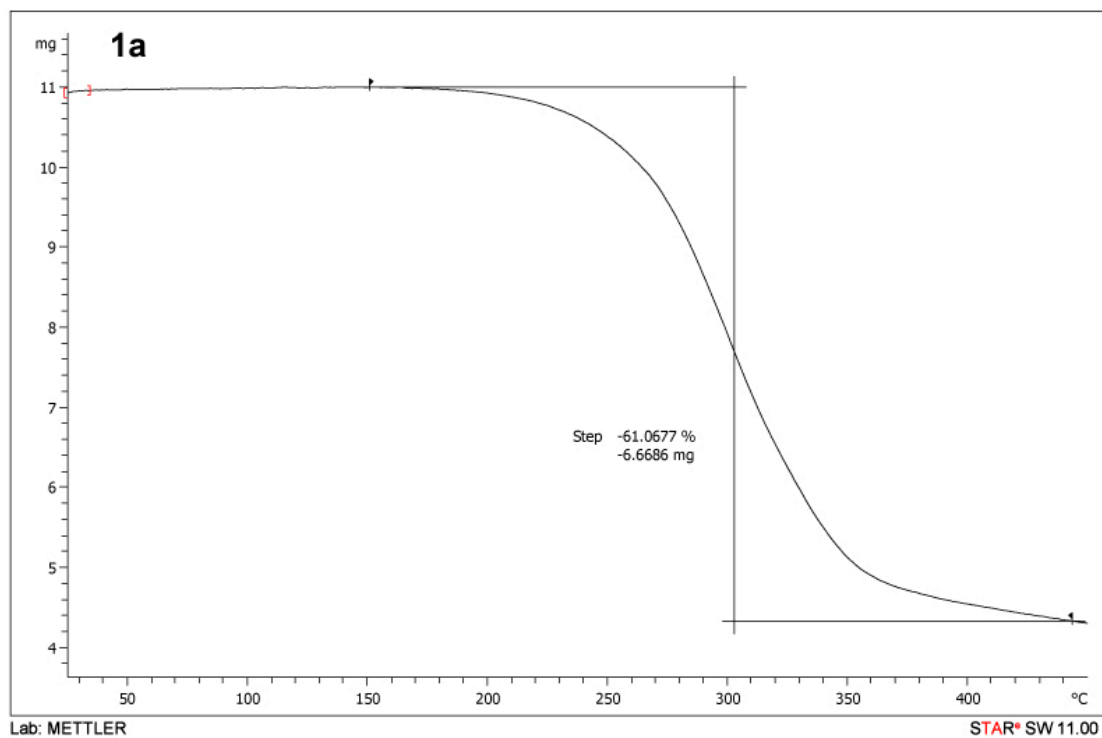


DSC of cocrystal between 5-fluorouracil+phenazine

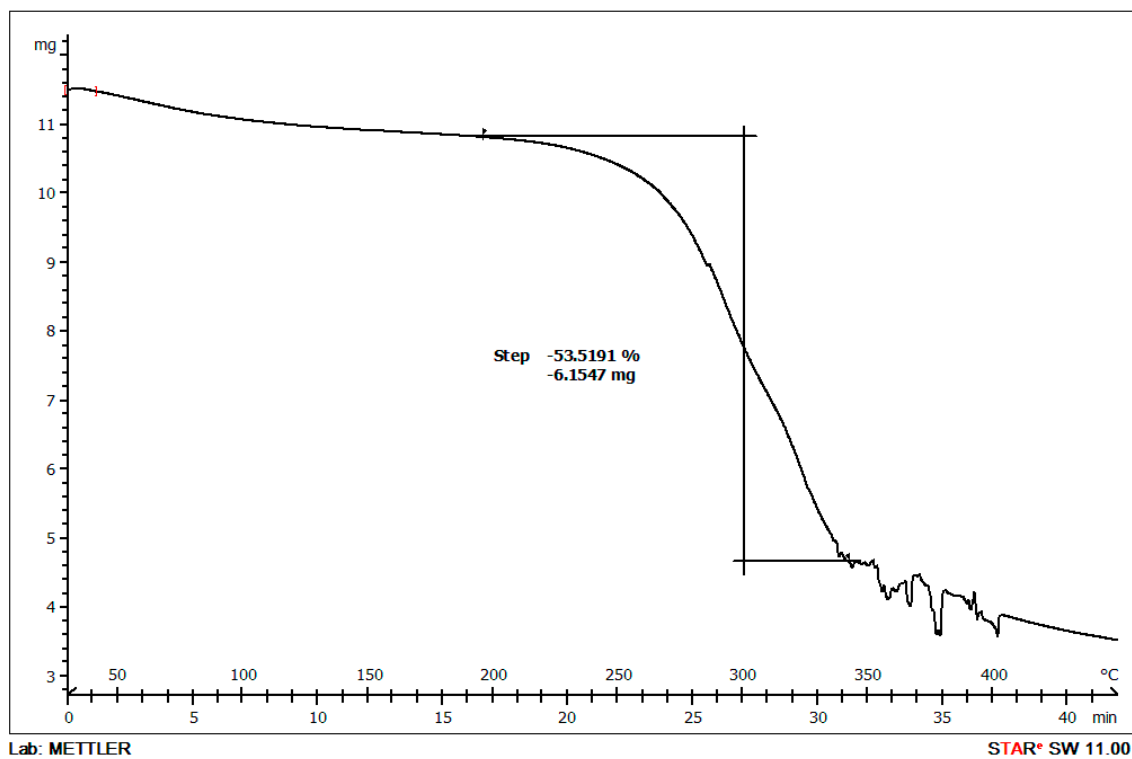


DSC of cocrystal between 5-fluorouracil+4,4-bispyridylethene

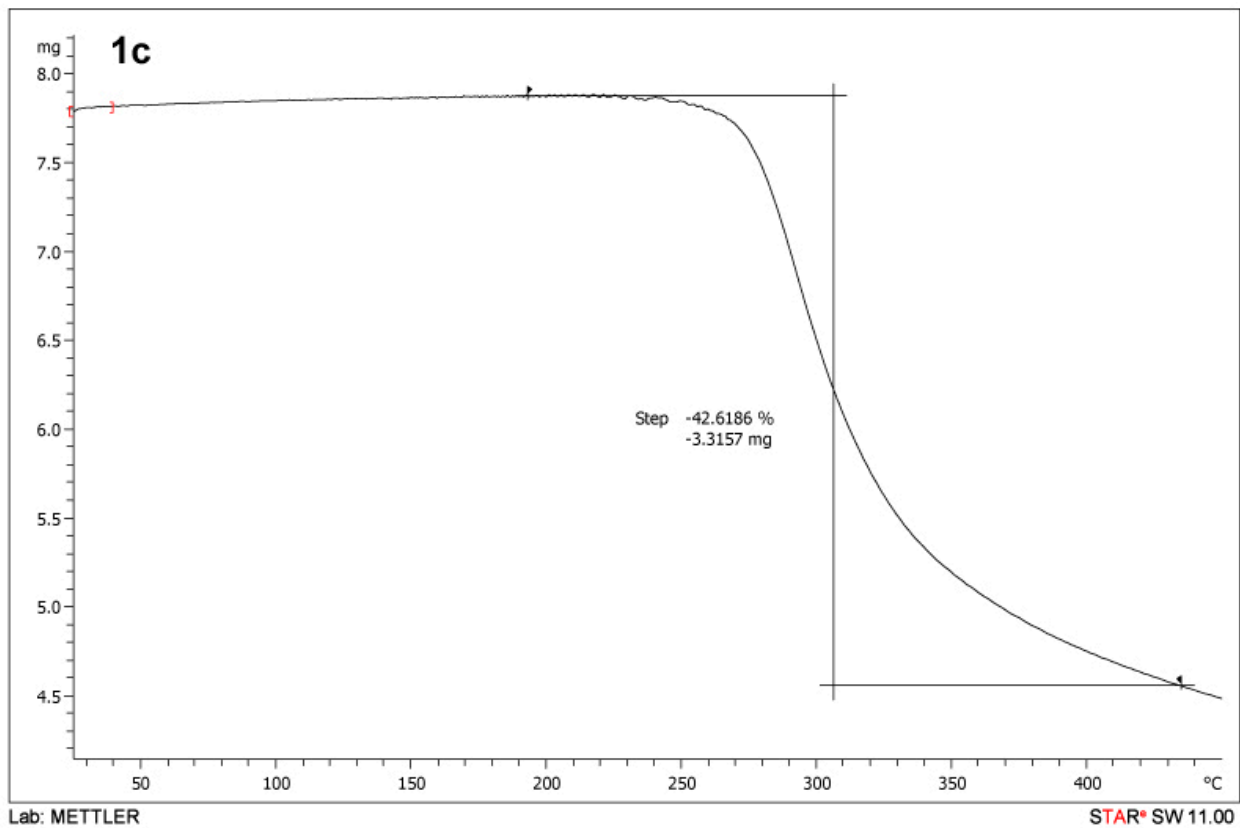
TGA:



TGA of cocrystal between 5-fluorouracil+acridine



TGA of cocrystal between 5-fluorouracil+ phenazine



TGA of cocrystal between 5-fluorouracil+4,4'- bispyridylethene

TEM details

Transmission electron microscopy characterization was performed at room temperature on a Philips CM30 instrument operating at 300 kV. Images and diffraction patterns were typically recorded using a magnification of 3,900x and camera length of 650 mm respectively. Data were collected on photographic films which were scanned in order to generate digital images. Samples were supported on holey-carbon films on 300 mesh copper grids held within a double tilt sample holder. The diffraction patterns were indexed by comparison with crystal structures held in the Cambridge Structural Database (CSD). The positions of reflections in experimental diffraction patterns were measured, converted to d-spacings and matched to calculated values for these CSD structures. The experimental diffraction patterns were then compared with simulated diffraction patterns of the appropriate zone axes to ensure a match. The simulations were carried out using CrystalMaker SingleCrystal v2.1.3 software which performs a rapid, kinematic calculation of the diffraction pattern.