Supplementary Information for

Structural and physicochemical aspects of hydrochlorothiazide co-crystals

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Table S1 Hydrogen bonding distances and angles for **1-4**

	D−H···A	H···A (Å)	D···A (Å)	∠D−H···A (°)	Symmetry code
1	N_2−H_2···O_3	2.26	2.911(8)	141	-x+1/2, -y+1, z-1/2
	N_6−H_{6A}···N_5	2.20	2.922(7)	141	x-1, y, z
	N_3−H_3···O_5	2.31	3.092(7)	150	x-1/2, -y+1/2, -z+1
	N_3−H_4···O_5	2.32	3.092(7)	149	x, y, z
2	O_{1S}−H_{1S}···N_4	2.00	2.825(4)	166	-x+1/2, y-1/2, -z+1/2
	O_{1S}−H_{2S}···N_5	2.03	2.847(4)	175	-x, -y, -z
	N_1−H_1···O_{1S}	1.96	2.815(4)	166	x, y, z
	N_3−H_4···O_{1S}	2.27	3.026(4)	162	x+1/2, -y+1/2, z-1/2
	N_3−H_3···N_6	2.17	2.933(41)	154	x-1/2, -y+1/2, z-1/2
3	N_1−H_1···N_5	1.83	2.836(6)	172	x-1, y, z-1
	N_3−H_4···N_4	2.15	2.993(8)	169	-x+1, -y, z
	N_2−H_2···O_2	2.36	3.077(5)	141	x, -y+1/2, z-1/2
4	N_1−H_1···N_4	2.39	2.868(8)	115	x-1, y, z
	N_3−H_3···N_5	2.38	3.169(13)	164	x, y, z
	N_3−H_4···N_6	2.10	2.991(12)	177	x-1, y-1, z-1
	$N_{1'}$−$H_{1'}$···N_7	2.43	2.866(9)	112	x, y+1, z
	$N_{3'}$−$H_{3'}$···N_8	2.15	2.950(12)	156	x, y, z

Table S2 Solubility and IDR of HCT, **1**–**4**, and the corresponding co-formers in pH = 2.0 phosphate buffer.

Solid form	Equilibrium solubility (mg/mL)	IDR (μg/min/cm^2)
HCT	0.59	47
pyrazinamide	0.59	
4,4'-bipyridine	25	
1,2-bis(4-pyridyl)ethane	9	
trans-1,2-bis(4-pyridyl)ethylene	19	
1	12	68
2	0.75	52
3	0.63	57
4	0.72	53

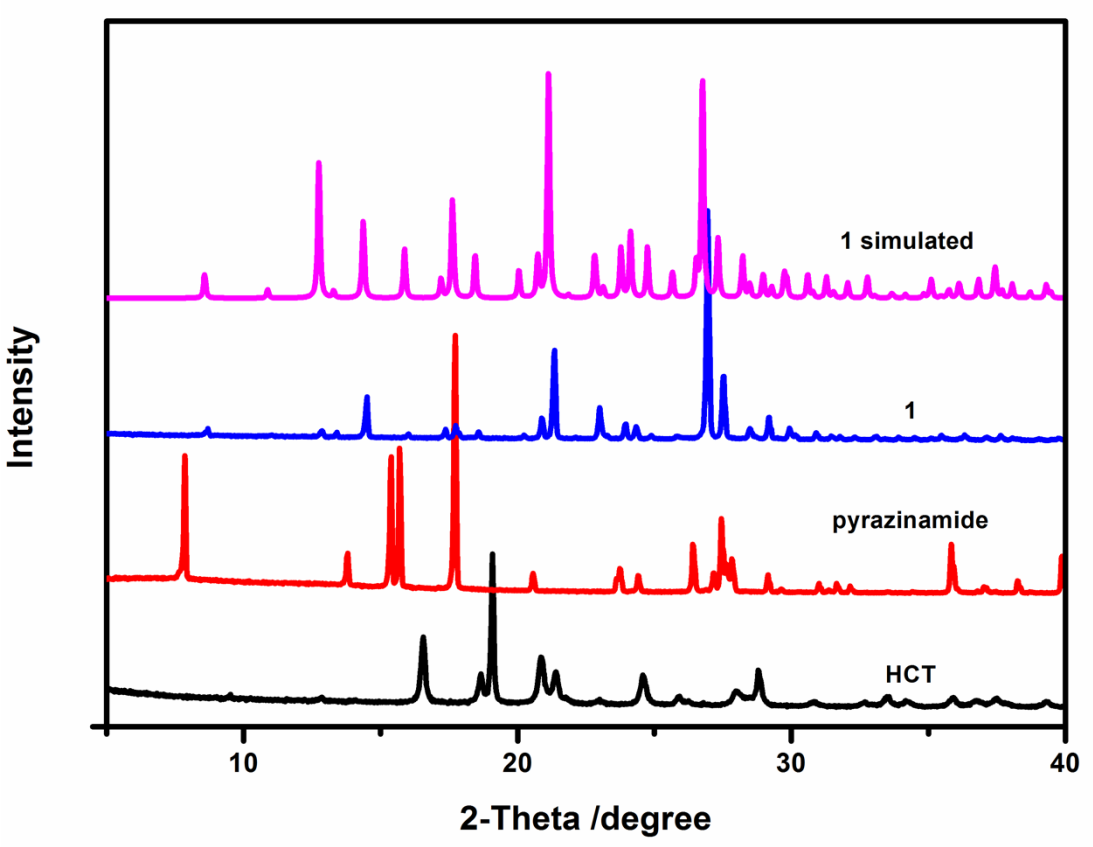

Figure S1 PXRD patterns of co-crystal **1**

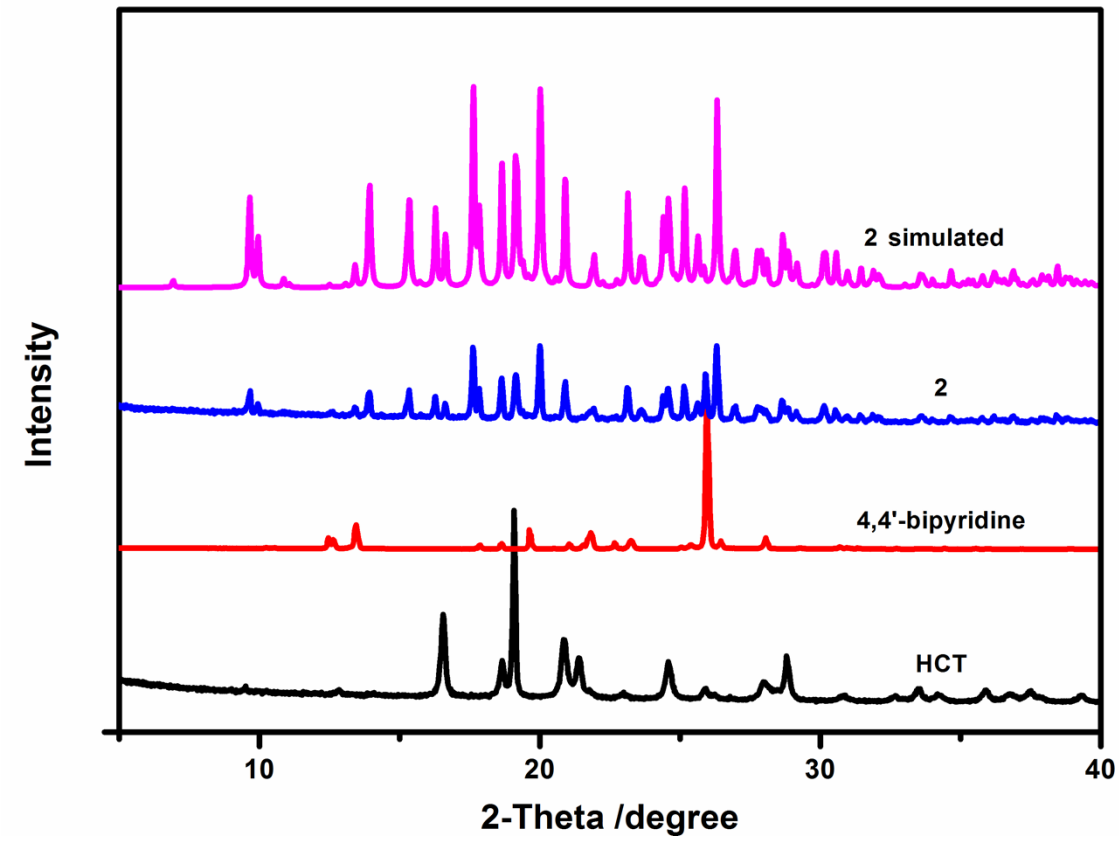

Figure S2 PXRD patterns of co-crystal **2**

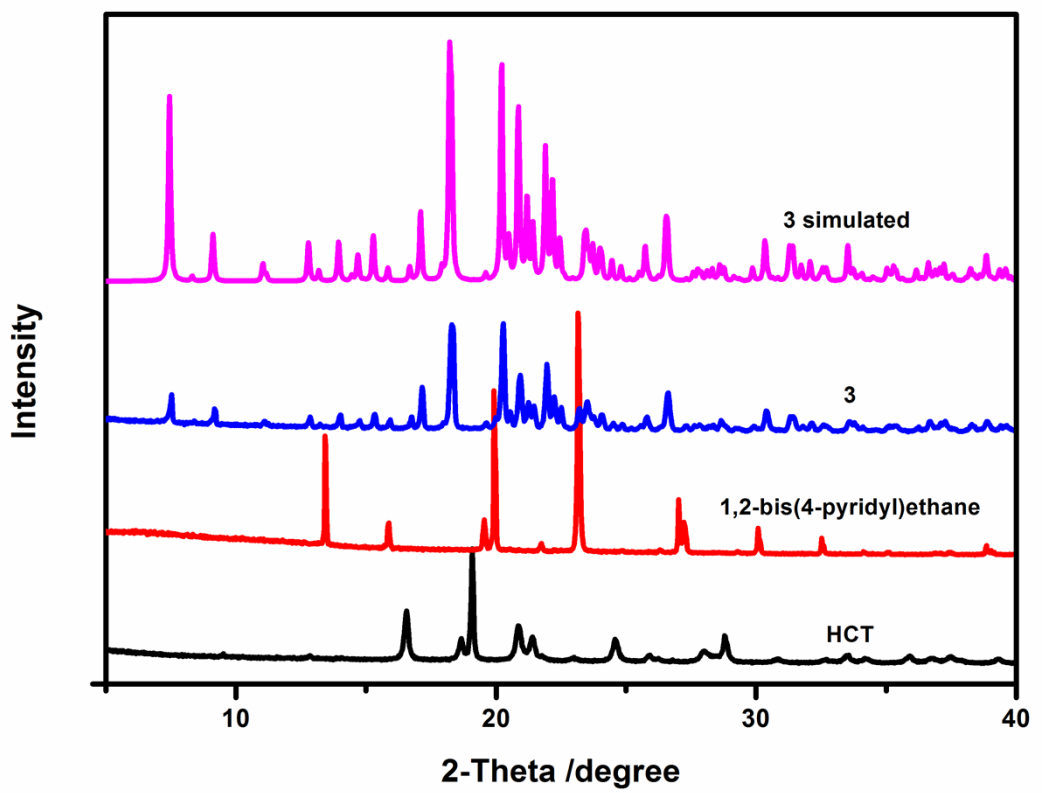

Figure S3 PXRD patterns of co-crystal **3**

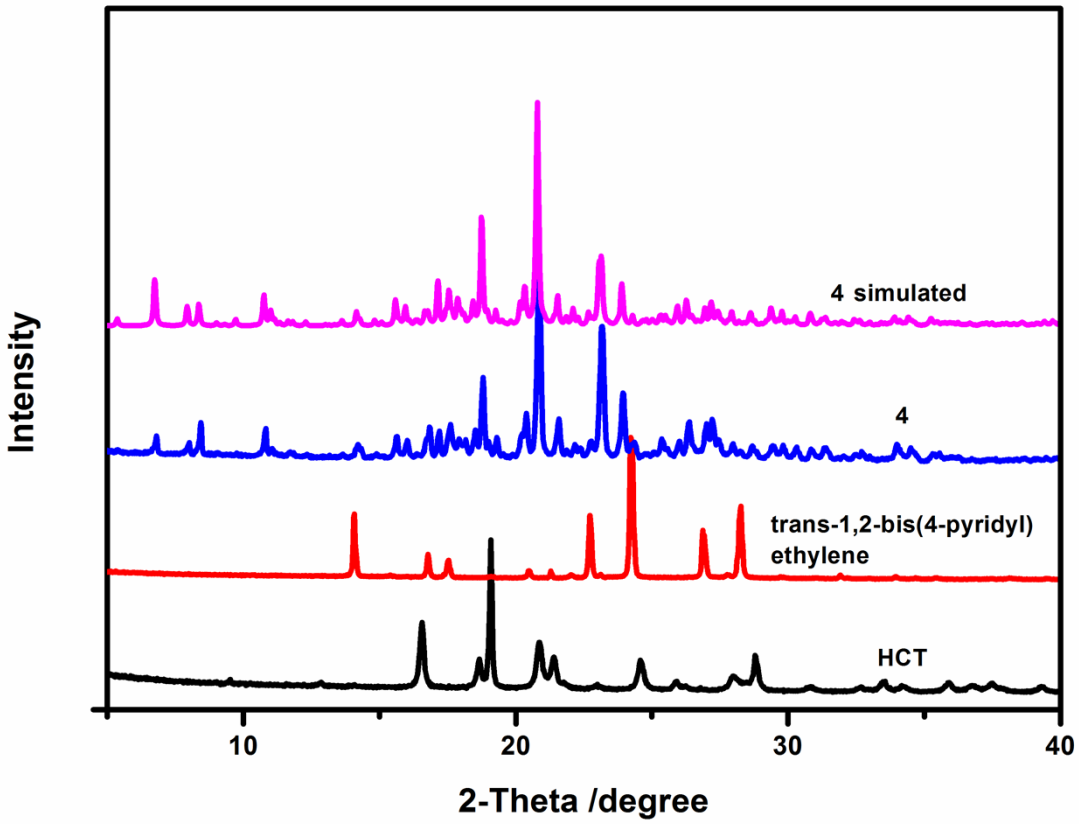

Figure S4 PXRD patterns of co-crystal **4**

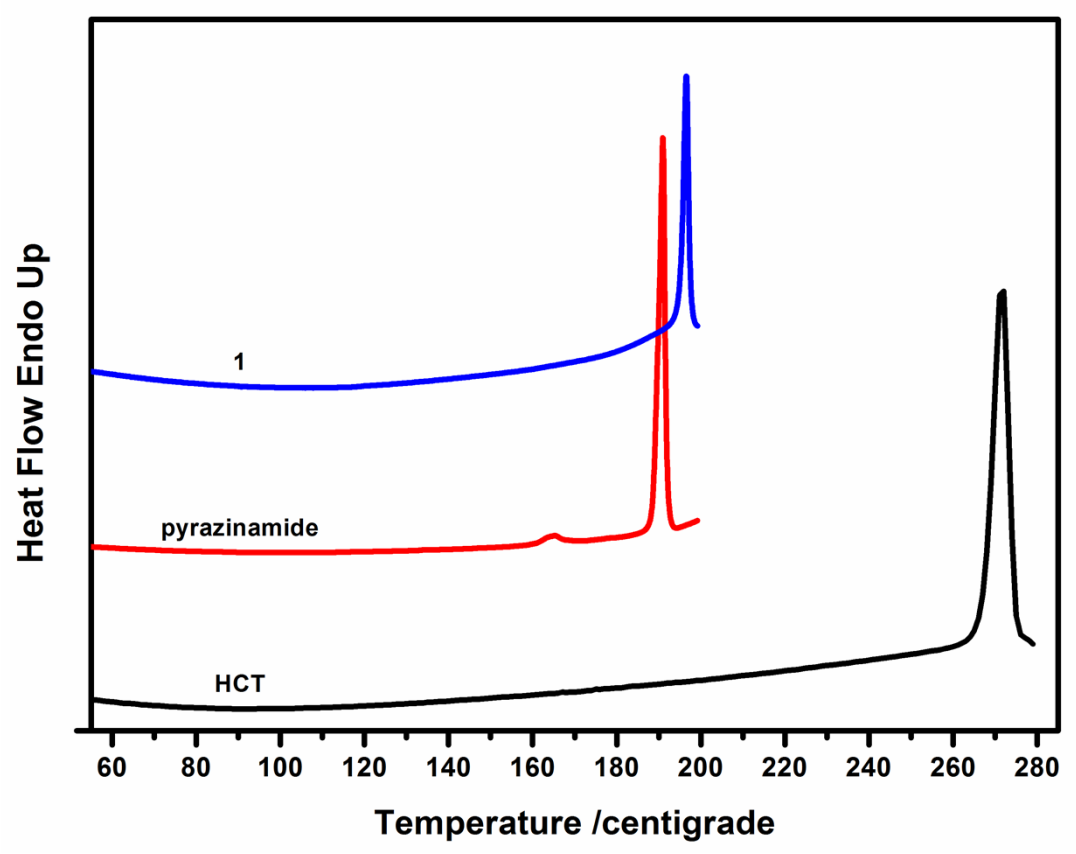

Figure S5 DSC patterns of co-crystal **1**

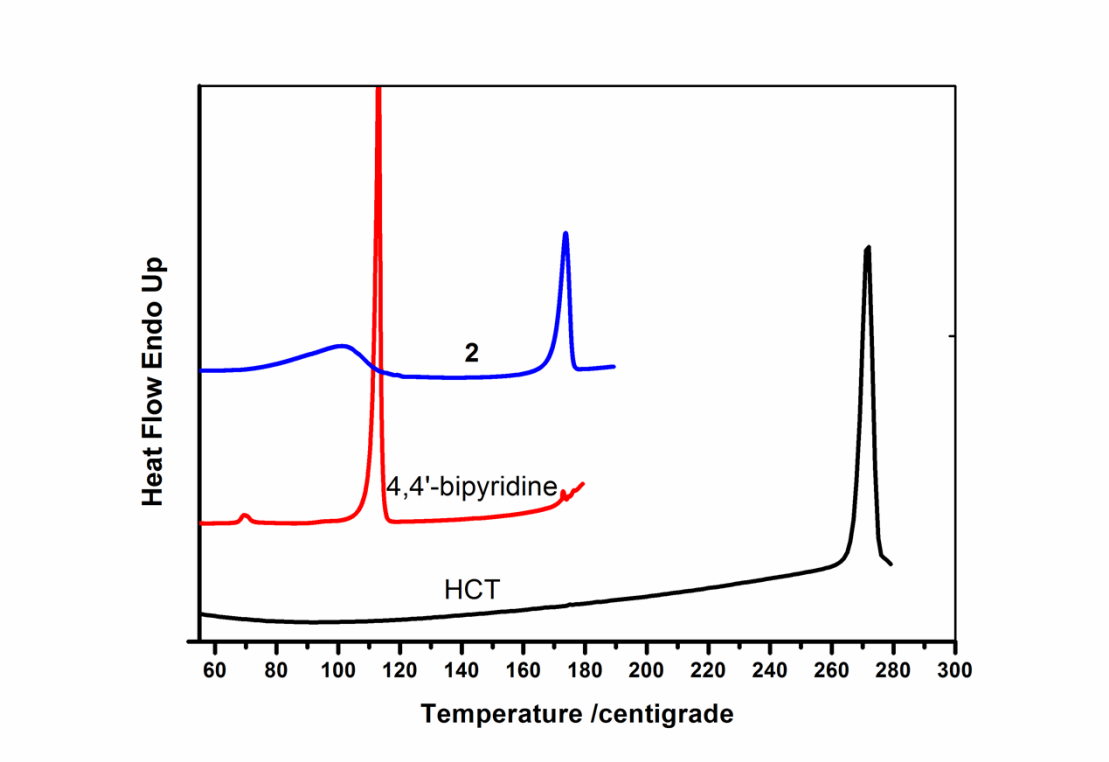

Figure S6 DSC patterns of co-crystal **2**

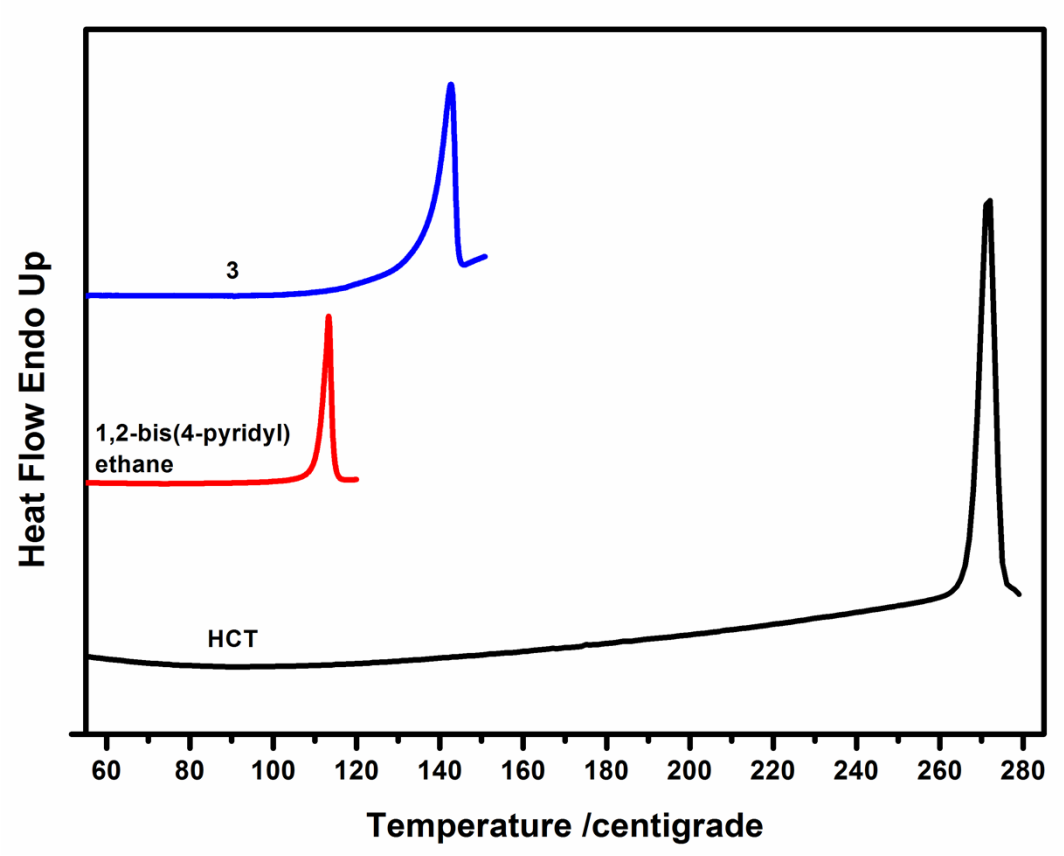

Figure S7 DSC patterns of co-crystal **3**

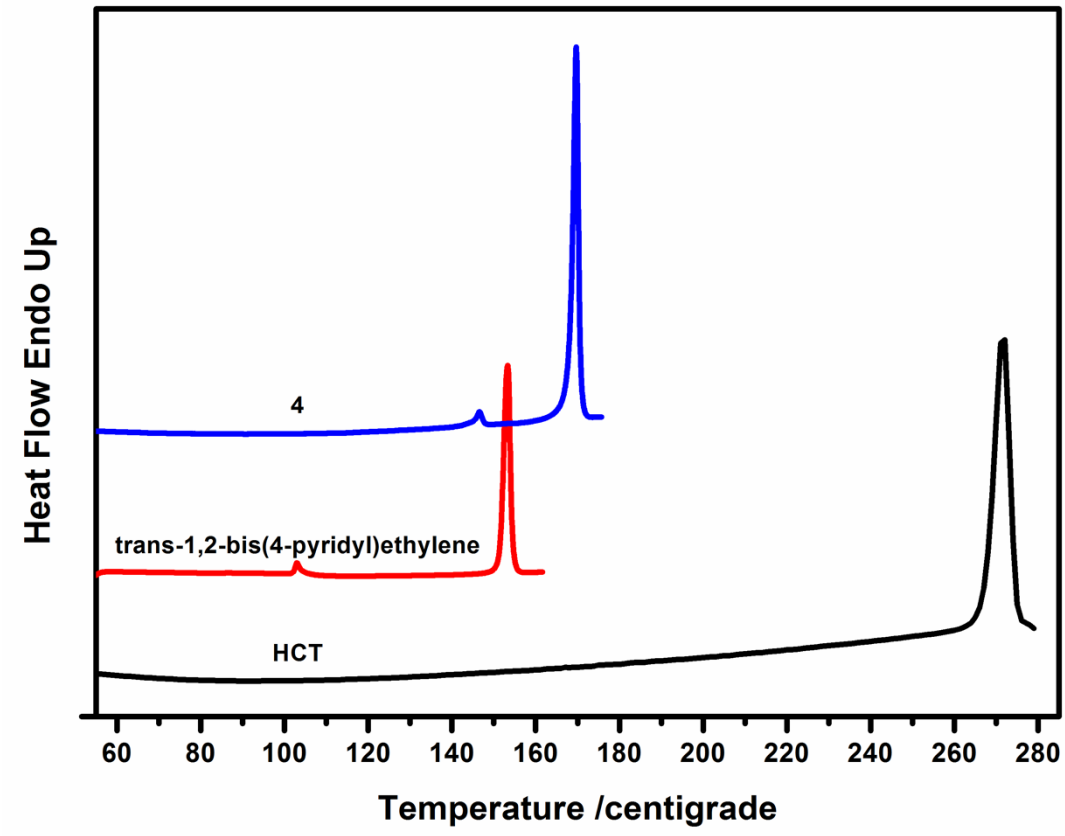

Figure S8 DSC patterns of co-crystal **4**

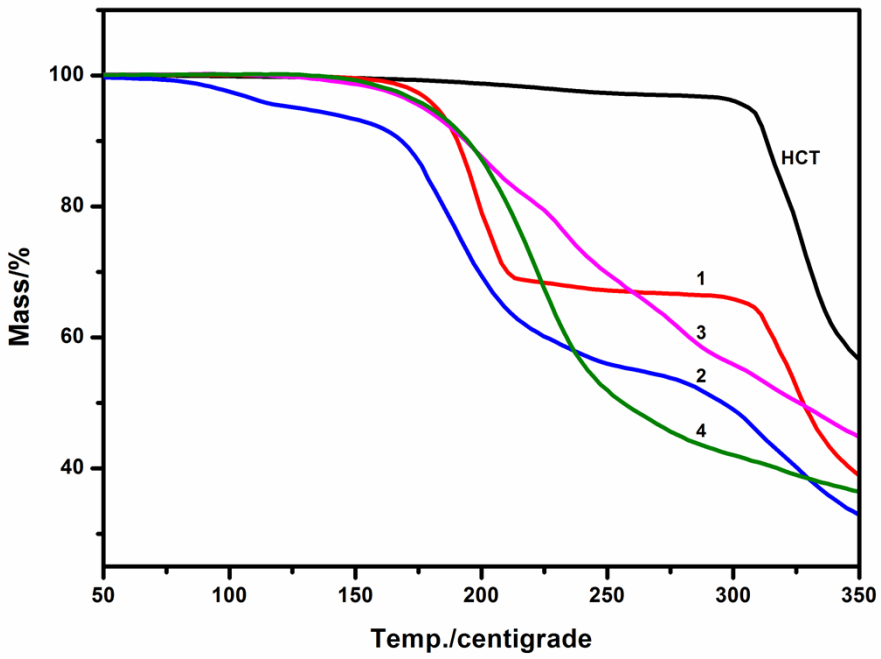

Figure S9 TGA patterns of HCT and co-crystals

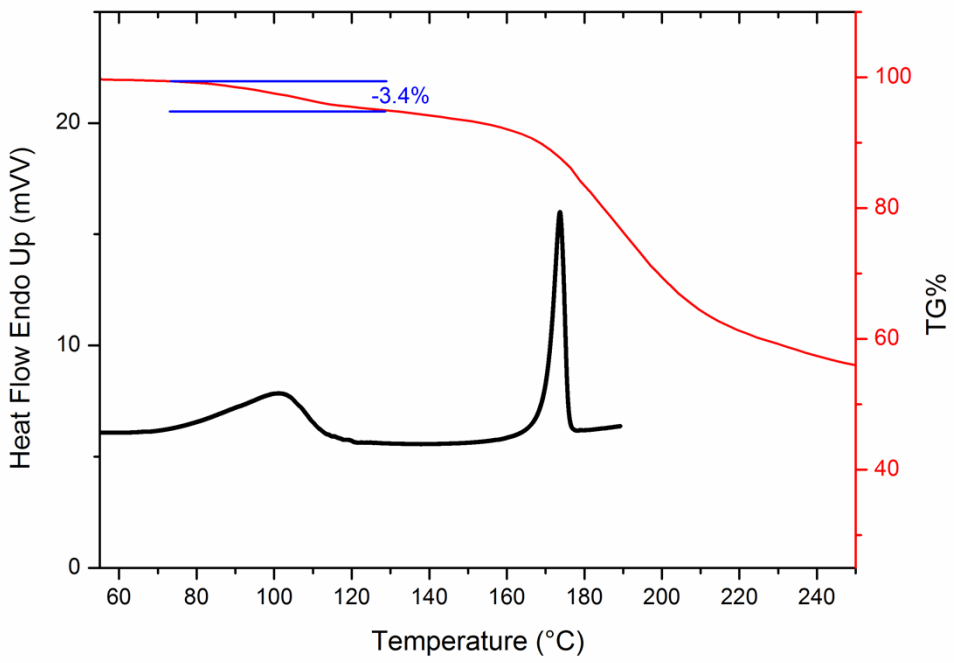

Figure S10 TGA compared with DSC of co-crystal **2**

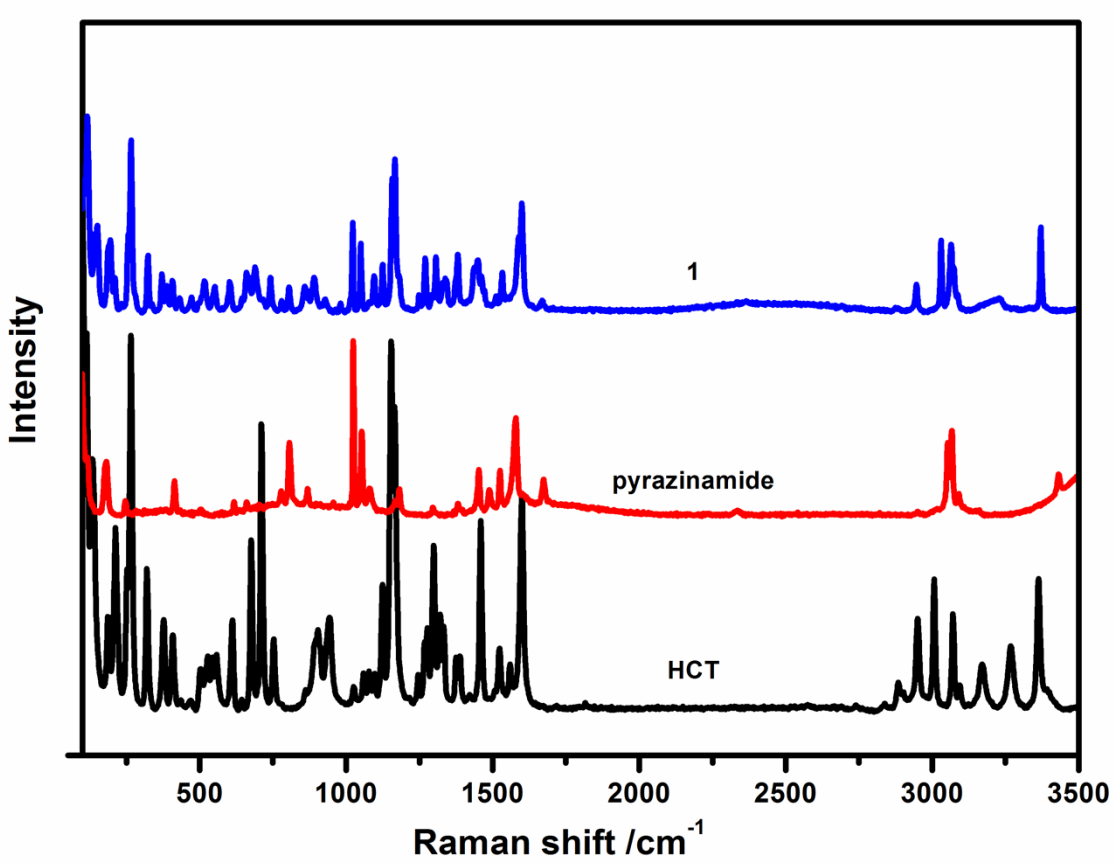

Figure S11 Raman spectroscopies of co-crystal **1**

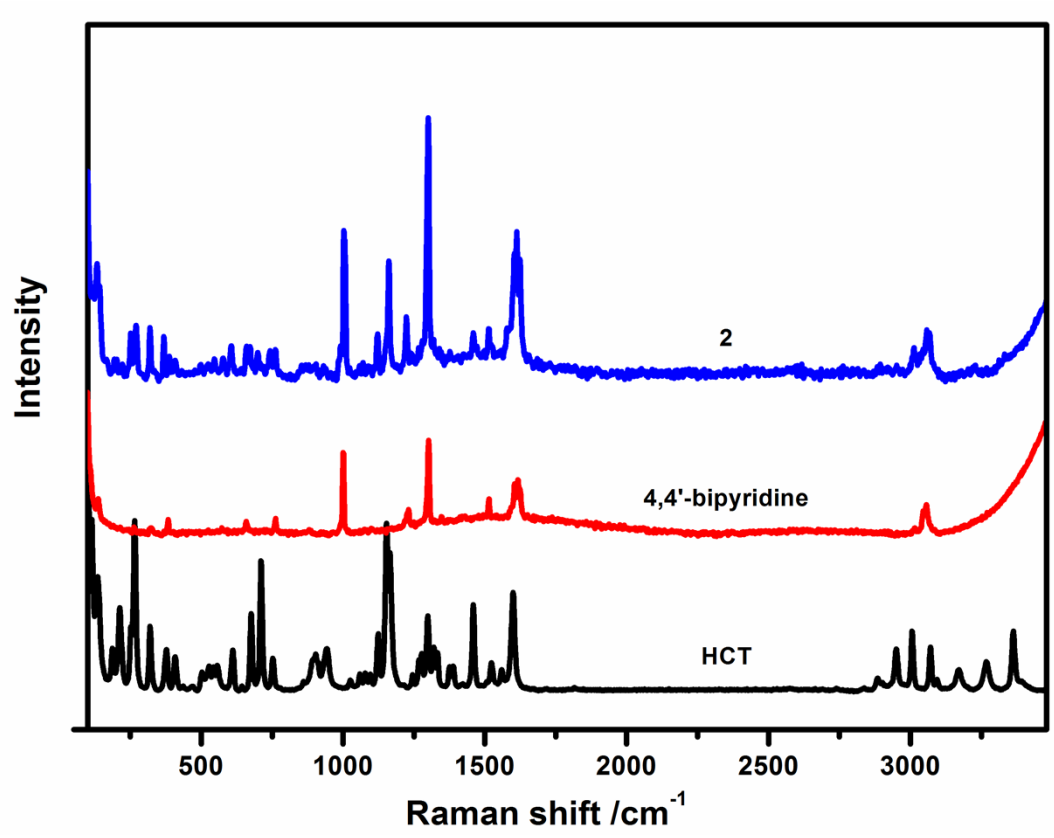

Figure S12 Raman spectroscopies of co-crystal **2**

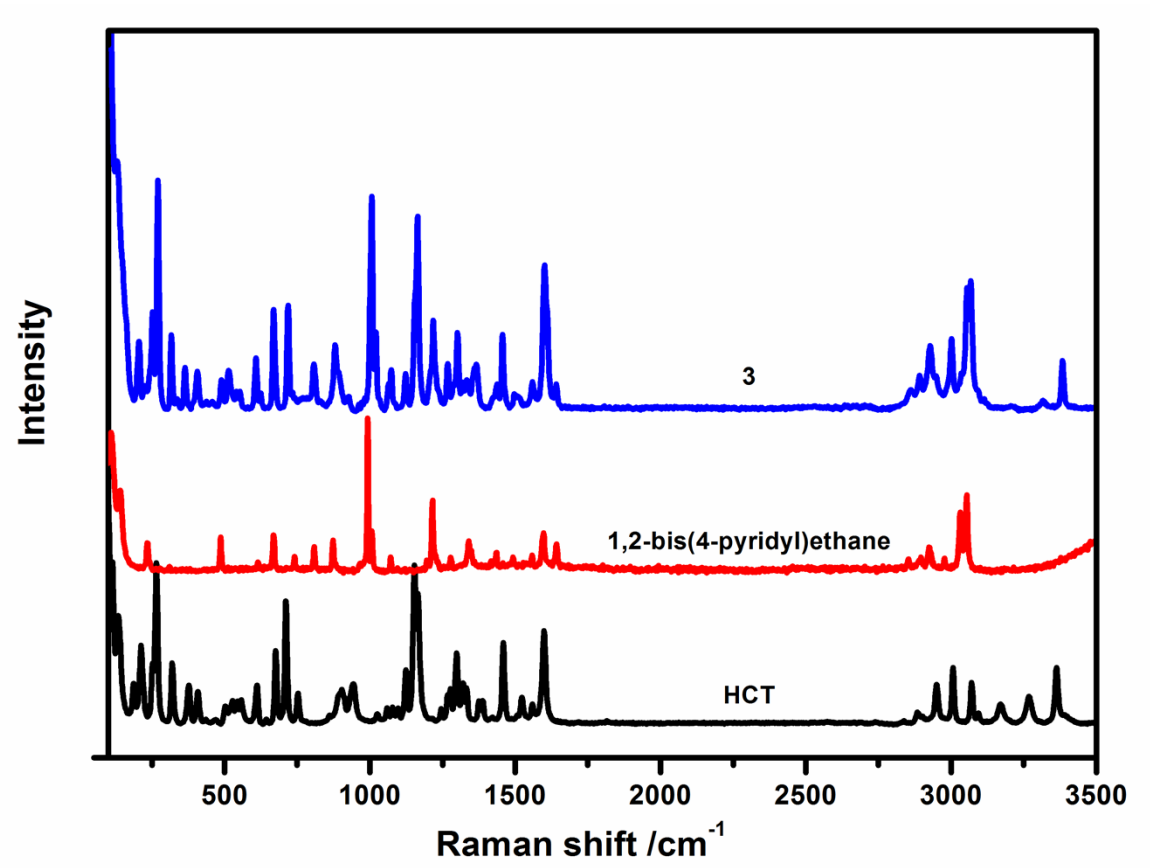

Figure S13 Raman spectroscopies of co-crystal **3**

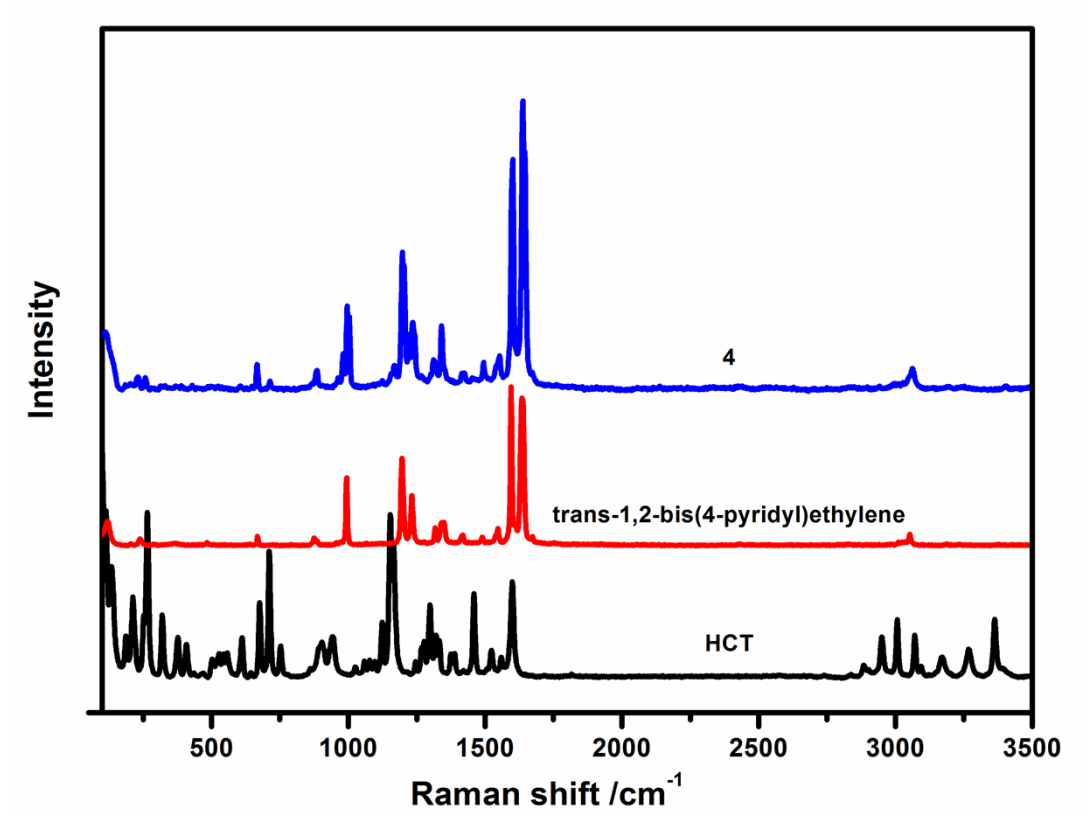

Figure S14 Raman spectroscopies of co-crystal **4**

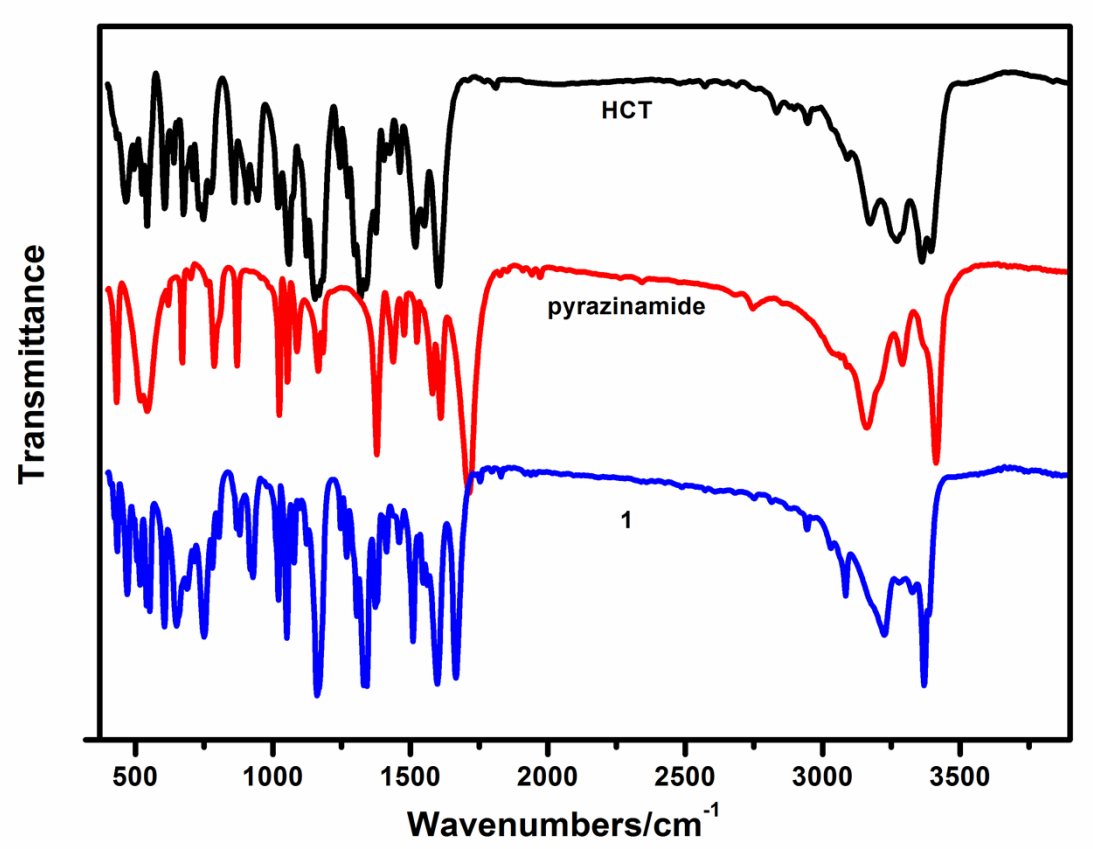

Figure S15 IR spectroscopies of co-crystal **1**

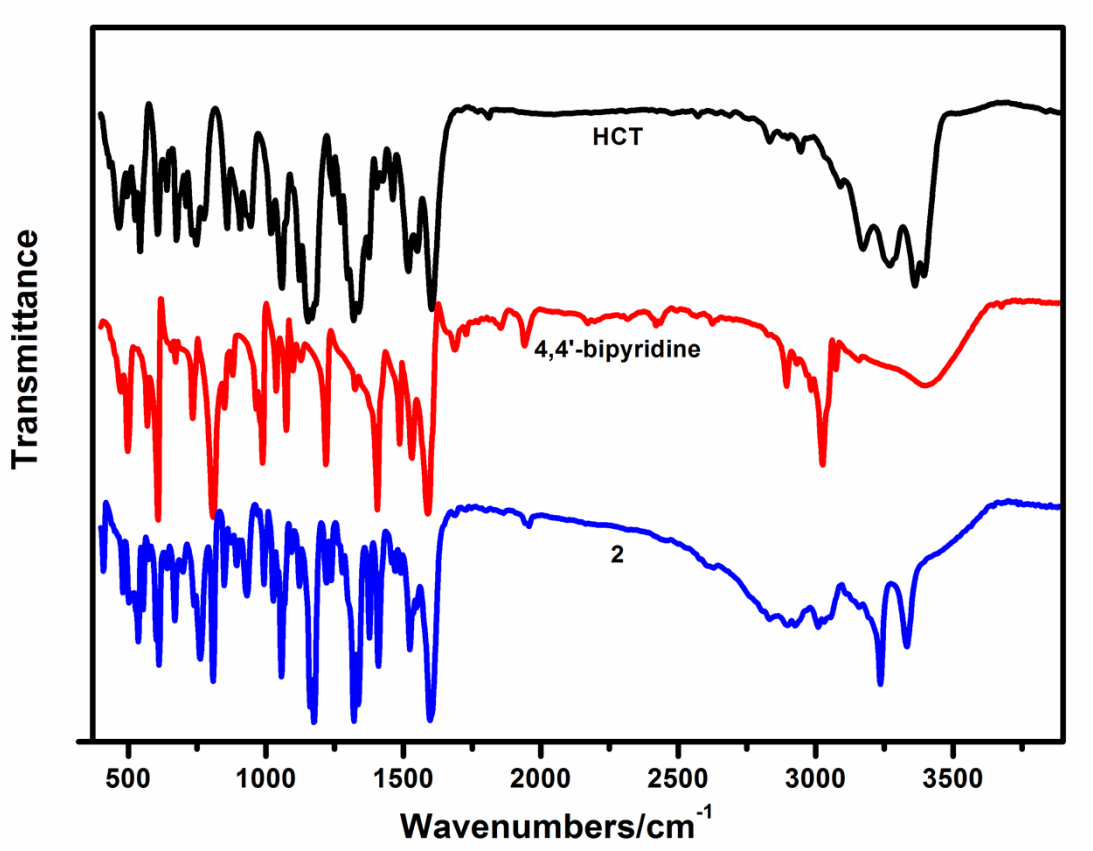

Figure S16 IR spectroscopies of co-crystal **2**

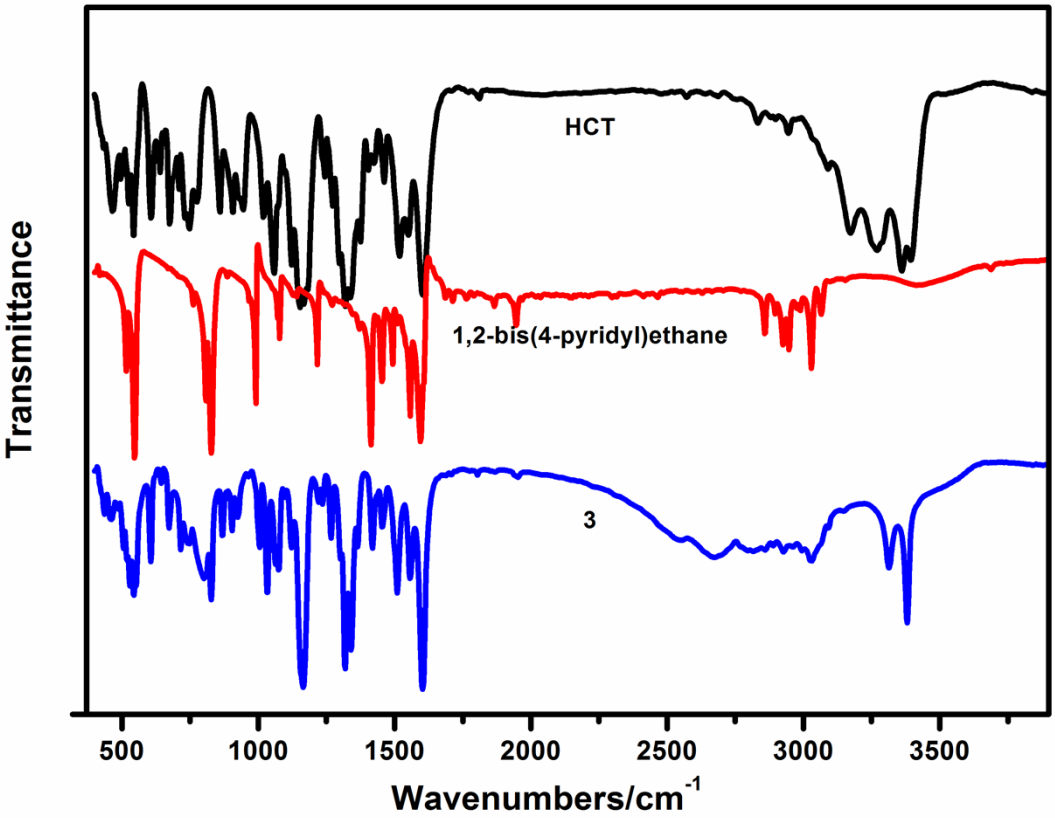

Figure S17 IR spectroscopies of co-crystal **3**

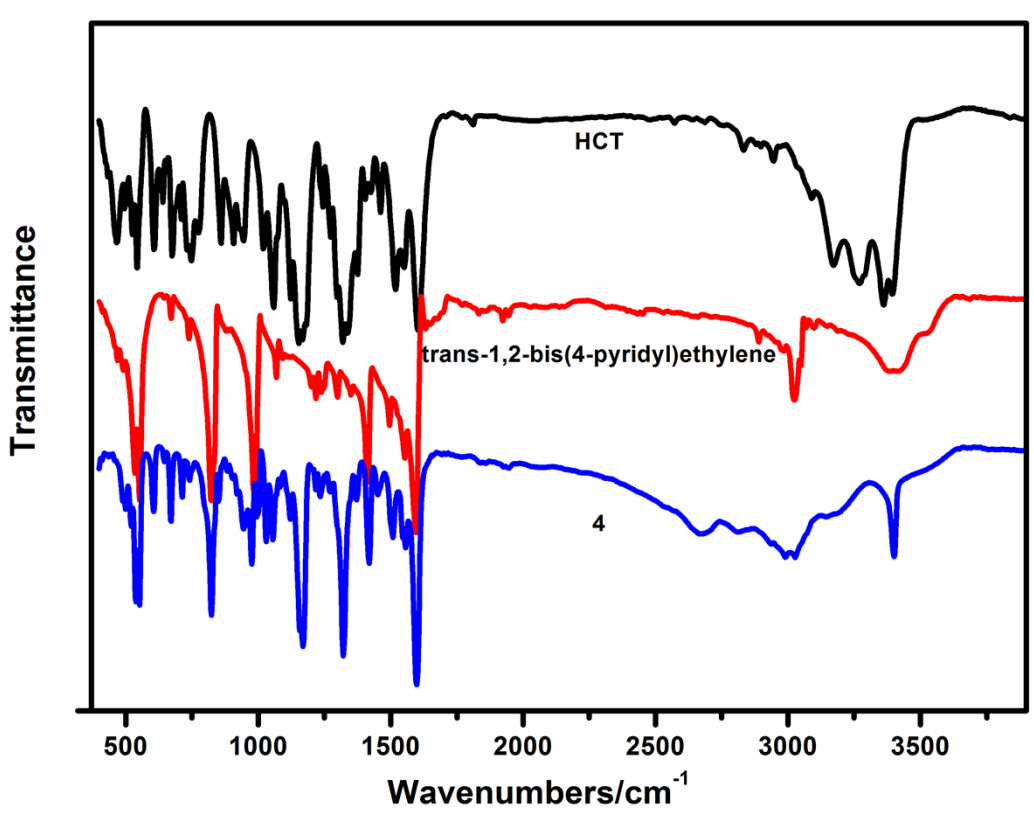

Figure S18 IR spectroscopies of co-crystal **4**

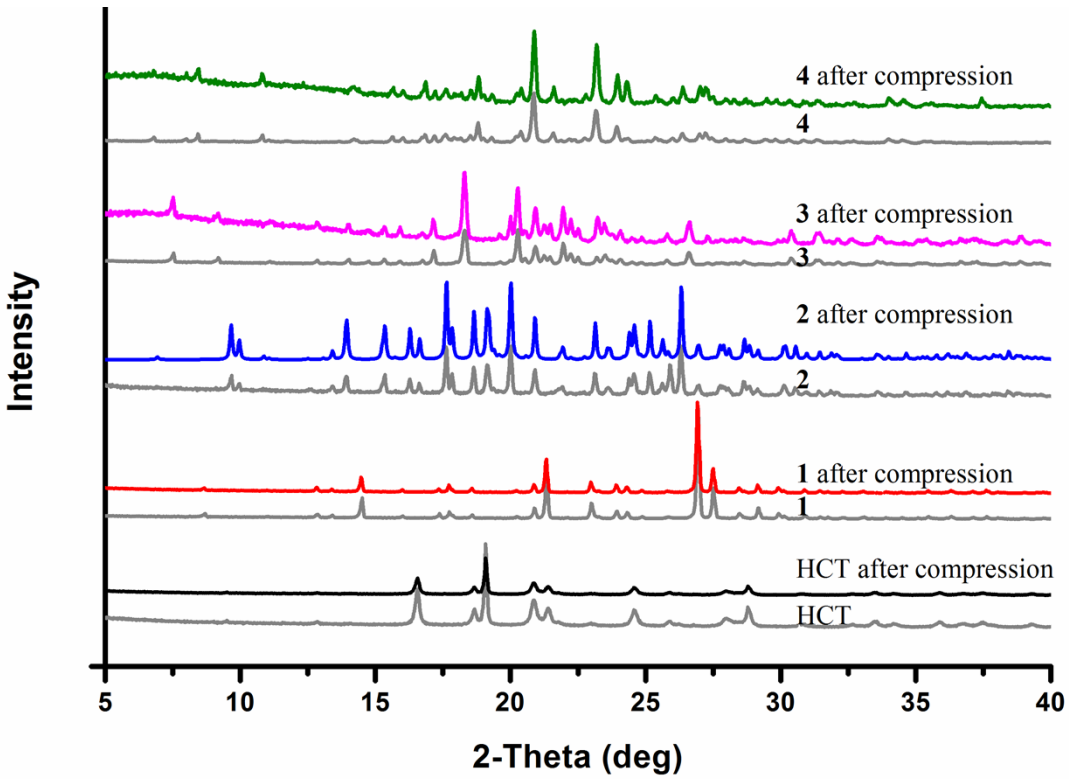

Figure S19 PXRD patterns of HCT and its co-crystals **1**−**4** after compression