

Supplementary Information for

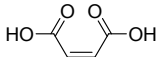
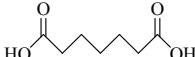
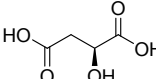
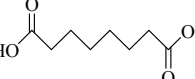
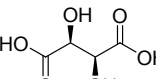
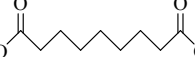
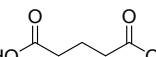
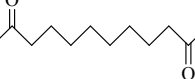
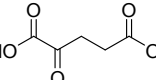
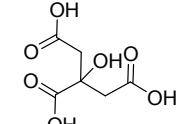
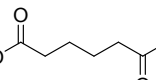
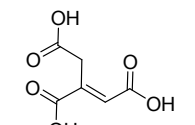
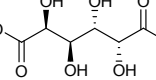
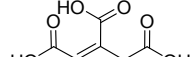
Pharmaceutical cocrystals of the anti-tuberculosis drug pyrazinamide with dicarboxylic and tricarboxylic acids†

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Table S1 Results of the screening experiments for the formation of cocrystals with PZA using dicarboxylic and tricarboxylic acids in MeOH, ethyl acetate (EA), and tetrahydrofuran (THF).

Cocrystal former	MeOH	EA	THF	Cocrystal former	MeOH	EA	THF
 maleic acid	X	X	X	 pimelic acid	X	X	X
 L-malic acid	X	X	X	 suberic acid	X	X	X
 L-tartaric acid	X	X	X	 azelaic acid	X	X	X
 glutaric acid	X	X	X	 sebacic acid	✓	✓	✓
 α -ketoglutaric acid	X	X	X	 citric acid	✓	✓	✓
 adipic acid	✓	✓	✓	 <i>trans</i> -aconitic acid	✓	✓	✓
 mucic acid	X	X	X	 <i>cis</i> -aconitic acid	X	X	X

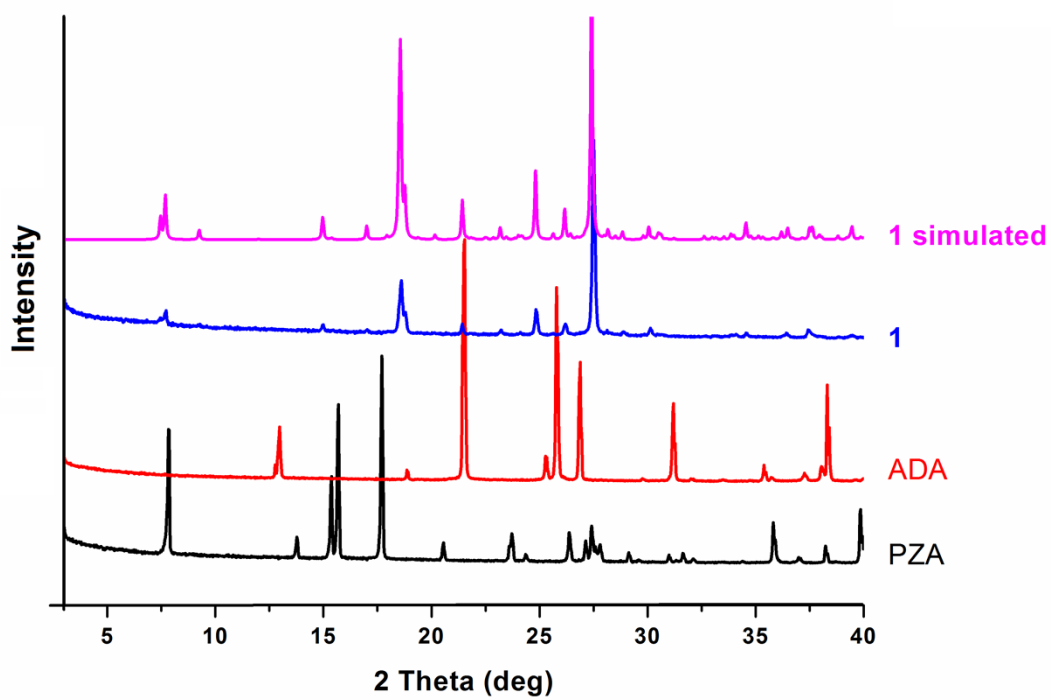


Fig. S1 PXR D patterns of cocystal 1

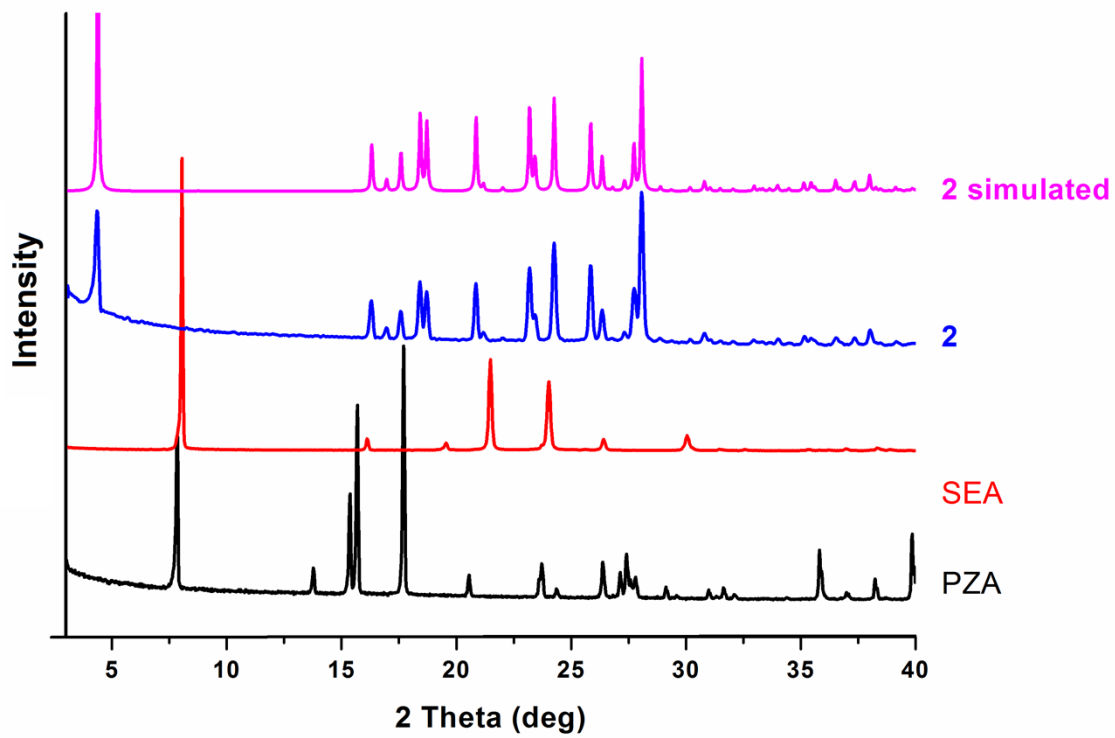


Fig. S2 PXR D patterns of cocystal 2

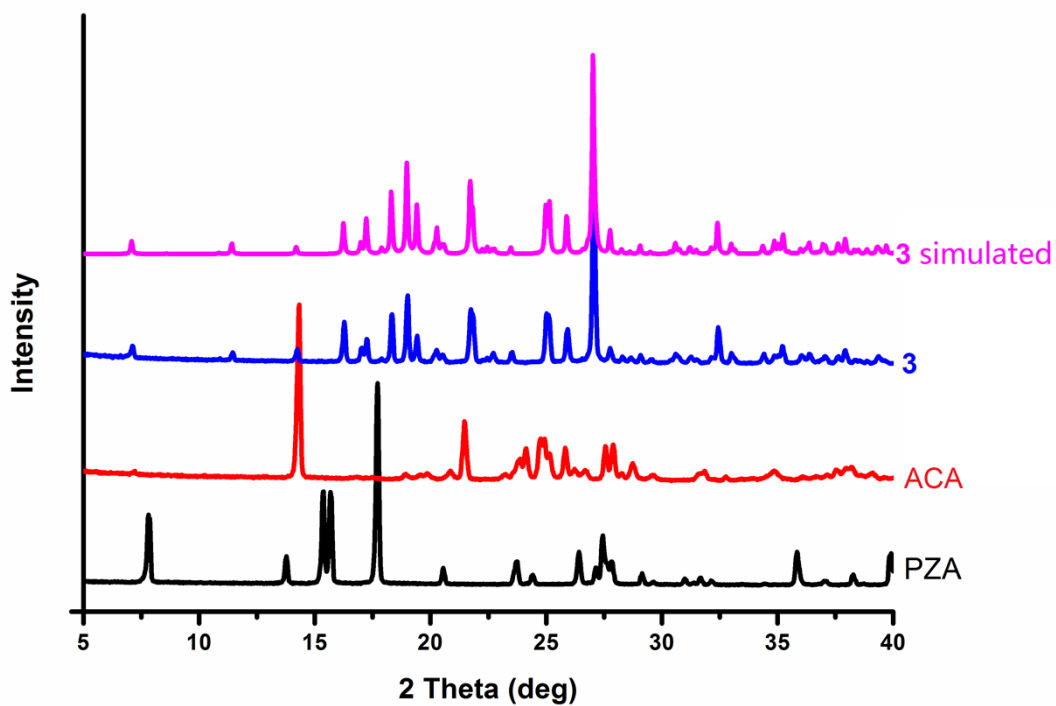


Fig. S3 PXRd patterns of cocystal 3

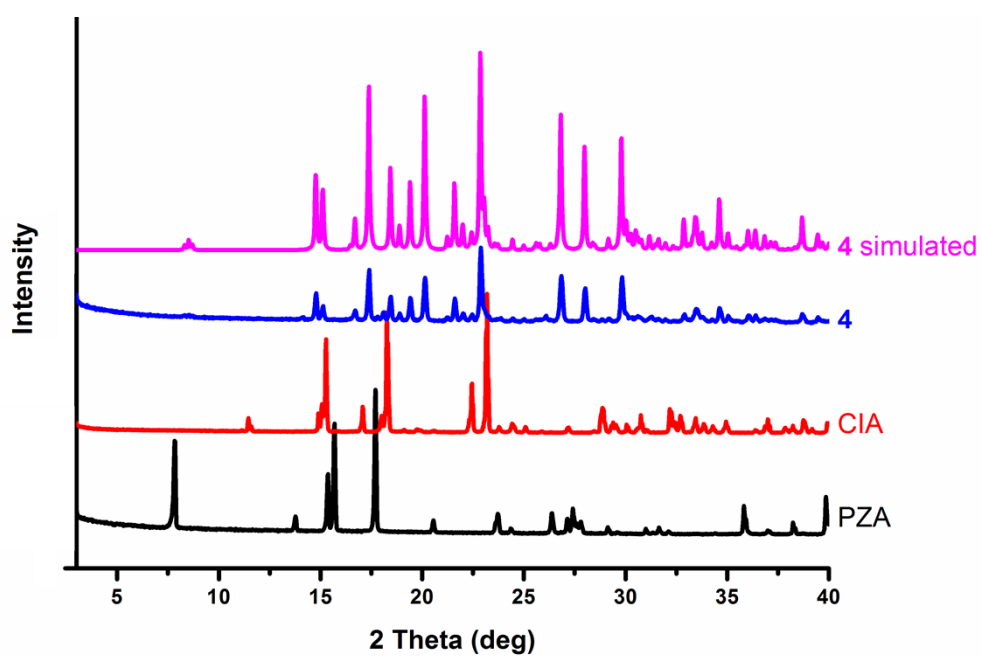


Fig. S4 PXRd patterns of cocystal 4

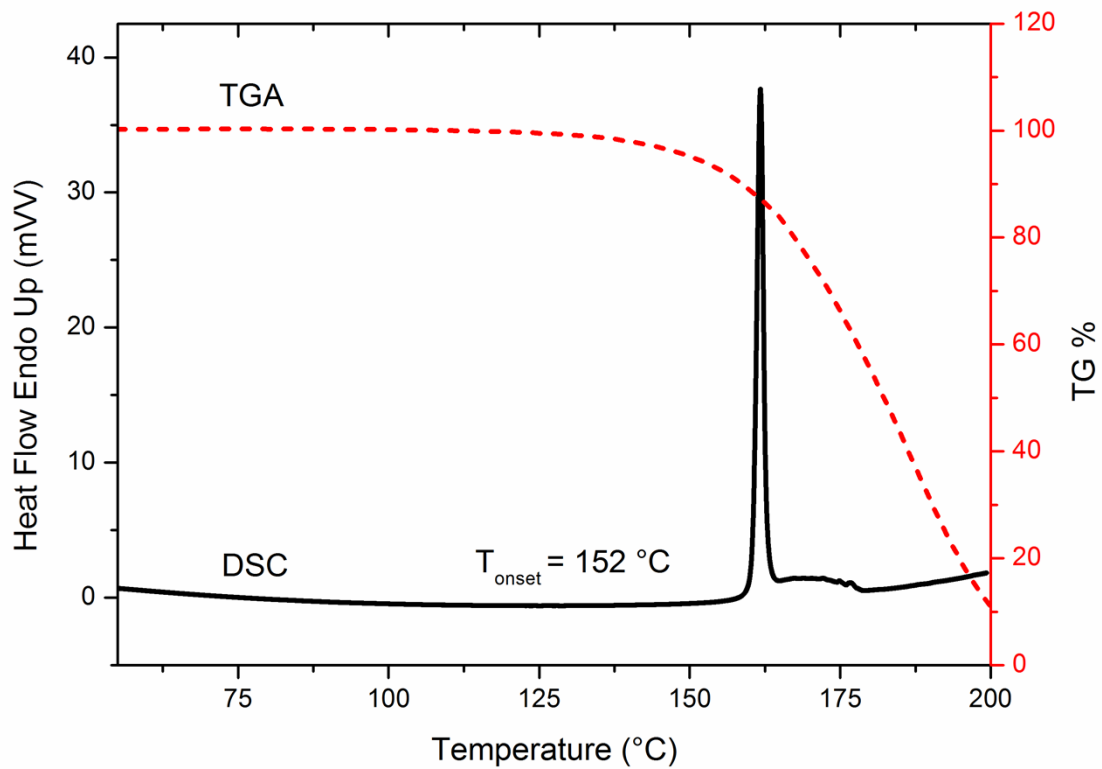


Fig. S5 TGA compared with DSC of cocystal 1

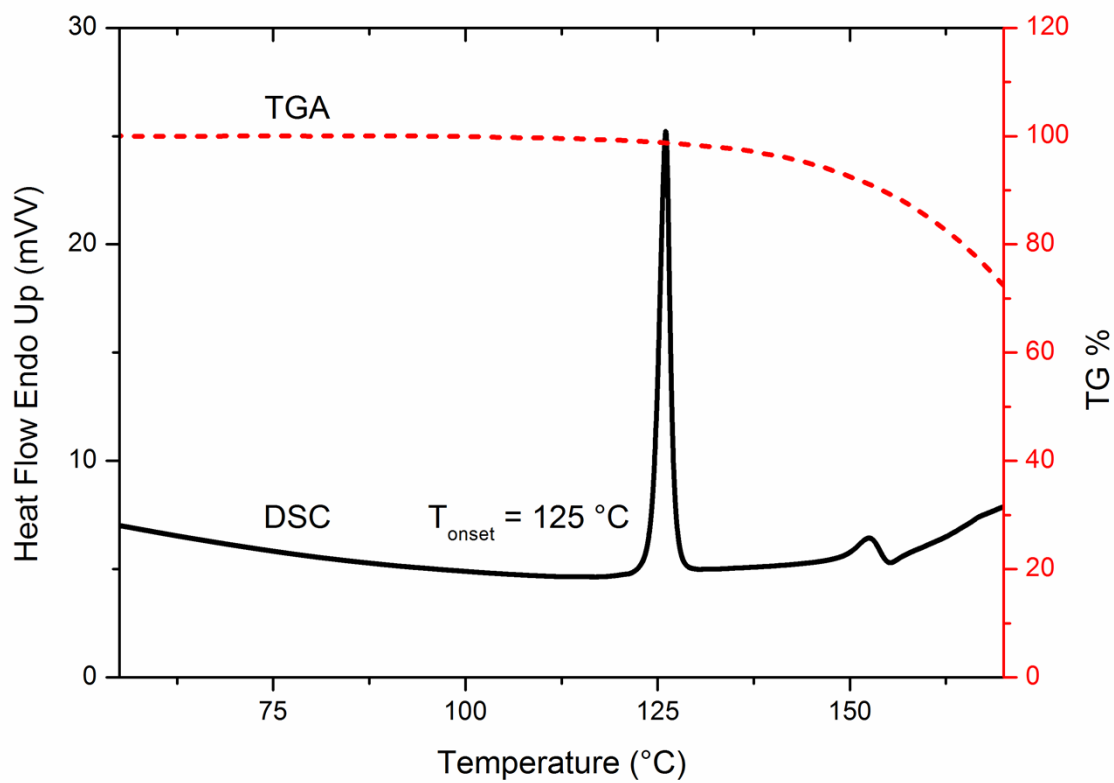


Fig. S6 TGA compared with DSC of cocystal 2

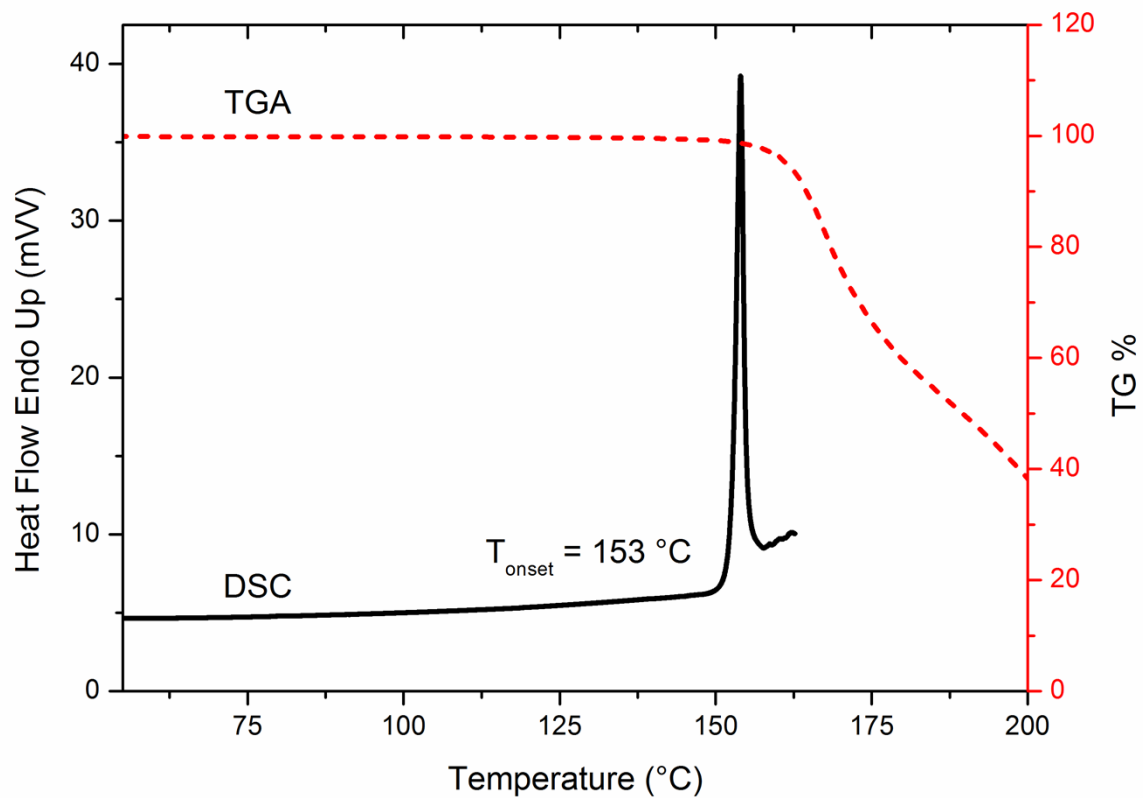


Fig. S7 TGA compared with DSC of cocrystal **3**

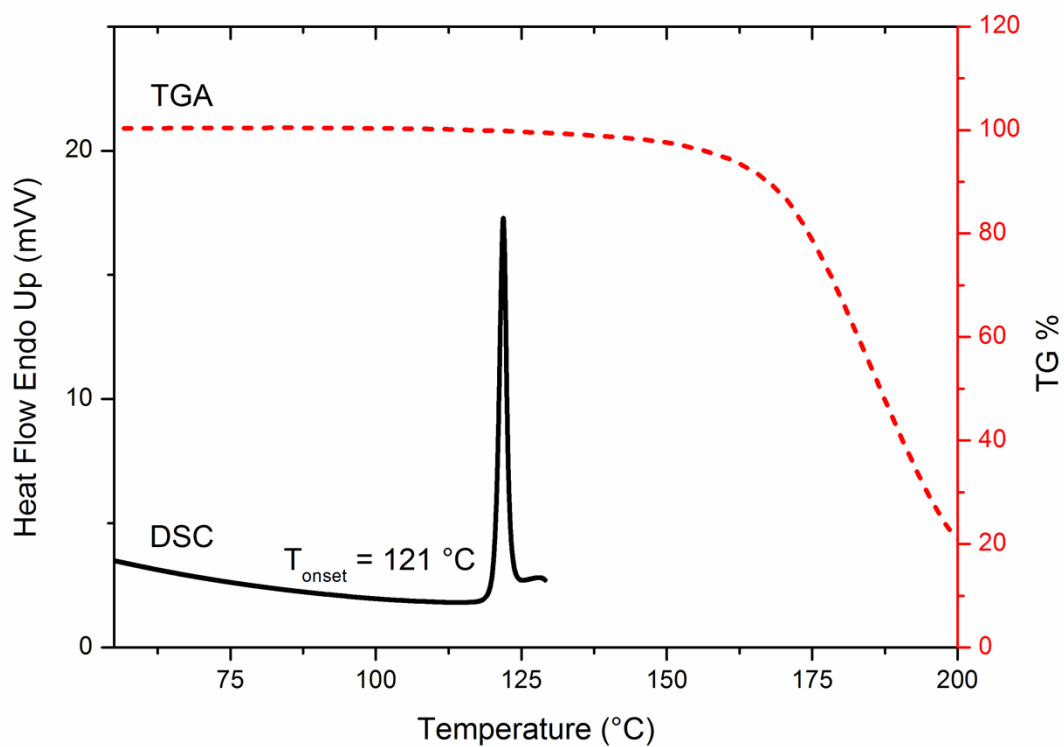


Fig. S8 TGA compared with DSC of cocrystal **4**

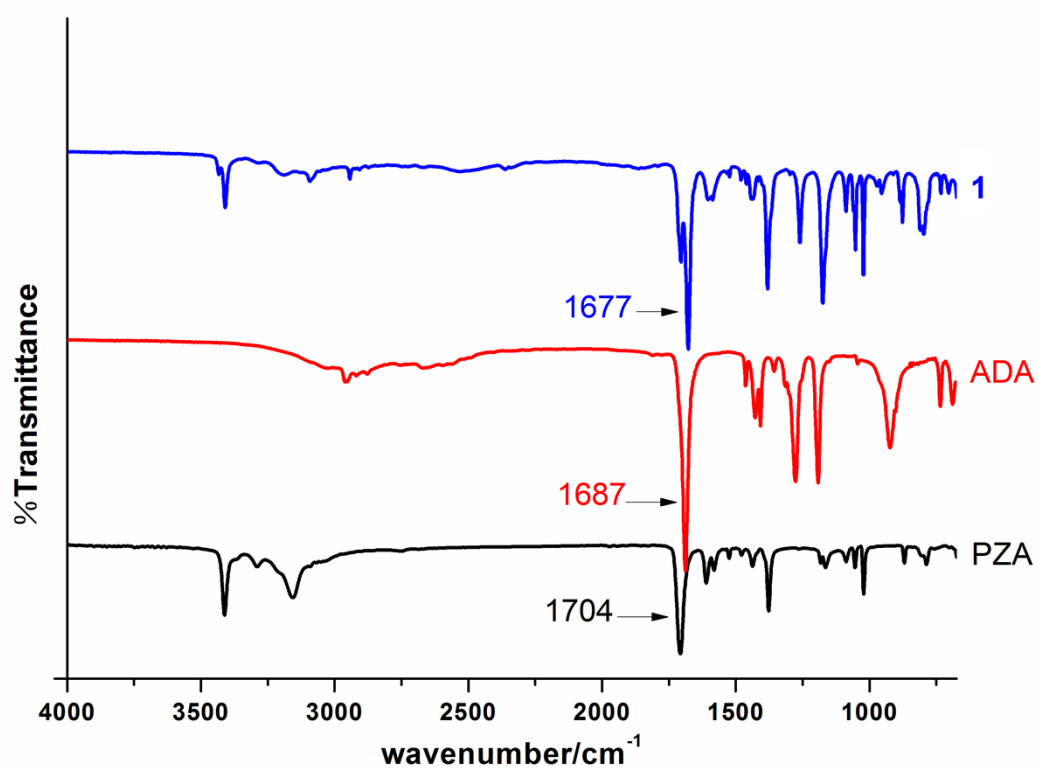


Fig. S9 IR spectra of PZA, ADA and cocystal 1

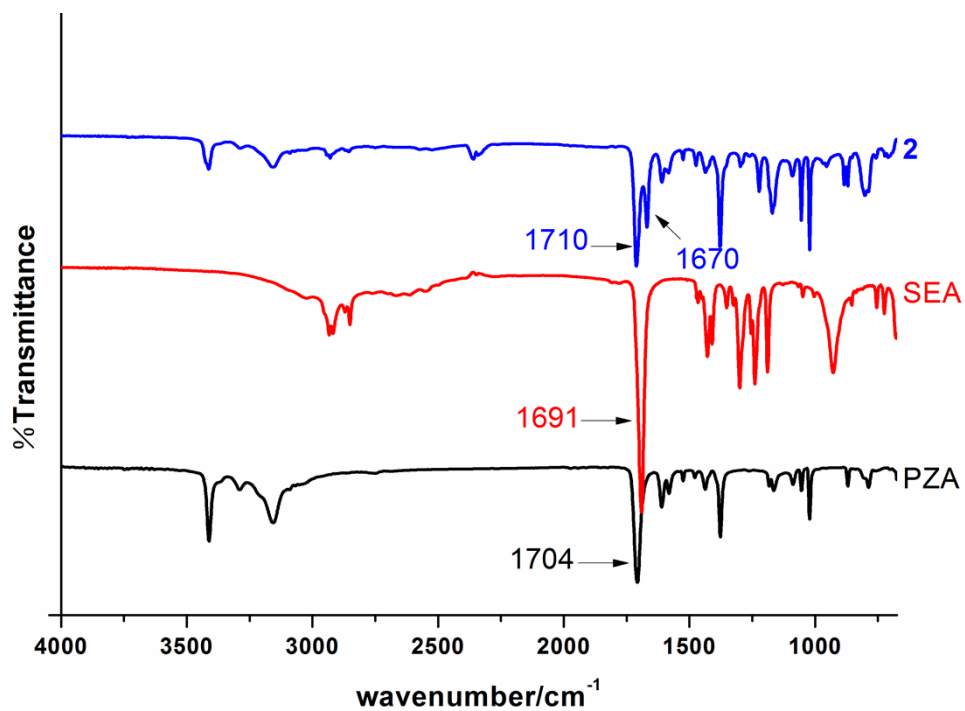


Fig. S10 IR spectra of PZA, SEA and cocystal 2

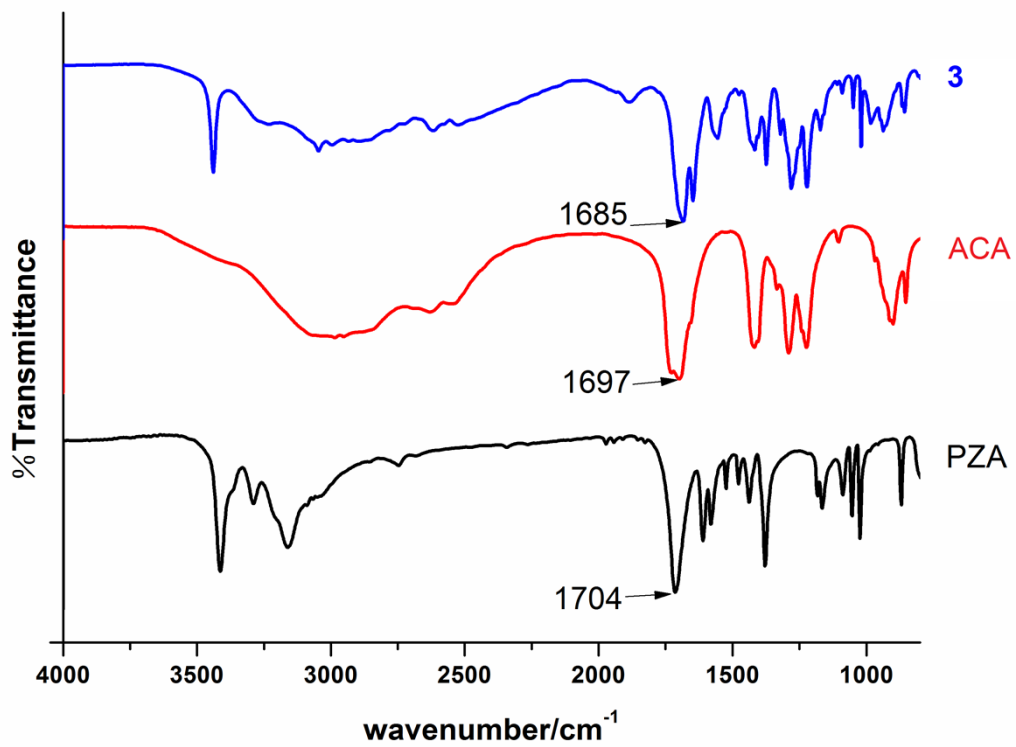


Fig. S11 IR spectra of PZA, ACA and cocrystal 3

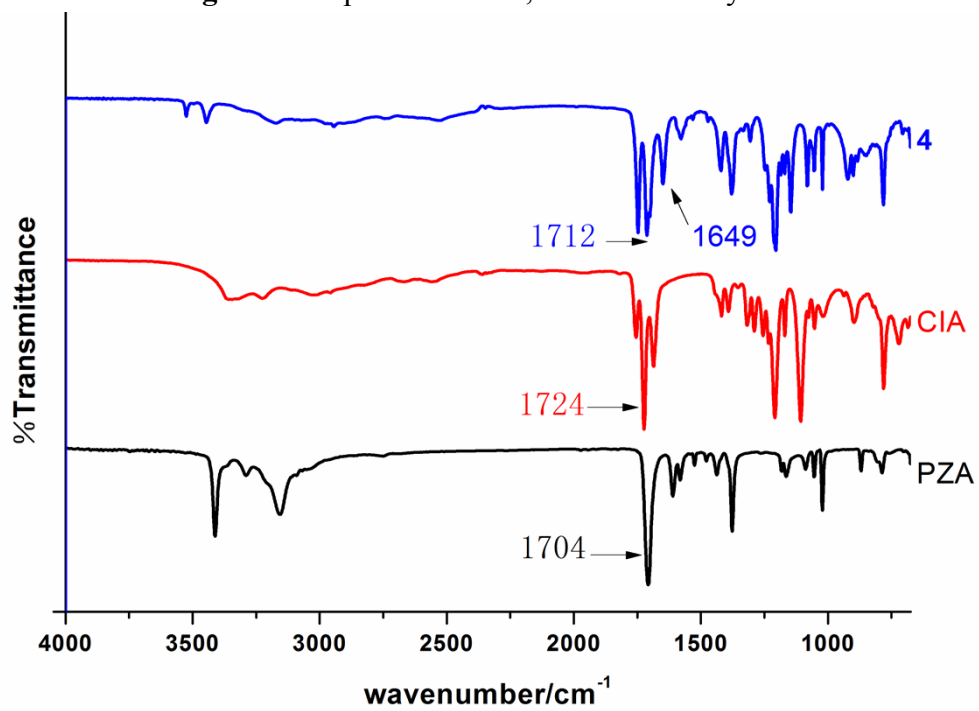


Fig. S12 IR spectra of PZA, CIA and cocrystal 4

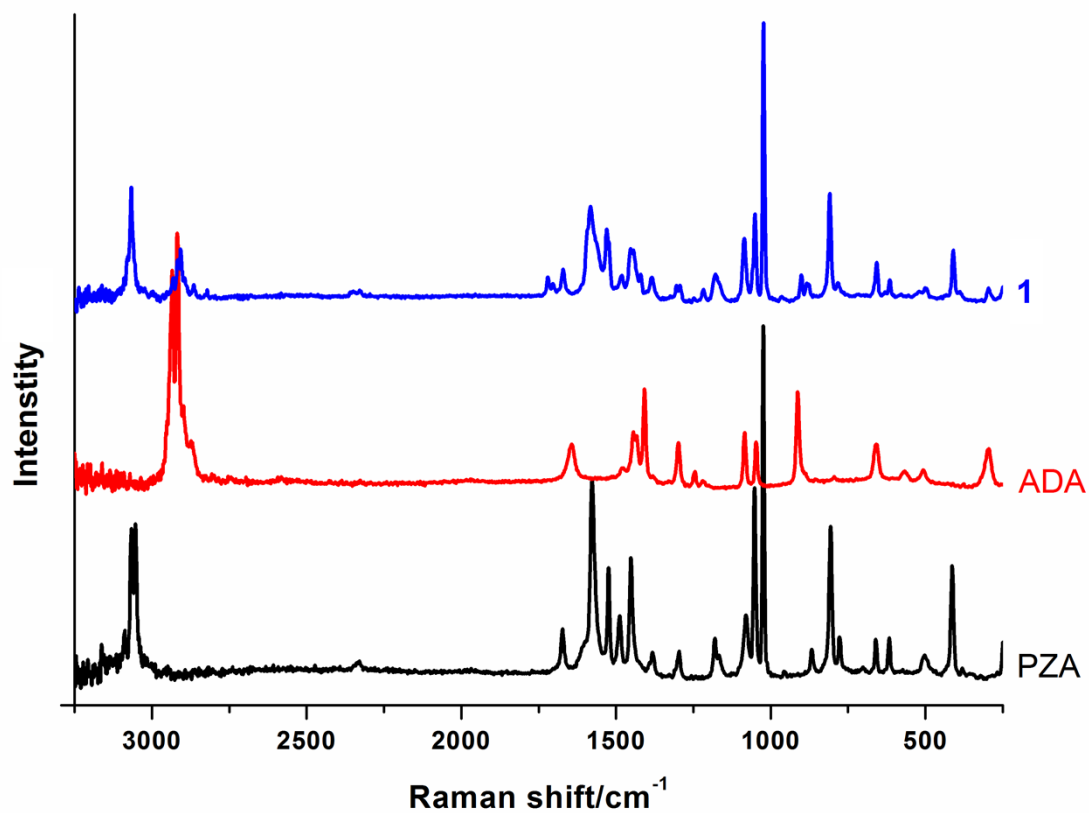


Fig. S13 Raman spectra of PZA, ADA and cocystal 1

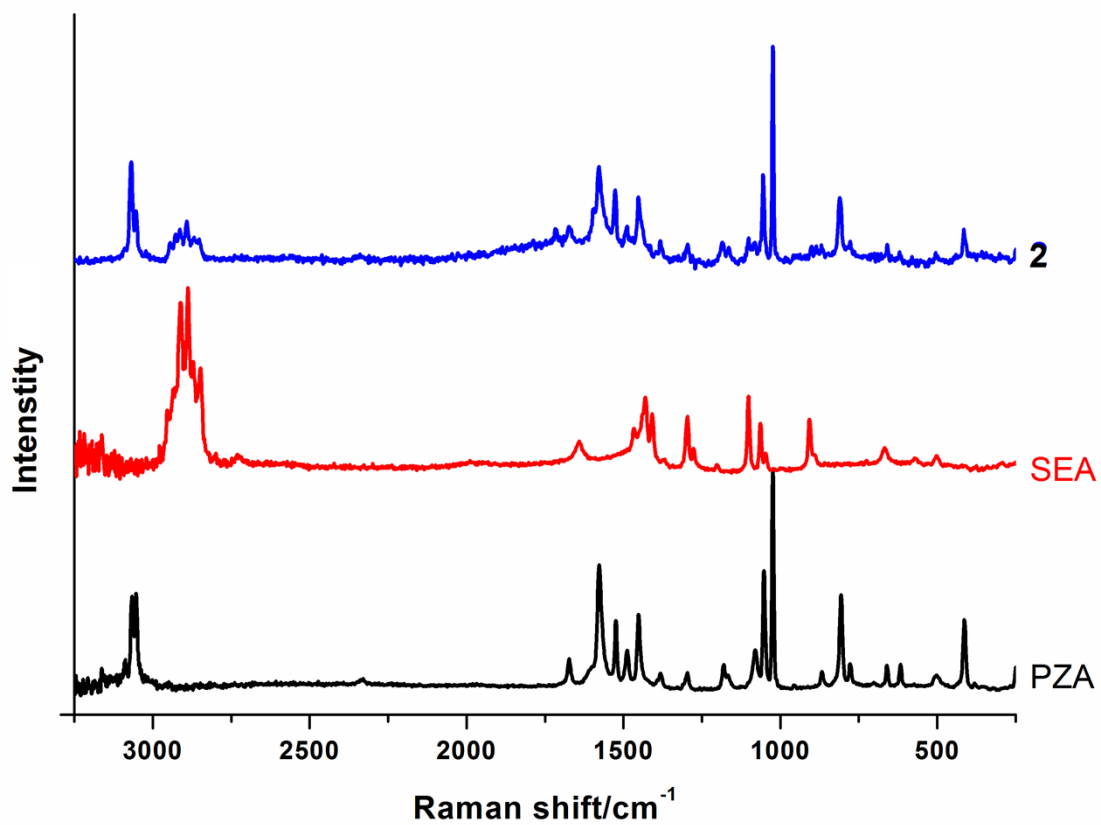


Fig. S14 Raman spectra of PZA, SEA and cocystal 2

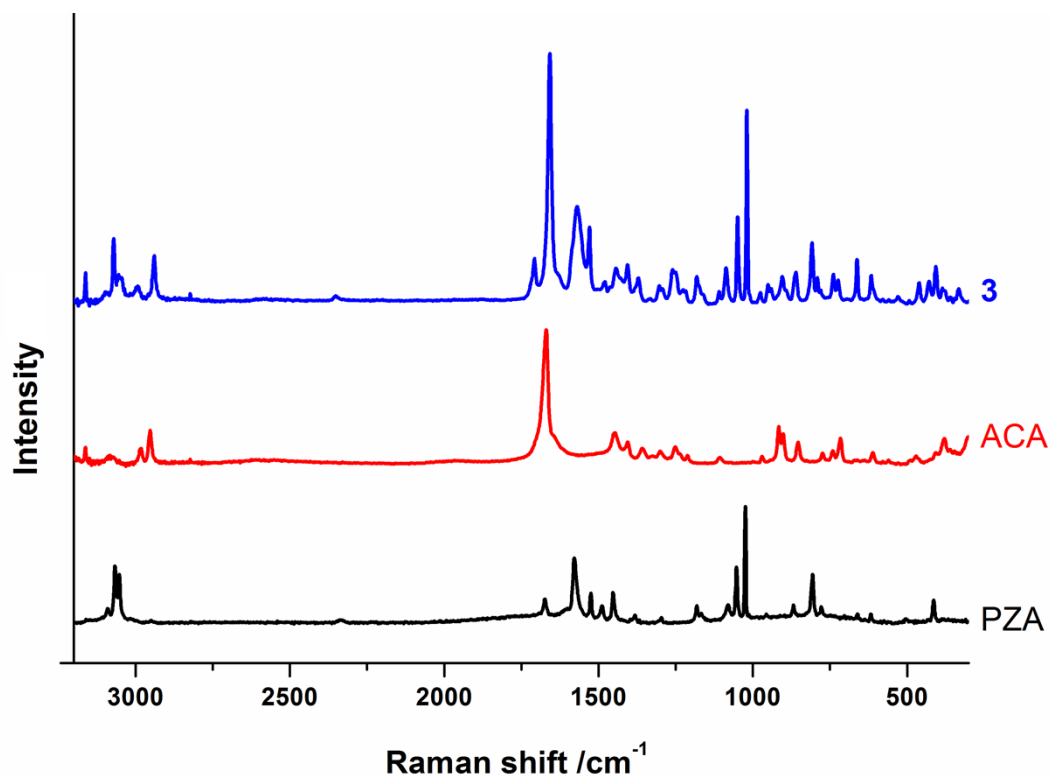


Fig. S15 Raman spectra of PZA, ACA and cocystal 3

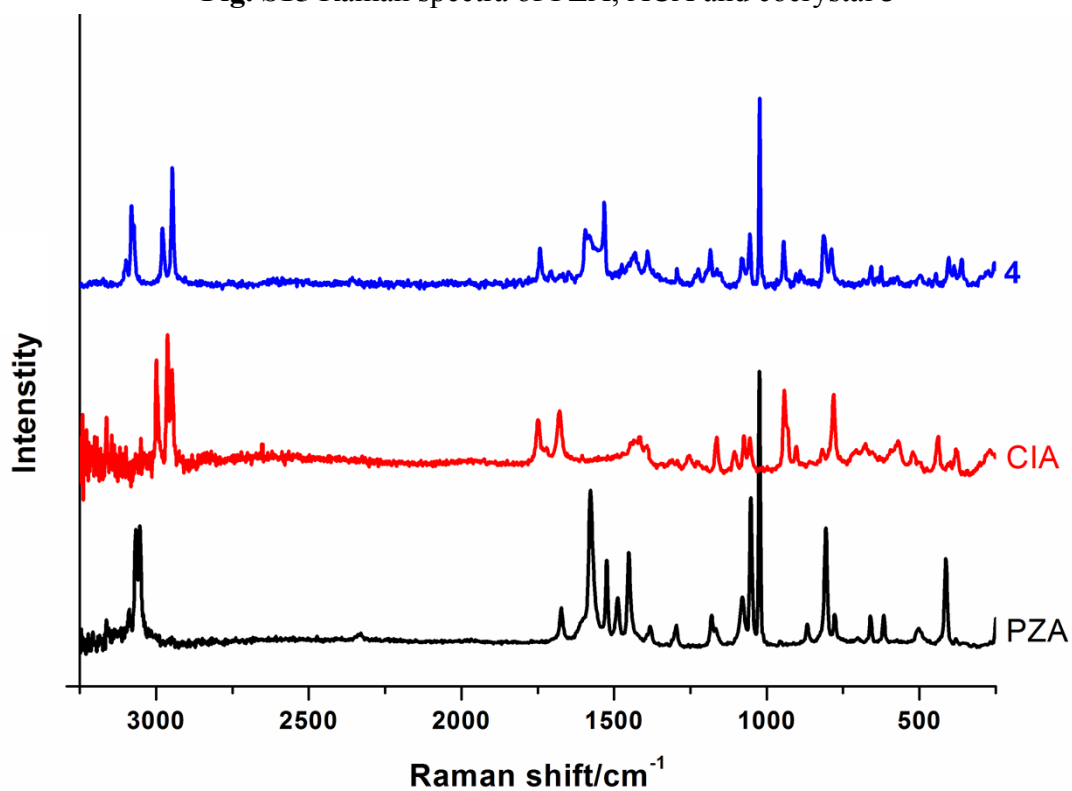


Fig. S16 Raman spectra of PZA, CIA and cocystal 4