

Crystal structures of pyrazinamide-*p*-amino benzoic acid cocrystal and their transamidation reaction product, 4-(pyrazine-2-carboxamido)benzoic acid in molten state

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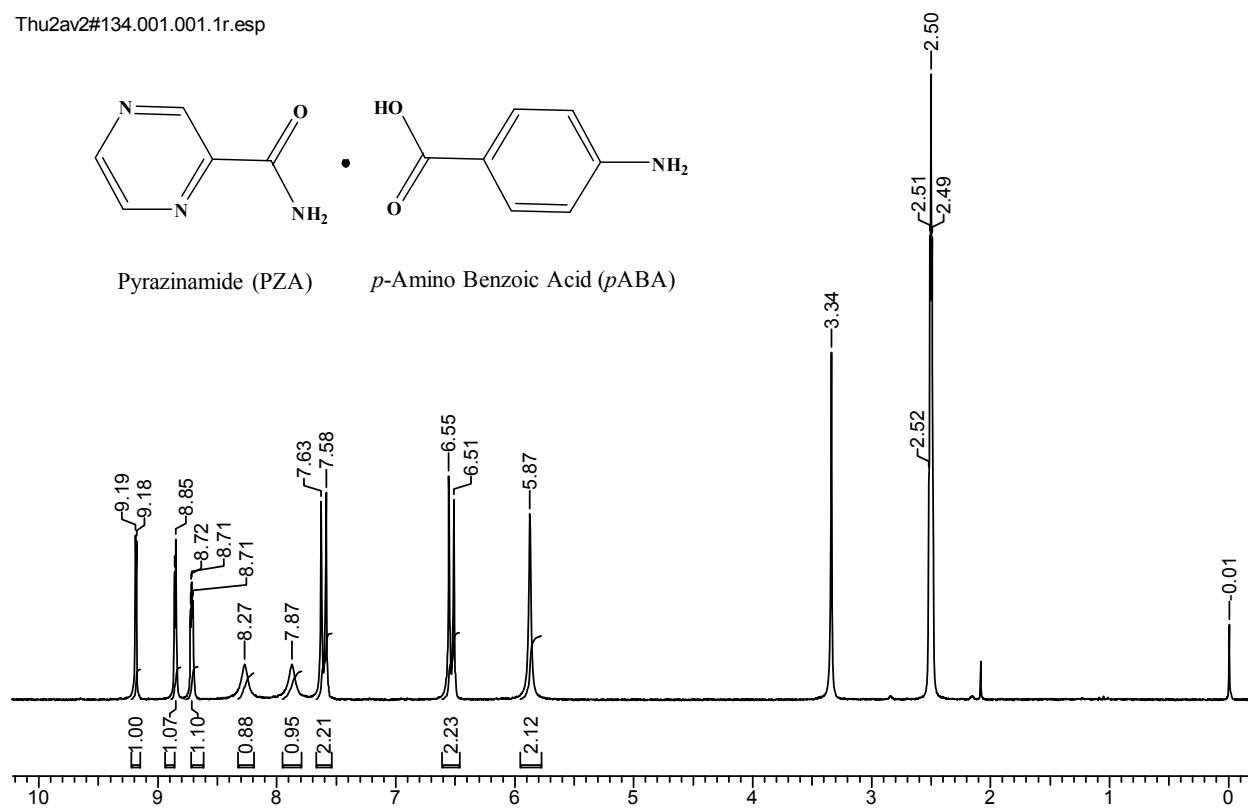


Figure S1. ¹H NMR of pyrazinamide (PZA) and *p*-amino benzoic acid (*p*ABA) cocrystal (**1**) recorded at 200 MHz in DMSO-*d*₆.

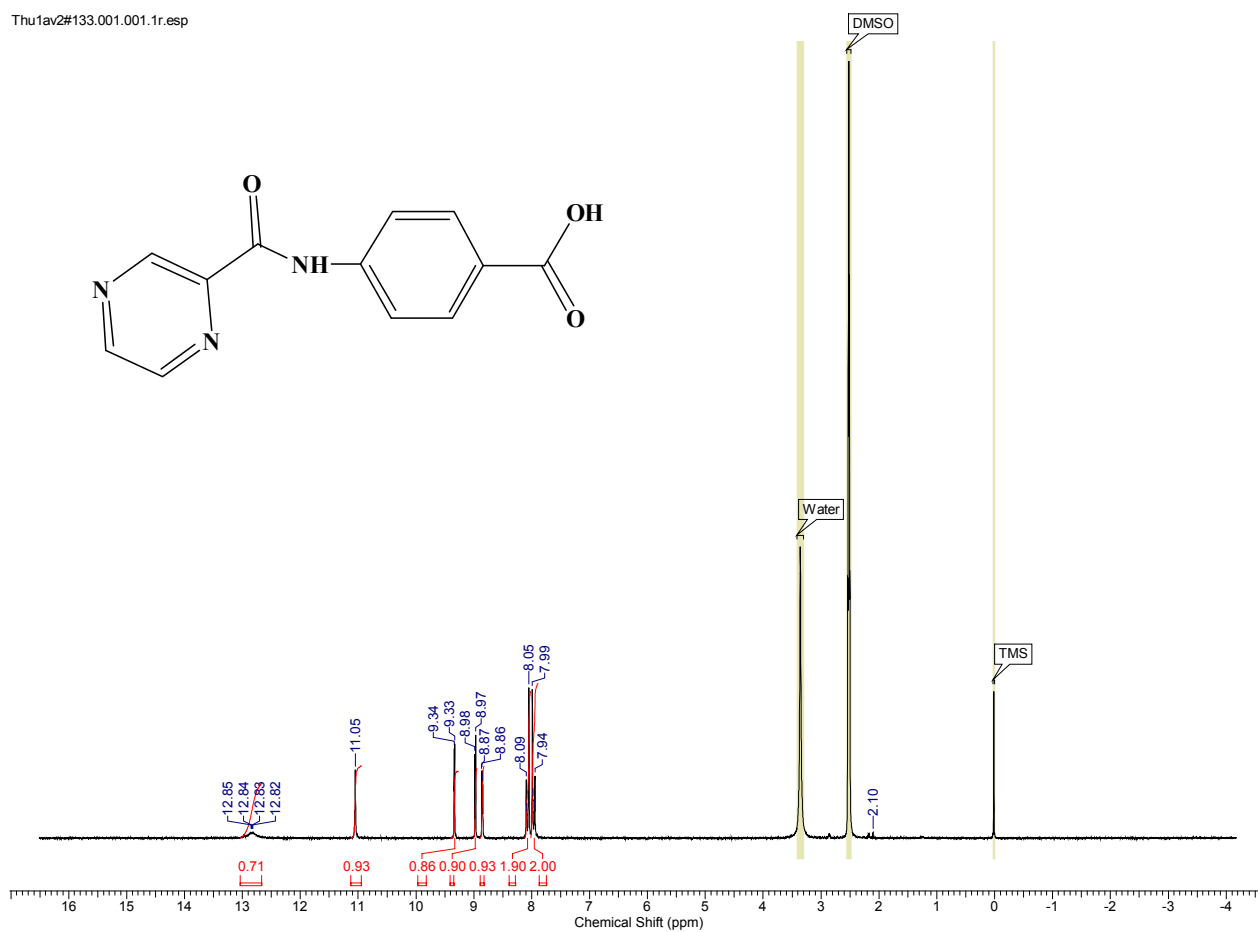


Figure S2. ¹H NMR of 4-(pyrazine-2-carboxamido) benzoic acid (**2**) recorded at 200 MHz in DMSO-*d*₆.

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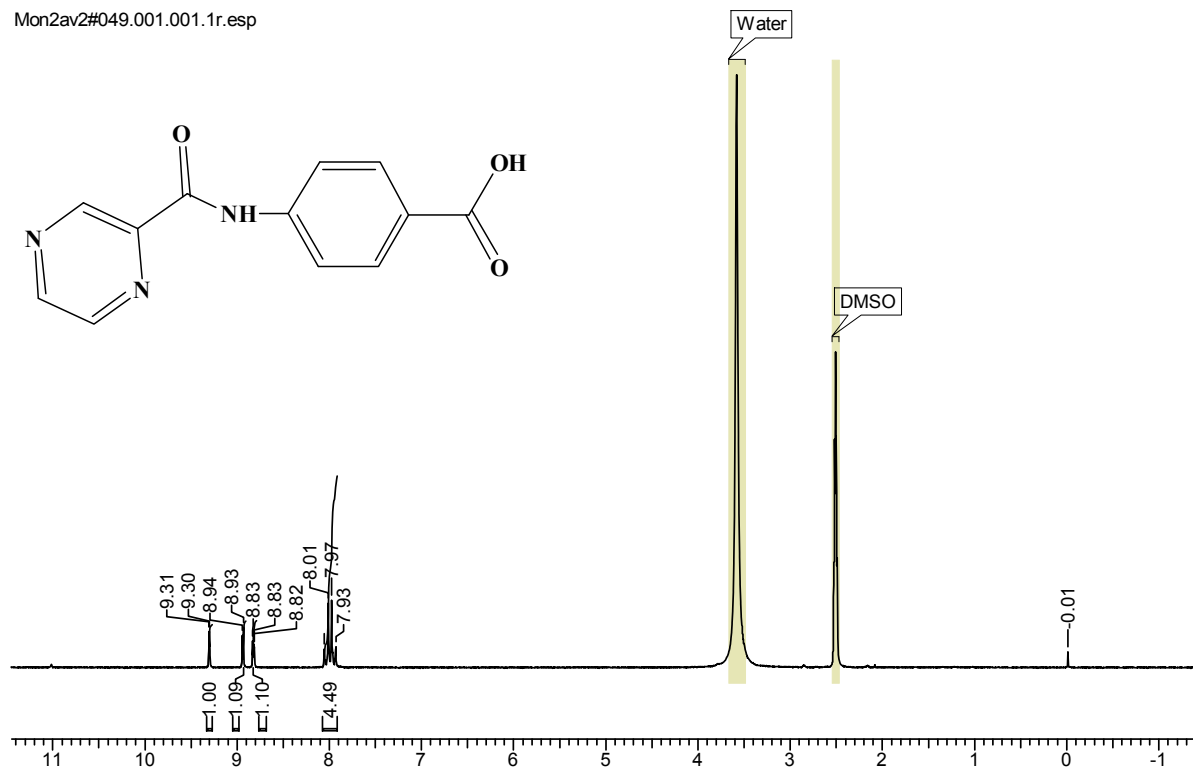


Figure S3. ¹H NMR of 4-(pyrazine-2-carboxamido) benzoic acid (**2**) recorded at 200 MHz in DMSO-*d*₆ with D₂O.

IR Analysis

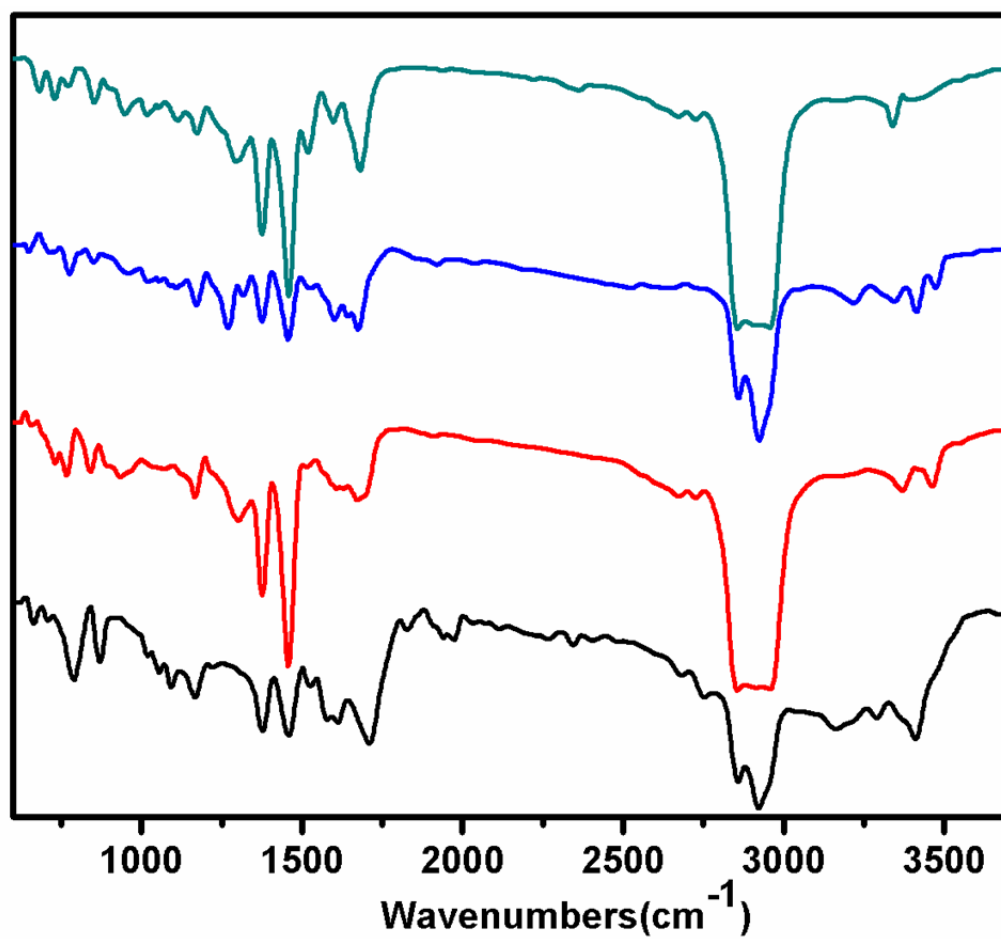


Figure S4. Infrared spectra of the PZA-*p*-ABA cocystal (**1**, blue), their molten product (**2**, green), pyrazinamide (PZA, black) and *p*-amino benzoic acid (*p*-ABA, red).

DSC analysis

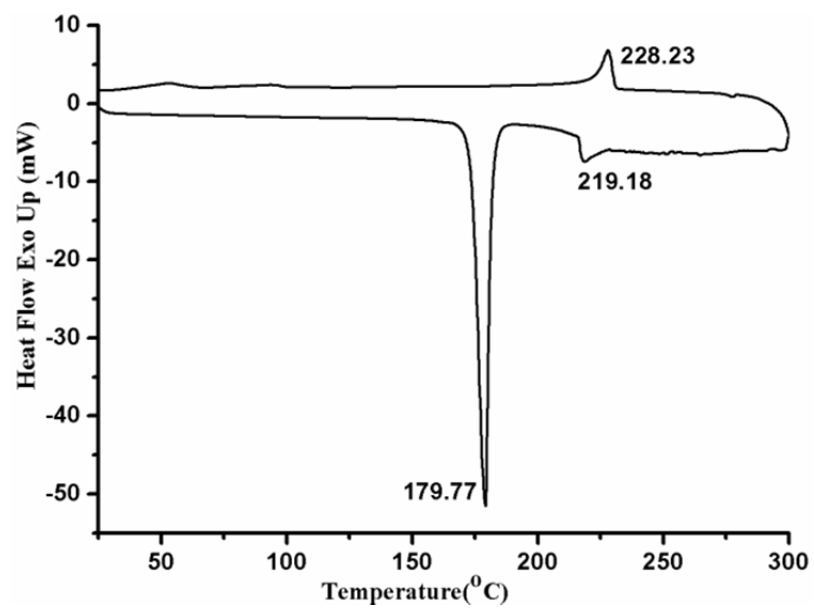


Figure S5. DSC profile of PZA – *p*-ABA cocrystal 1.

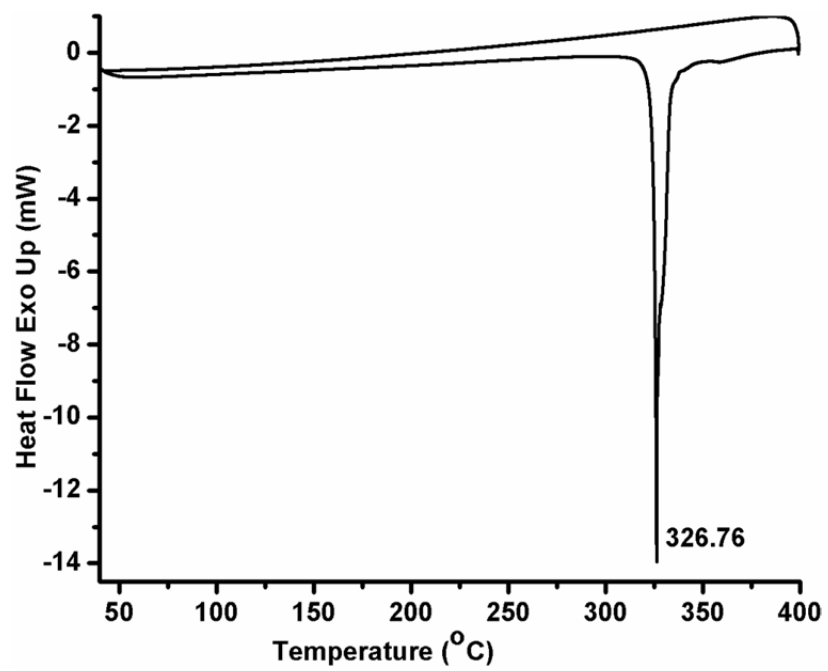


Figure S6. DSC profile of carboxamide 2.

PXRD analysis

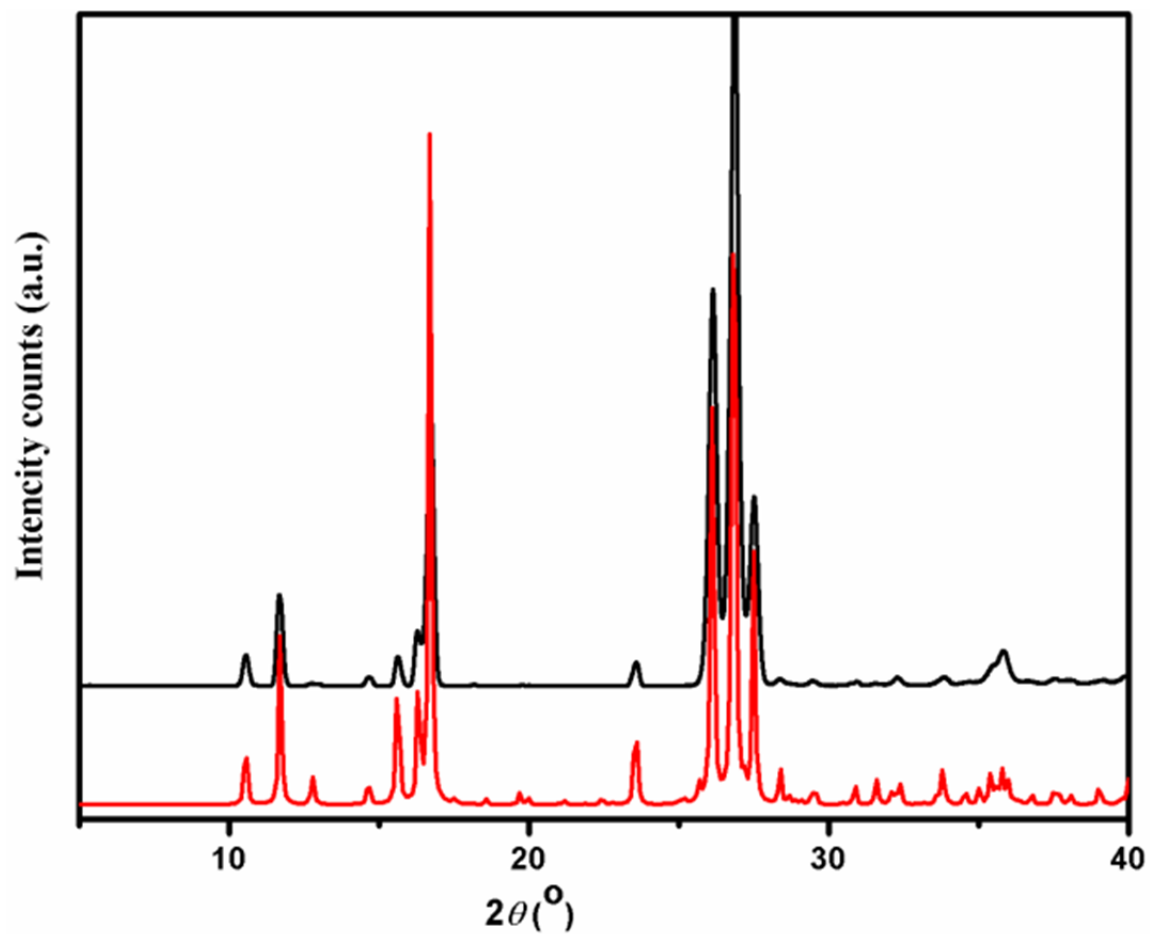


Figure S7. Overlay of PXRD patterns of cocrystal **1**, experimental (black) and simulated from single crystal diffraction data (red).

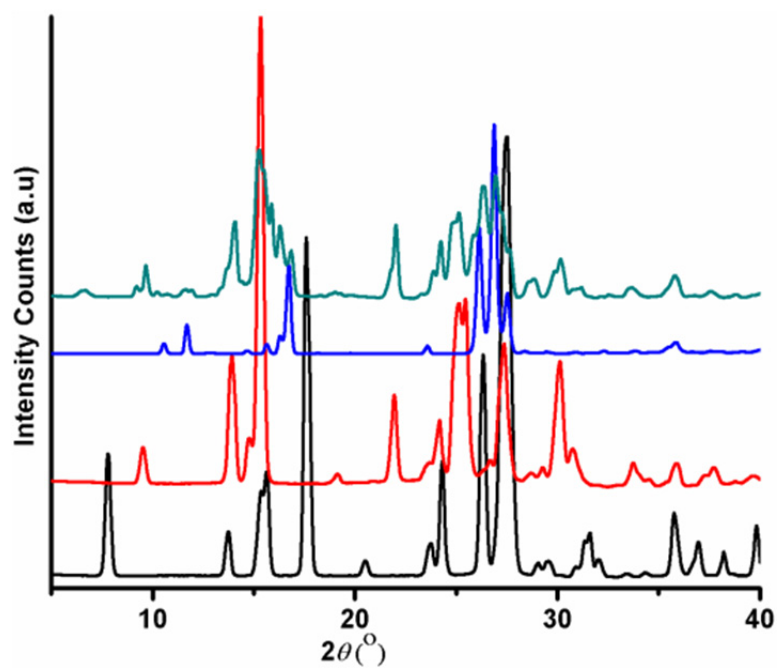


Figure S8. Overlay of PXRD patterns of cocystal **1** (blue), carboxamide **2** (green), PZA (black), *p*ABA (red).

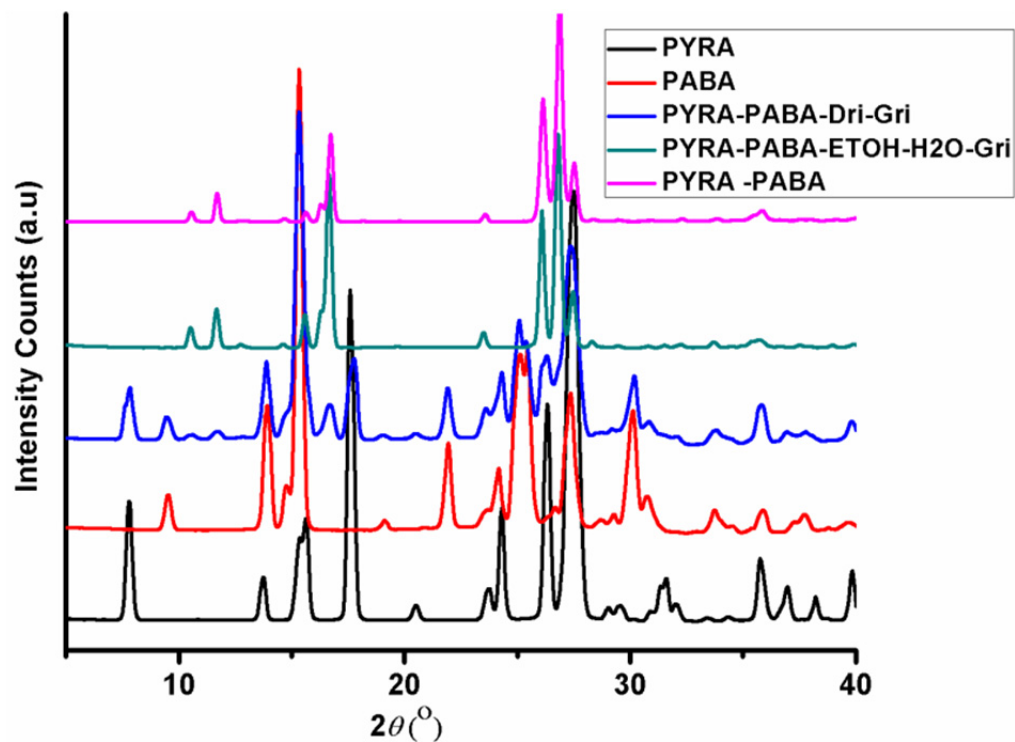


Figure S9. PXRD patterns of cocystal **1** prepared by dry grinding (blue), liquid assisted grinding (green) and their comparison with PXRD patterns of cocystals **1** produced from solution crystallization (magenta), PZA (black) and *p*ABA (red).

TGA Study

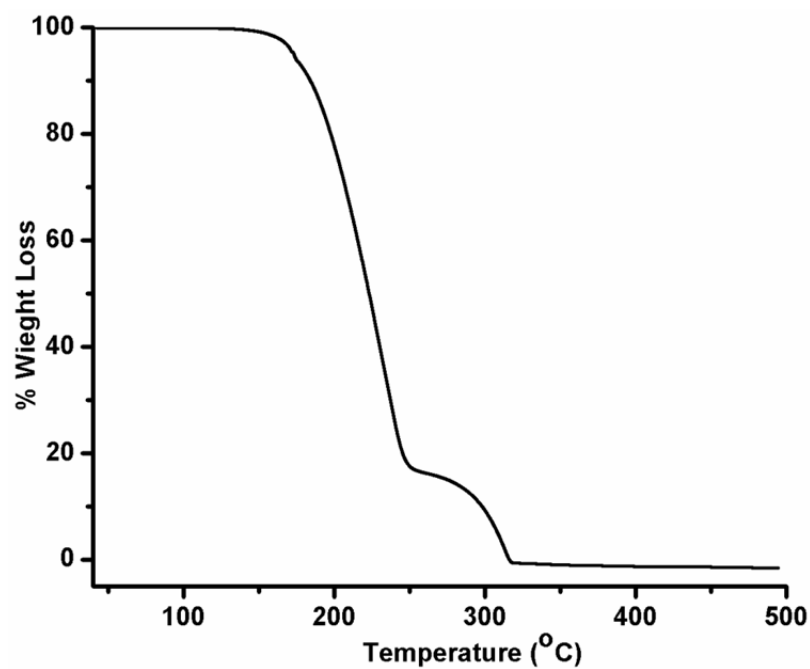


Figure S10. TGA plot of cocrystal **1** showing slight weight loss around melting attributed to the release of ammonia molecules as the byproduct of transamidation reaction in molten state.

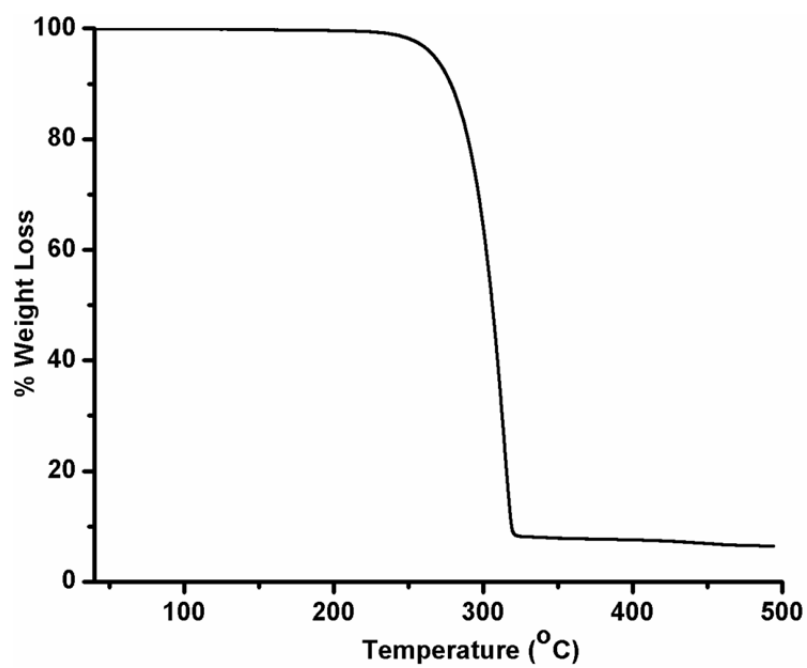


Figure S11. TGA plot of carboxamide **2**.

HSM Analysis

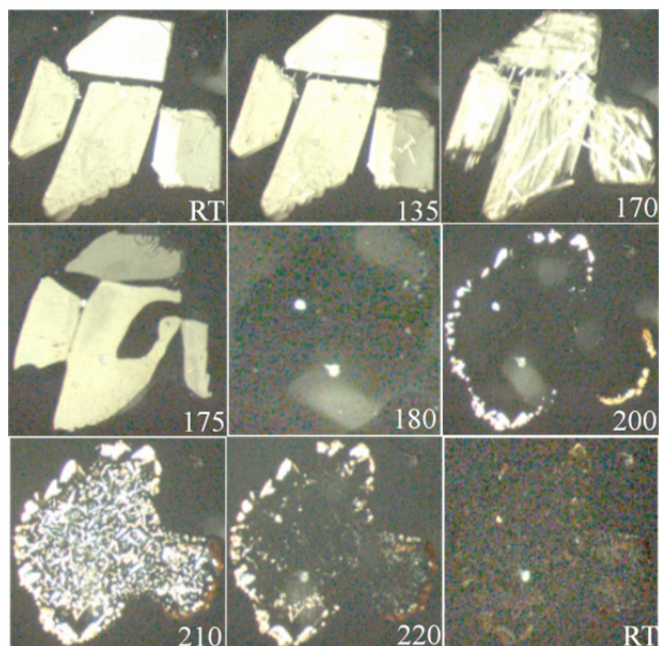


Figure S12. Photomicrographs of the cocrystal **1** grabbed during heating experiment showing thermal response at different temperatures.