Novel solid forms of the anti-tuberculosis drug, Isoniazid: ternary and polymorphic cocrystals

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Fig. S1 Comparison of the PXRD patterns of the products obtained from neat grinding and solvent-drop grinding (SDG) of INH and HBA with simulated powder patterns of INH•HBA hydrate polymorphs and INH•HBA anhydrous cocrystal. Notice that neat grinding produces the anhydrous cocrystal and SDG produces the Form II of INH•HBA hydrate.



Fig. S2 Comparison of PXRD patterns of the products obtained from neat grinding and SDG of INH and FA with simulated powder patterns of INH•FA cocrystal polymorphs. Notice that both grinding methods produce Form I of the cocrystal.



Fig. S3 Comparison of PXRD patterns of the products obtained from neat grinding and SDG of INH, NA and FA with simulated powder pattern of INH•NA•FA cocrystal. Notice that both grinding methods produce the cocrystal.



Fig. S4 Comparison of PXRD patterns of the products obtained from neat grinding and SDG of INH, NA and SA with simulated powder pattern of INH•NA•SA cocrystal. Notice that both grinding methods produce the cocrystal.



Fig. S5 Comparison of PXRD patterns of the INH•HBA hydrate after dehydration with simulated patterns of anhydrous INH•HBA cocrystal and INH•HBA hydrate. Notice that the INH•HBA hydrate converts to anhydrous cocrystal upon dehydration.



Fig. S6 DSC thermogram of INH•NA•FA cocrystal. The melting point of INH: 170 °C, NA: 128 °C, and FA: 287 °C.



Fig. S7 DSC thermogram of INH•NA•SA cocrystal. The melting point of INH: 170 °C, NA: 128 °C, and SA: 184 °C.



Fig. S8 Comparison of PXRD patterns of the INH•HBA anhydrous and hydrate cocrystal samples stored at accelerated test conditions (40 °C, 70 % RH). Notice that the anhydrous cocrystal converts to the hydrate within 2 days.



Fig. S9 Comparison of PXRD patterns of the INH•FA cocrystal (Form I) stored at accelerated test conditions (40 °C, 70 % RH). Notice that the cocrystal is stable.



Fig. S10 Comparison of PXRD patterns of the INH•NA•FA cocrystal sample stored at accelerated test conditions (40 °C, 70 % RH). Notice that the cocrystal is stable.



Fig. S11 Comparison of PXRD patterns of the INH•NA•SA cocrystal sample stored at accelerated test conditions (40 °C, 70 % RH). Notice that the cocrystal is stable.

Table S1 The observed retention times of INH and coformers in HPLC using differentMeOH: H_2O mobile phases.

HPLC mobile phase ratio	Retention time (min)				
(MeOH:H ₂ O)	INH	HBA	NI	FA	SA
60:40	2.496	2.304			
20:80	3.292		3.818	2.332	
5:95	5.527		7.957		4.570