Polymorphs, Hydrates and Solvates of a Co-crystal of Caffeine with Anthranilic Acid

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Supplementary Material

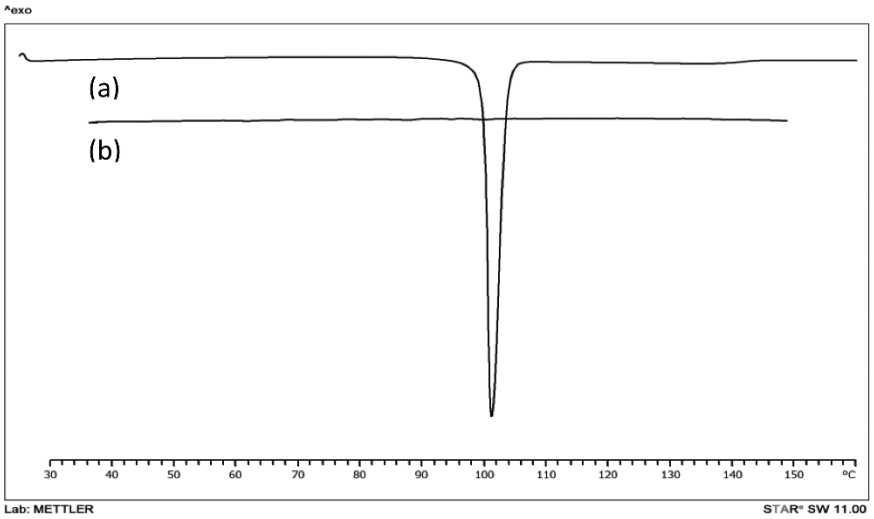

Figure S1 DSC trace (a) and TGA thermogram (b) for Form I of the caffeine:anthranilic acid co-crystal.

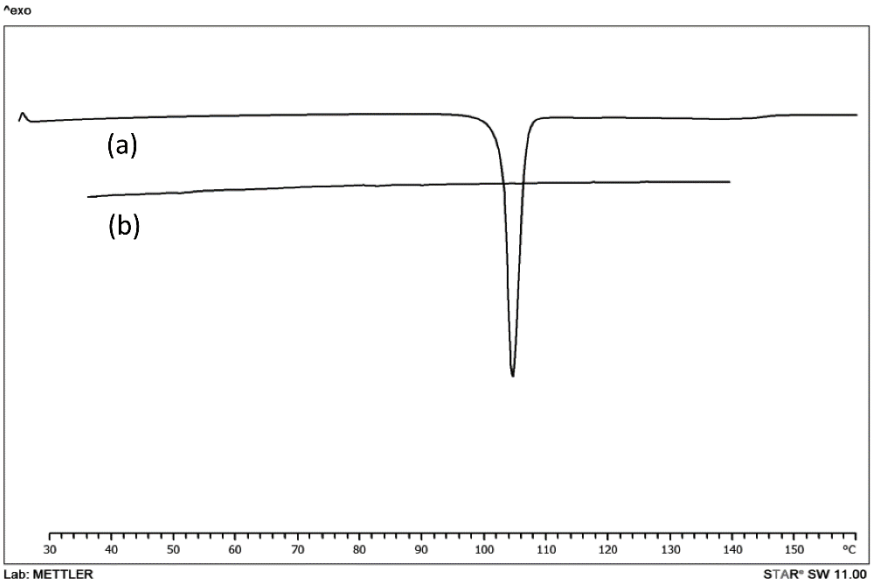

Figure S2 DSC trace (a) and TGA thermogram (b) for Form II of the caffeine:anthranilic acid co-crystal.

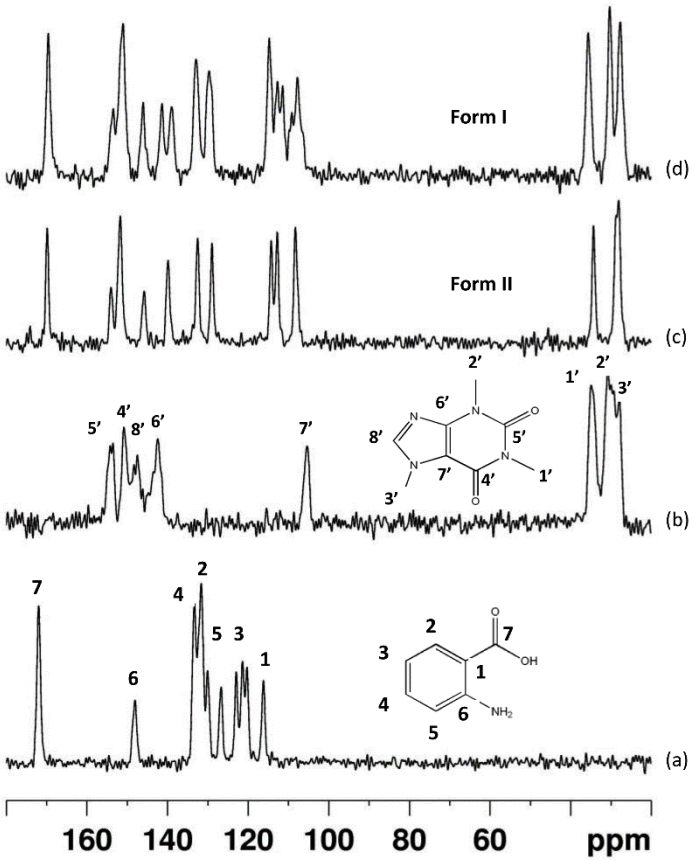

Figure S3 ^{13}C solid-state NMR spectrum of (a) anthranilic acid (b) caffeine (c) Form I of the caffeine:anthranilic acid co-crystal and (d) Form II of the caffeine:anthranilic acid co-crystal.

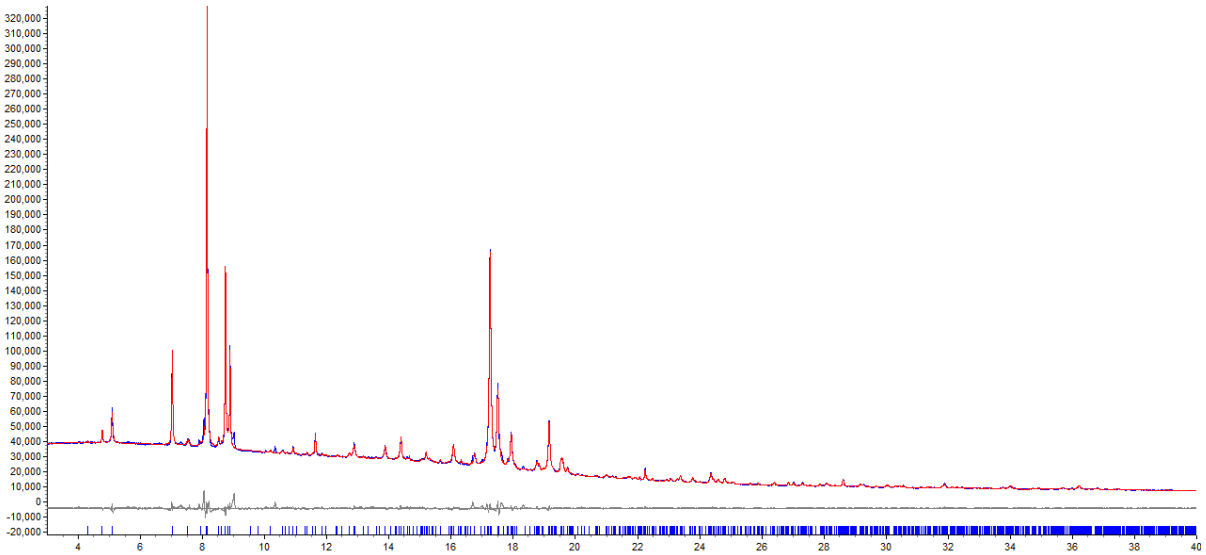

Figure S4 Experimental (blue), calculated (red), and difference (bottom) synchrotron powder diffraction profiles for the Rietveld refinement of **caf:ana** Form I.

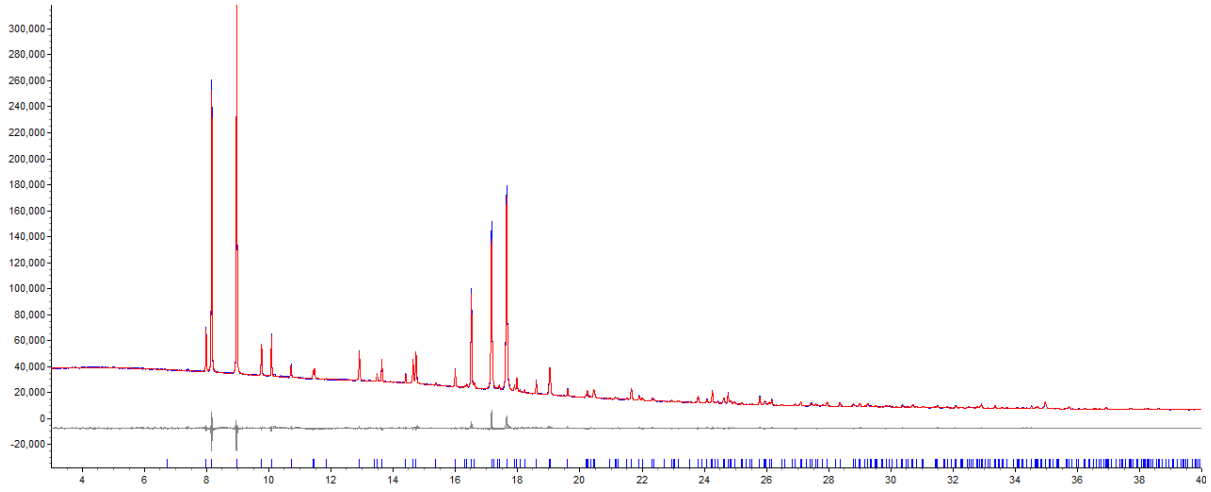

Figure S5 Experimental (blue), calculated (red), and difference (bottom) synchrotron powder diffraction profiles for the Rietveld refinement of **caf:ana** Form II.

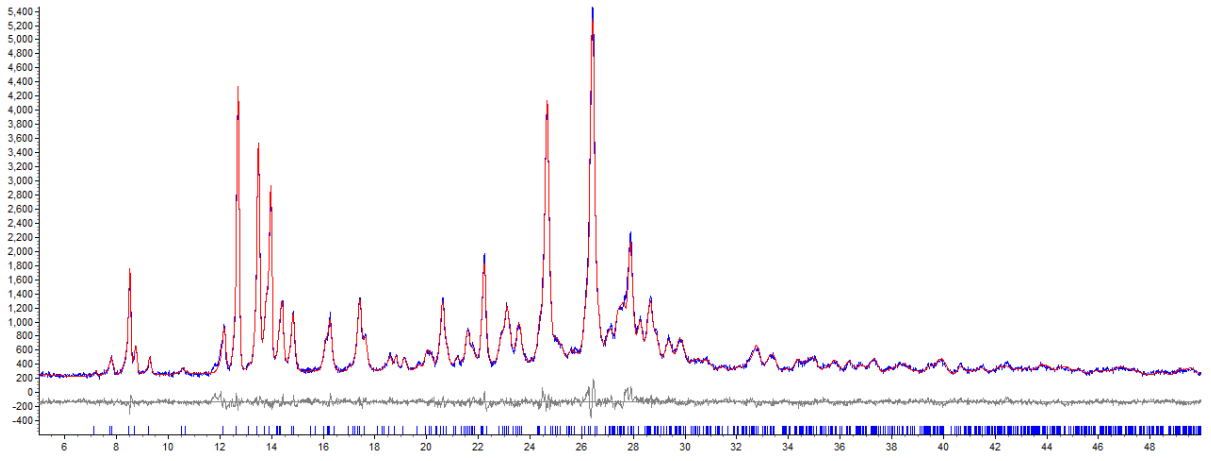

Figure S6 Experimental (blue), calculated (red), and difference (bottom) powder diffraction profiles for the Rietveld refinement of the **caf:ana** bromobenzene hemisolvate.

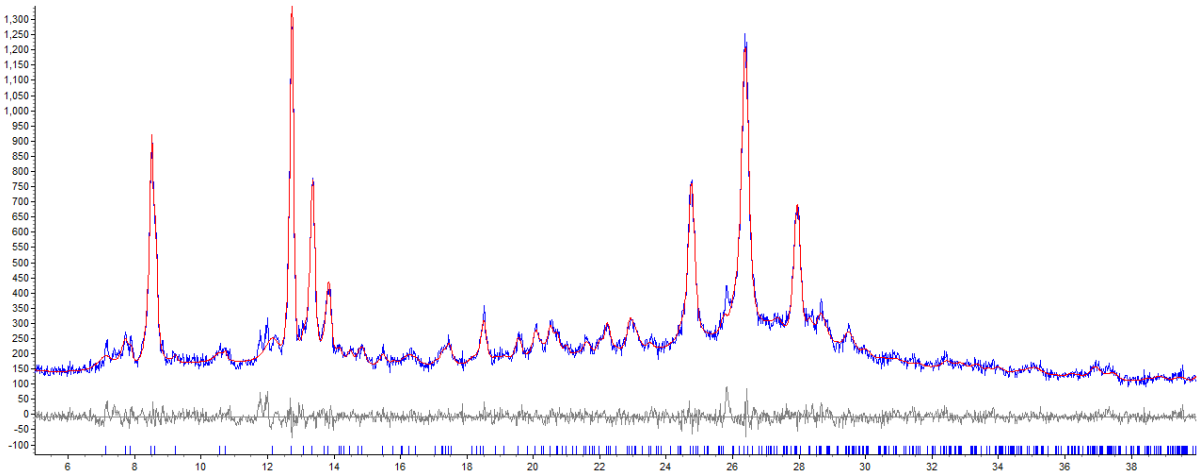

Figure S7 Experimental (blue), calculated (red), and difference (bottom) powder diffraction profiles for the Rietveld refinement of the **caf:ana** toluene hemisolvate.

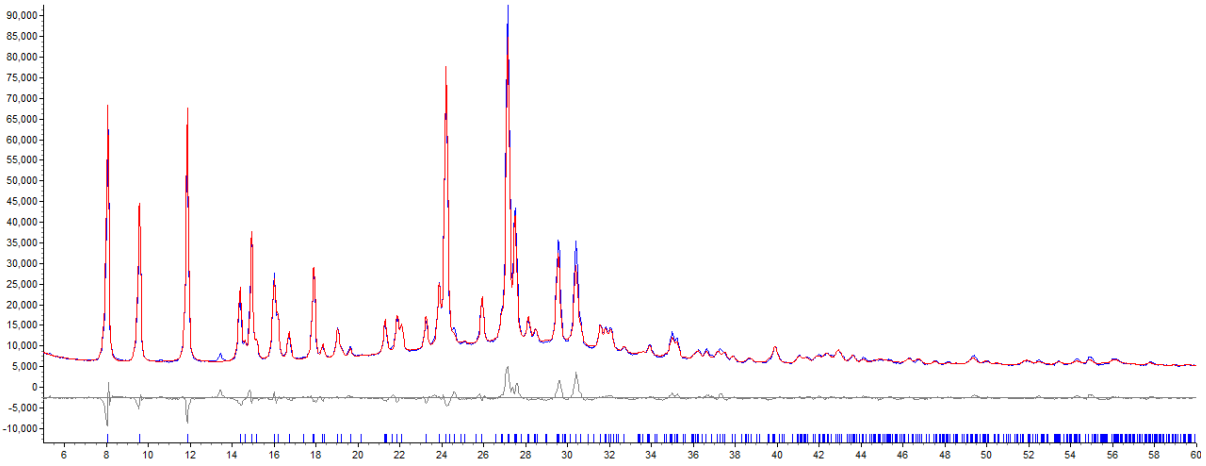

Figure S8 Experimental (blue), calculated (red), and difference (bottom) powder diffraction profiles for the Rietveld refinement of the **tbn:ana** co-crystal.