Supplementary Information to accompany "Co-crystallisation of cytosine with 1,10-phenanthroline : computational screening and experimental realisation"

Co-crystal screening by ball-milling

In order to explore the formation of co-crystals between DNA bases and the 1,10-phen, we employed solid-state neat grinding methods described in literature. Starting materials were transferred to a 12 mL jar and milled for 1 hour under neat condition in a Retsch PM 100 ball mill. Two stainless steel balls of 10mm diameter were used for milling. The reaction conditions here are sufficient for the stainless steel balls and mill to react with 1,10-phenanthroline-containing mixtures. Protracted milling in the presence of 1,10-phenanthroline leads to a colour change in the sample from white to pink. Extensive grinding, uv-vis, IR, and ICP experiments have shown that this colour is due to an iron-phenanthroline complex present in very small amounts. This does not interfere with structural studies. Grinding by hand in an agate pestle and mortar yields an identical transformation to that described for the cytosine:phenanthroline mixture but without any emergence of a pink colouration.

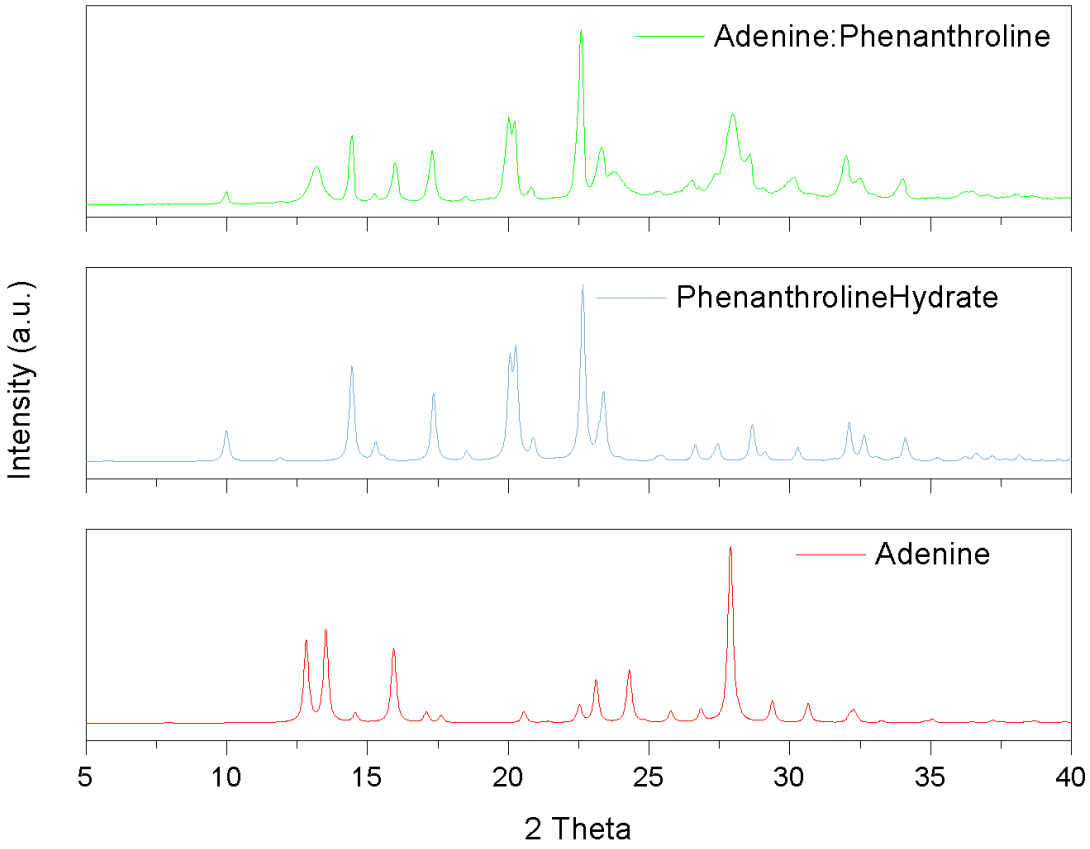

Figure S1: Simulated X-ray powder diffraction patterns of adenine and 1,10-phenanthroline hydrate, and experimental pattern obtained after milling their mixture.

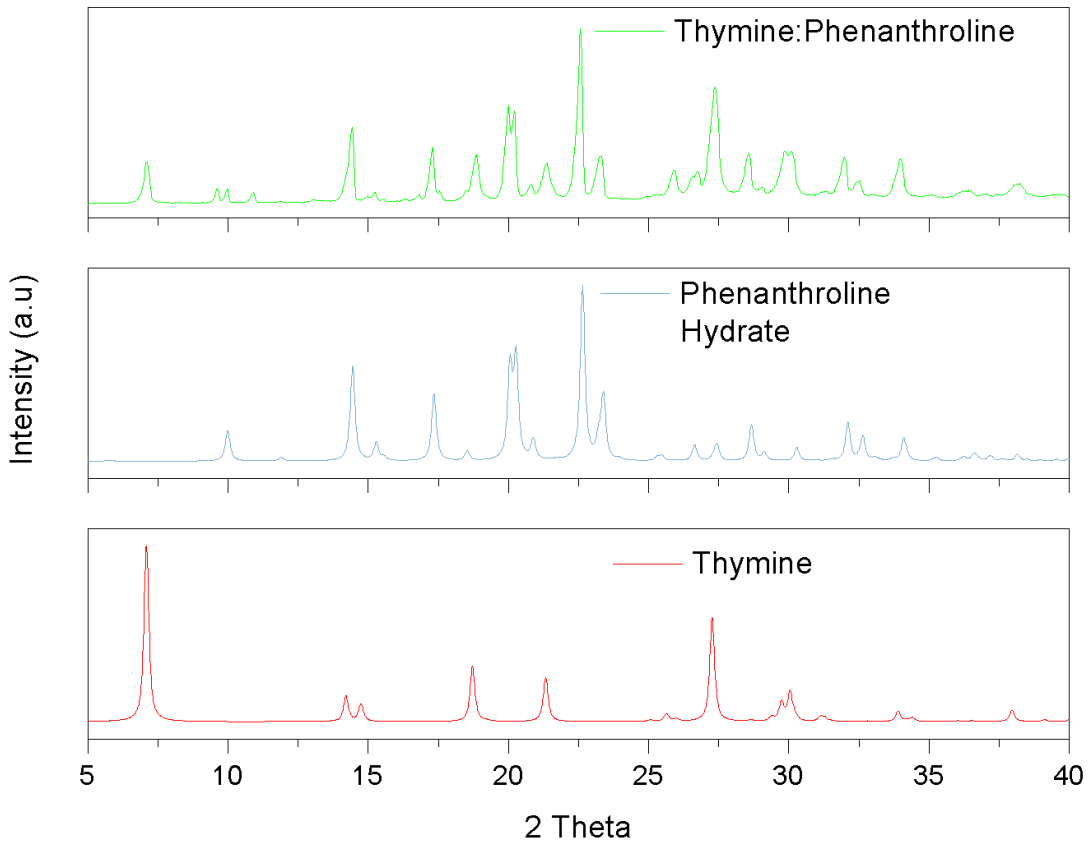

Figure S2: Simulated X-ray powder diffraction patterns of thymine and 1,10-phenanthroline hydrate, and experimental pattern obtained after milling their mixture.

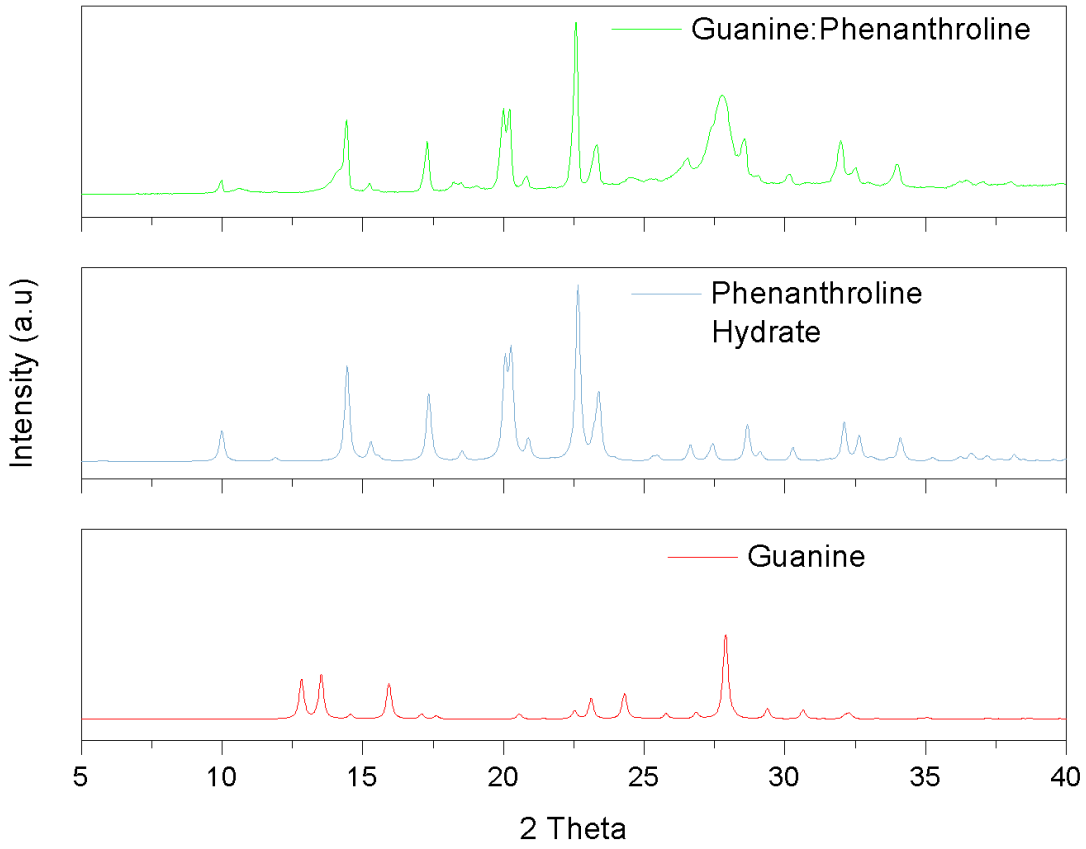

Figure S3: Simulated X-ray powder diffraction pattern of 1,10-phenanthroline hydrate and experimental patterns of guanine and the product of milling of a mixture of the two.

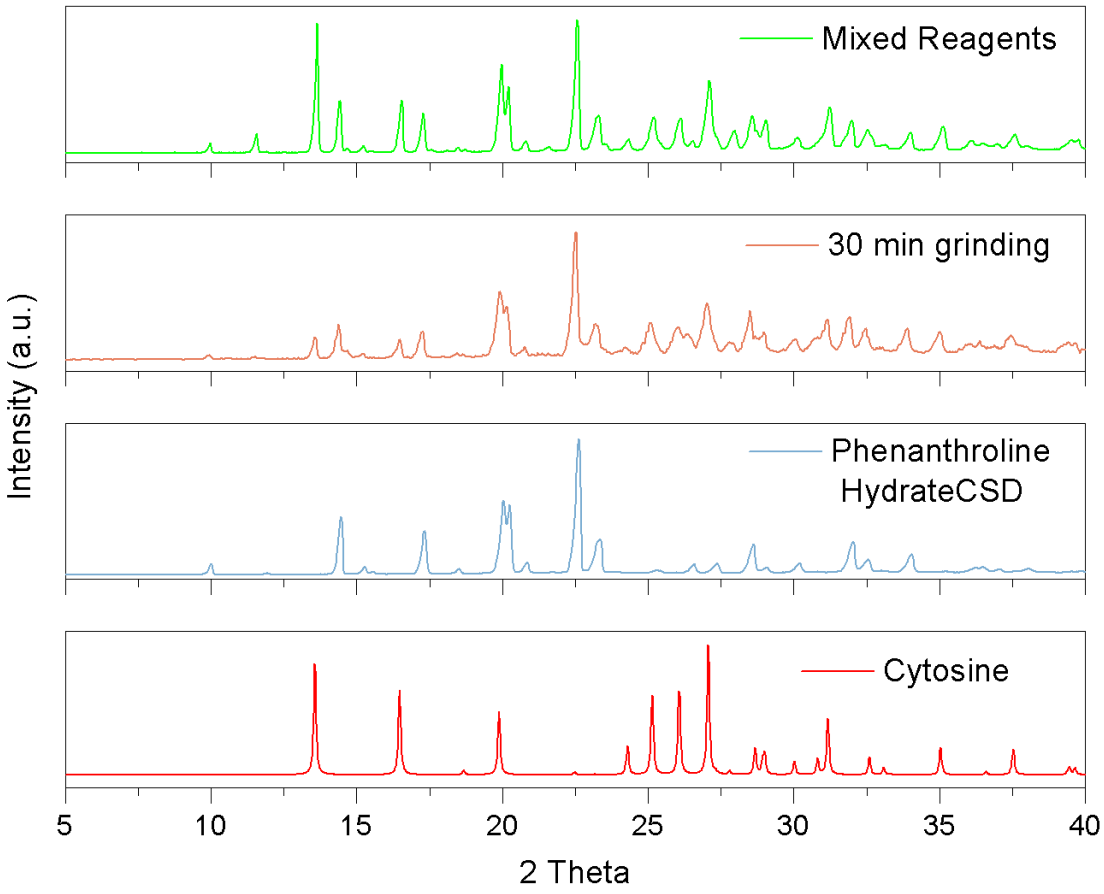

Figure S4: Comparison of XRD patterns of mixed reagents, 30 min milling and starting materials.

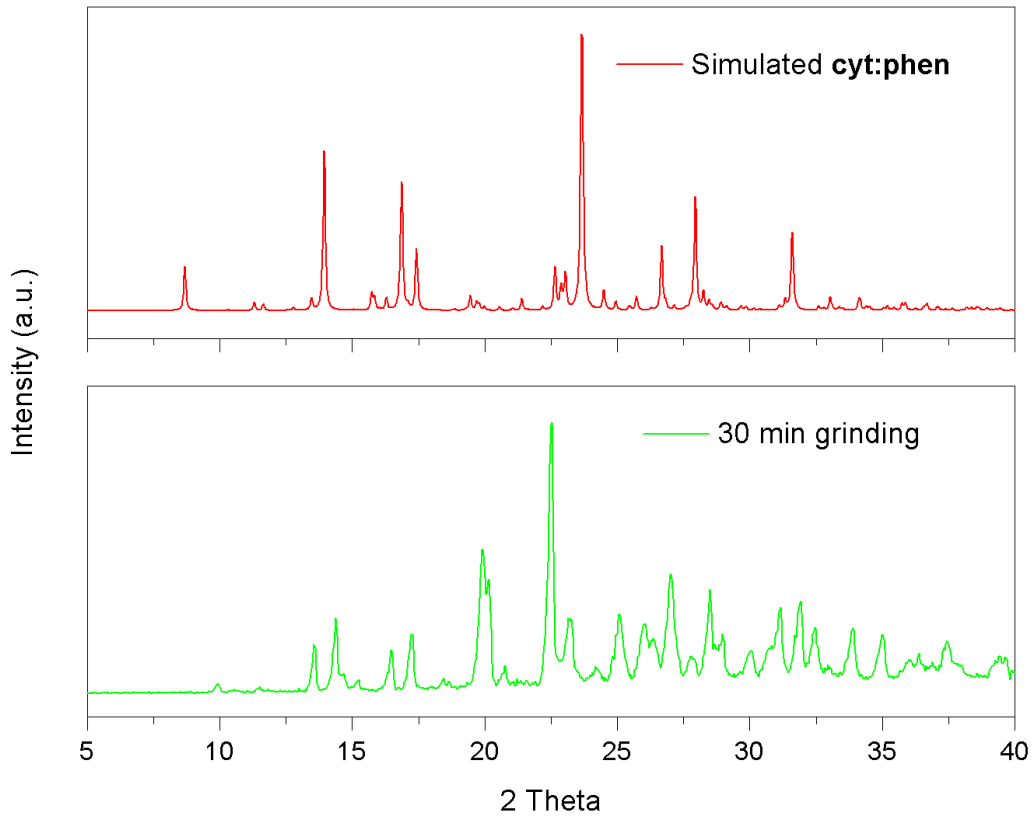

Figure S5: XRD patterns showing that 30 min grinding is not sufficient to achieve phase transformation to the cyt:phen co-crystal

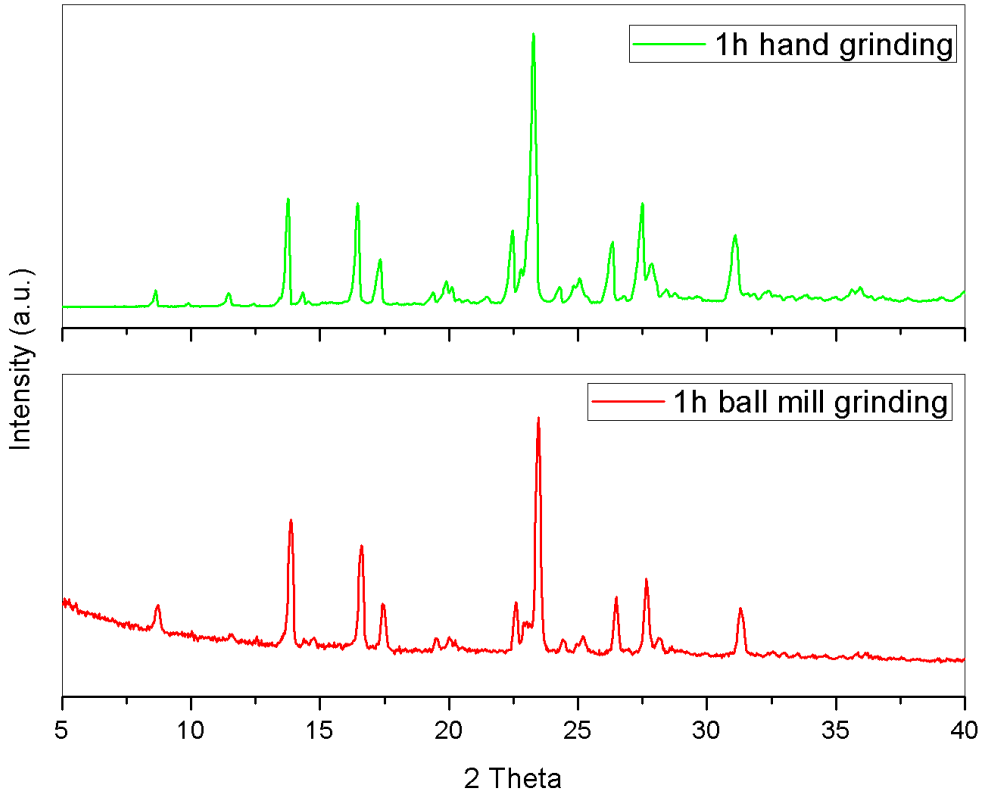

Figure S6: XRD patterns collected from sample ball-milled for 60 minutes and one ground by hand for 60 minutes. In each case all of the diffraction peaks can be indexed using the structure of the cyt:phen co-crystal.

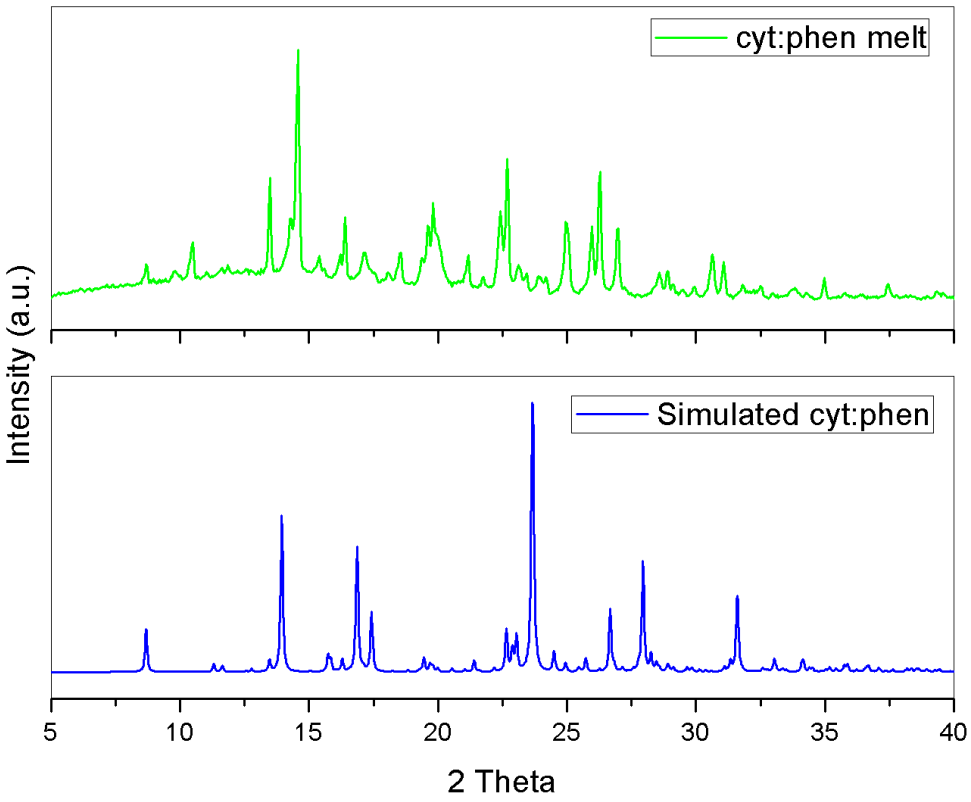

Figure S7: XRD pattern of product of melting cyt:phen (green) compared with simulated pattern for the pristine phase.

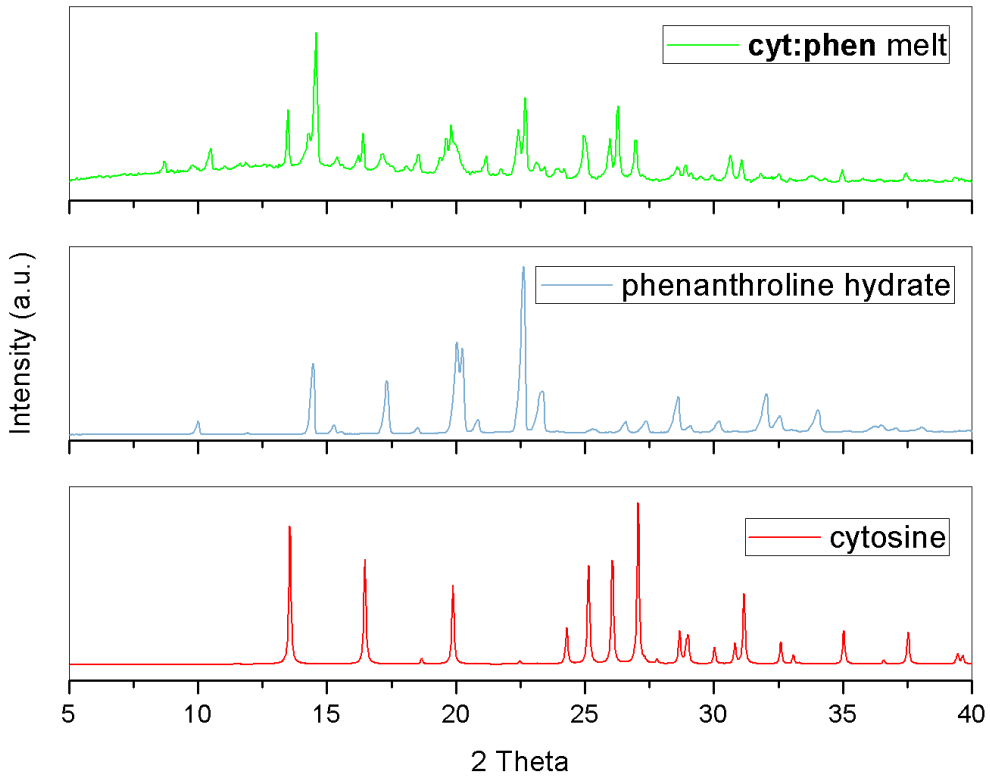

Figure S8: XRD pattern of product of melting cyt:phen (green) compared those for cytosine and phenanthroline hydrate.