

The solvates and a salt of an antibiotic agent, nitrofurantoin: Structural, thermochemical and desolvation studies†

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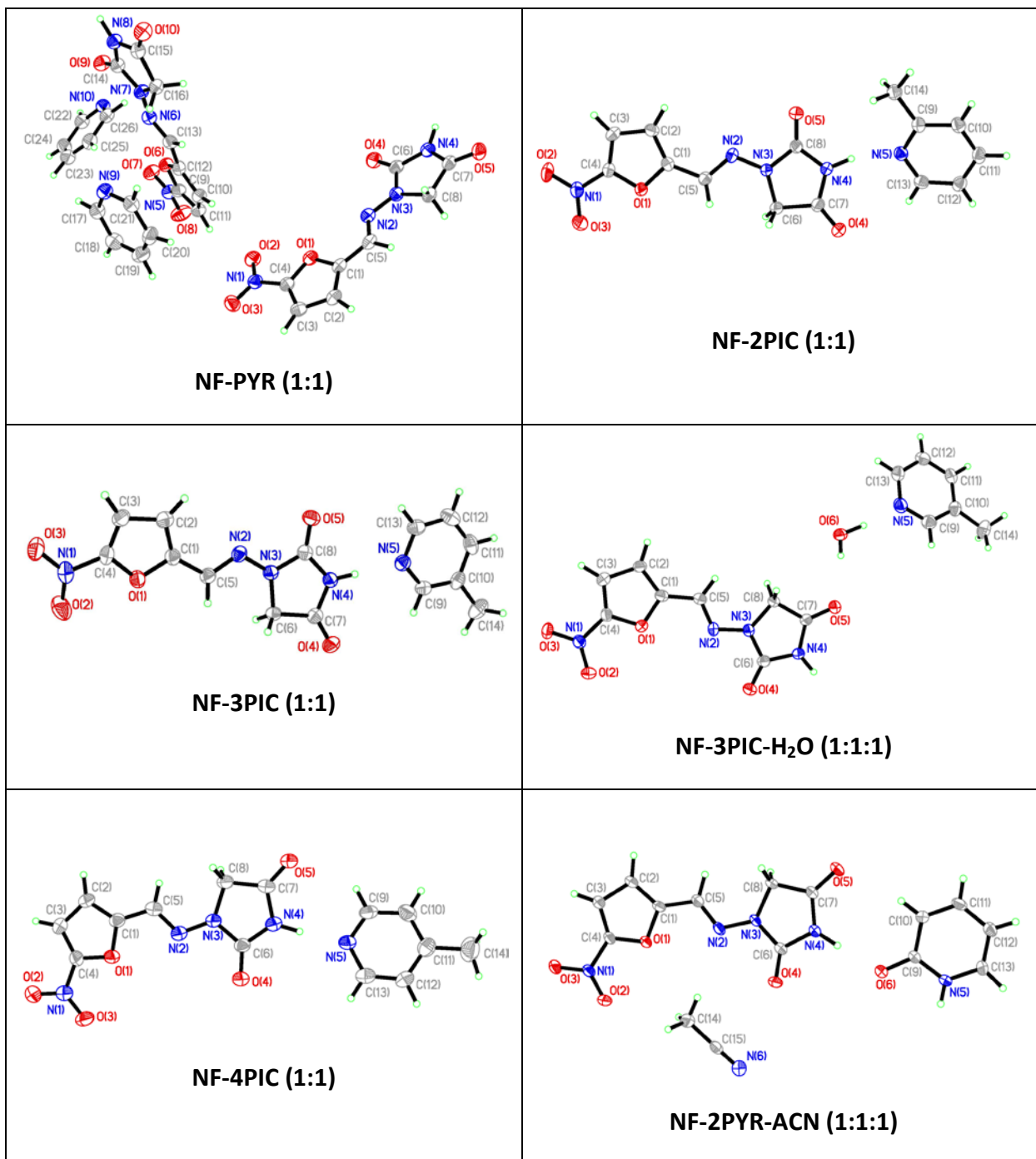
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Electronic Supplementary Information (ESI)

(7 pages)

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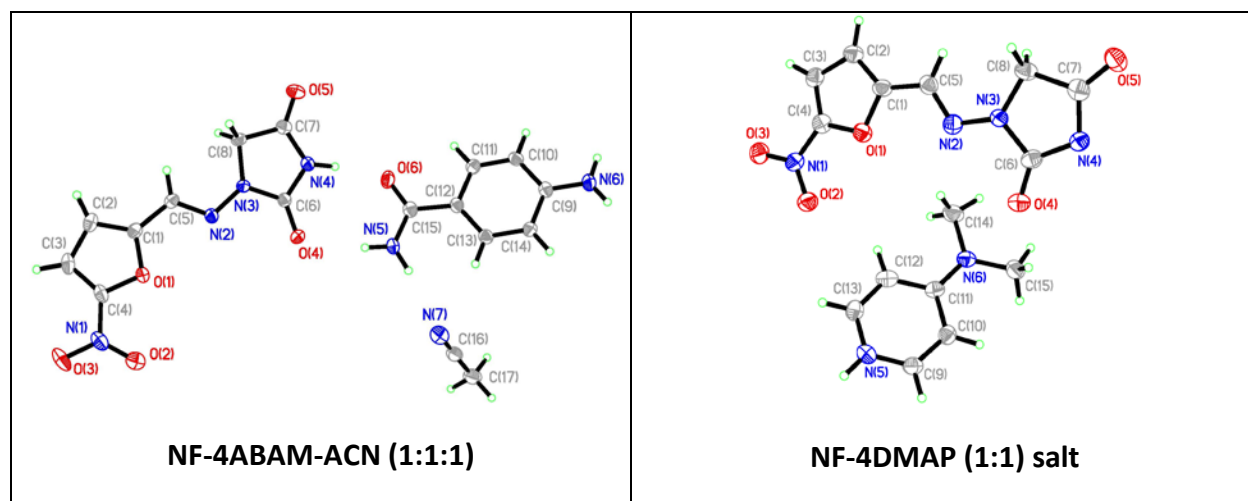


Fig. S1 ORTEP diagrams plotted at 50% probability level for the multi-component crystals reported in this study.

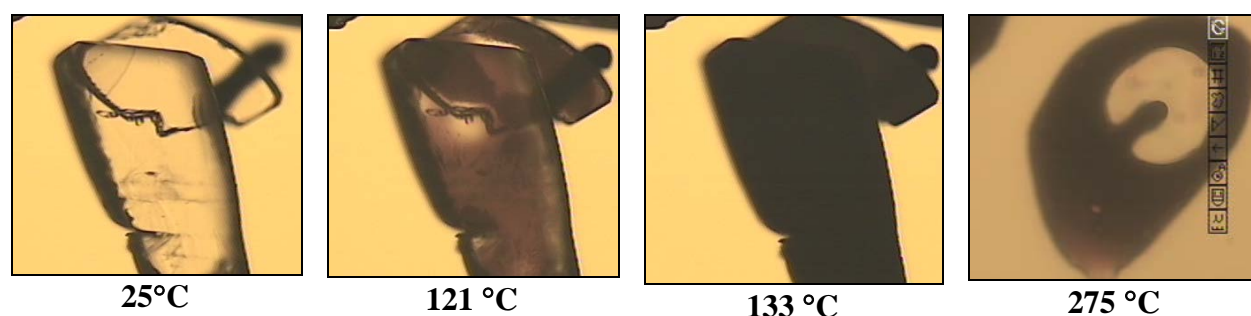


Fig. S2 Hot-stage microscopy images obtained with a crystal of NF-2PIC at 25, 121, 133, and 275 °C.

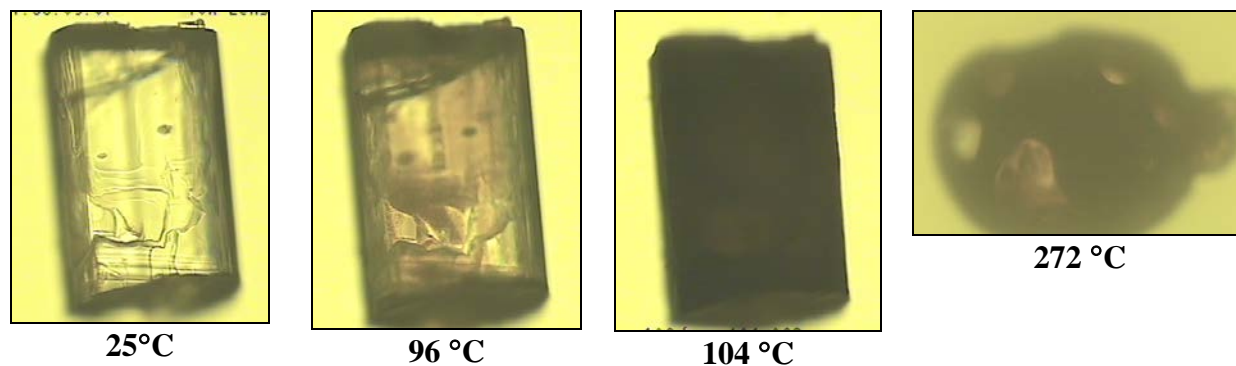


Fig. S3 Hot-stage microscopy images obtained with a crystal of NF-3PIC at 26, 96, 104, and 276 °C.

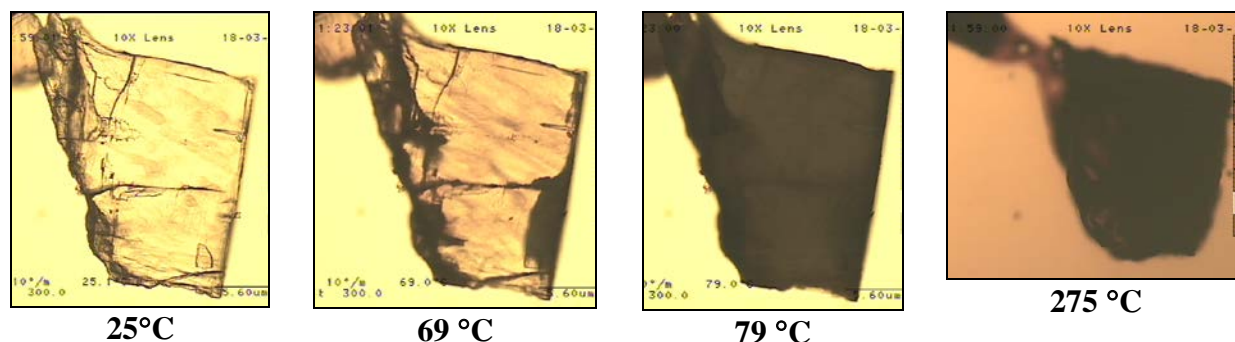


Fig. S4 Hot-stage microscopy images obtained with a crystal of NF-3PIC-H₂O at 25, 69, 79, and 275°C.

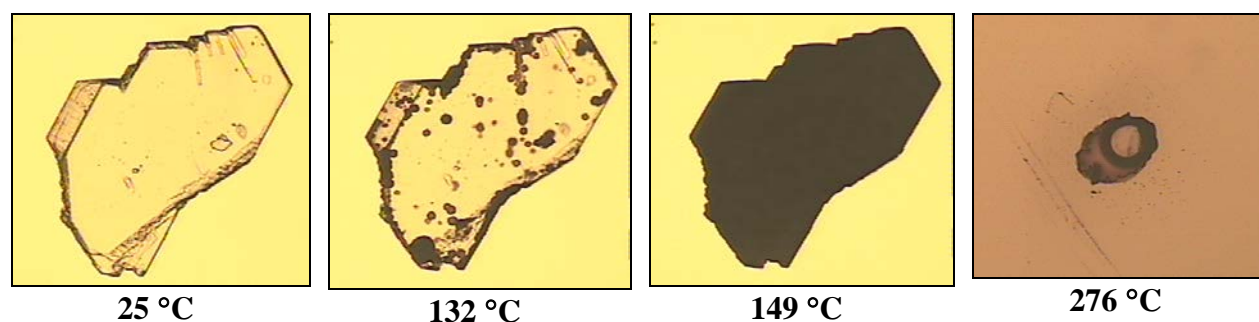


Fig. S5 Hot-stage microscopy images obtained with a crystal of NF-4PIC at 28, 132, 148, and 276°C.

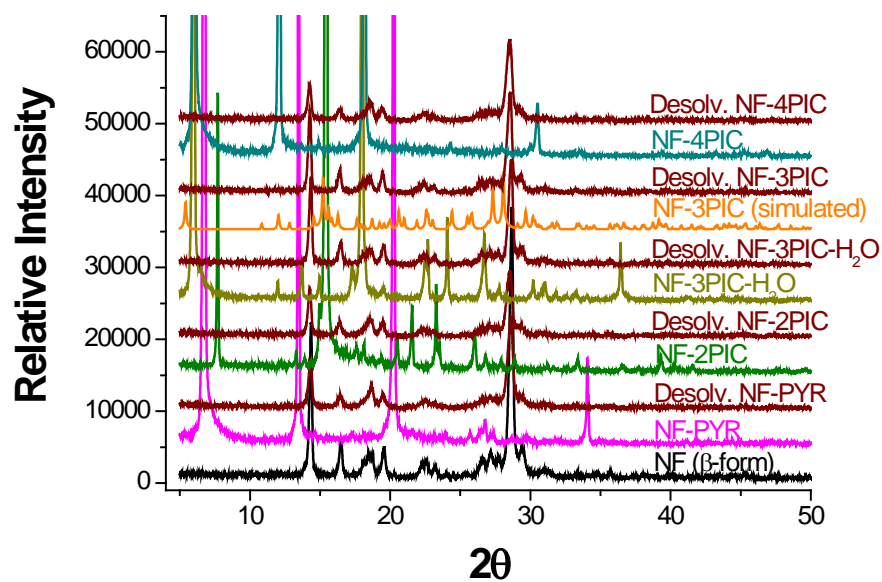


Fig. S6 Desolvated products of NF-PYR, NF-2PIC, NF-3PIC-H₂O, NF-3PIC and NF-4PIC shown to be matching with pure NF (β-form).

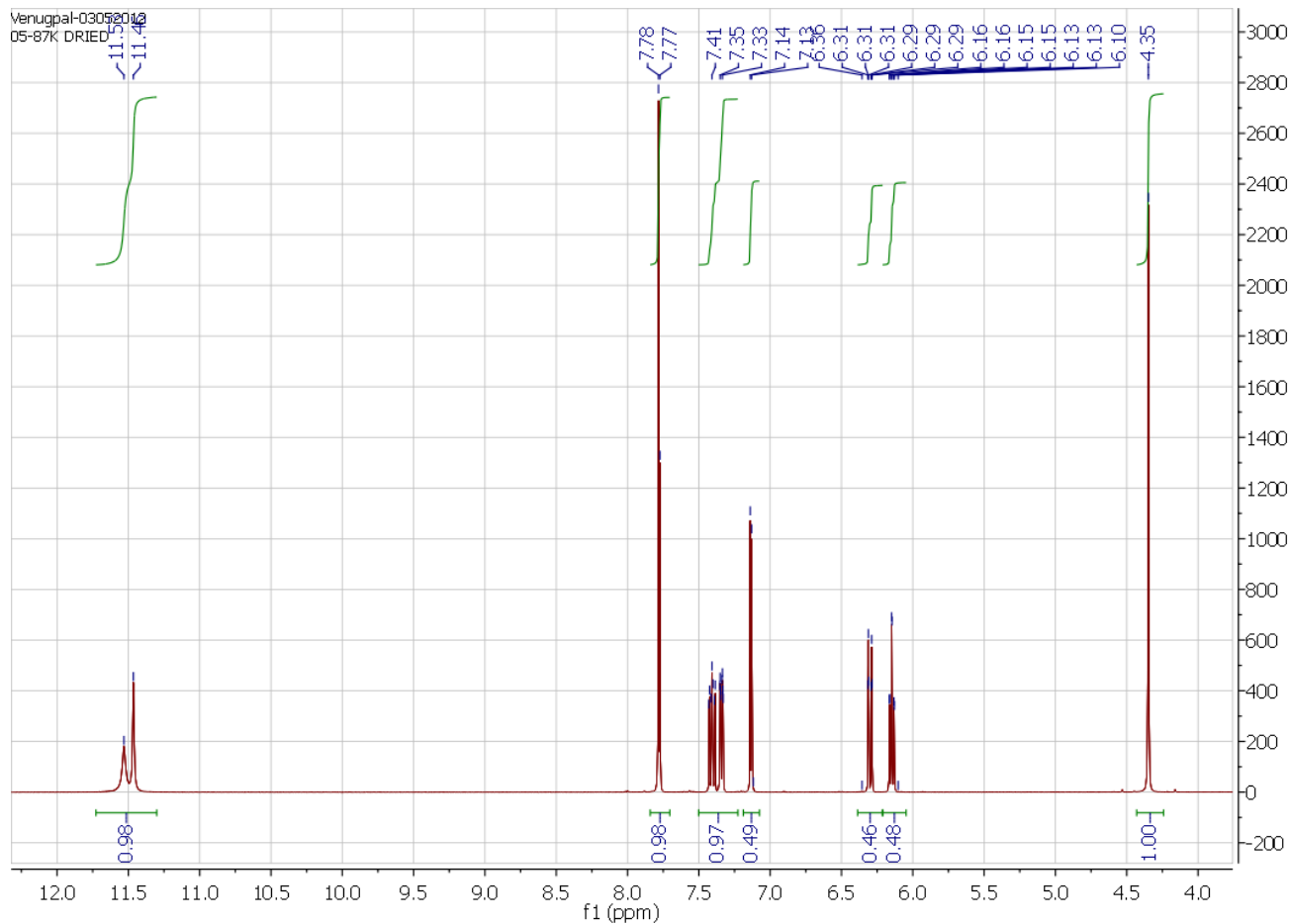


Fig. S7 ^1H NMR spectra of a dehydrated NF-2PYR-ACN at 90 °C in a vacuum oven at RT for two days. Notice the chemical shifts in δ ppm at 4.3 (2H), 7.1 (1H), 7.8 (2H) and 11.4 (1H) for NF and at 7.7 (2H), 8.7 (2H) for BIPY and an integration indicated for a 1:1 stoichiometry for a co-crystal.

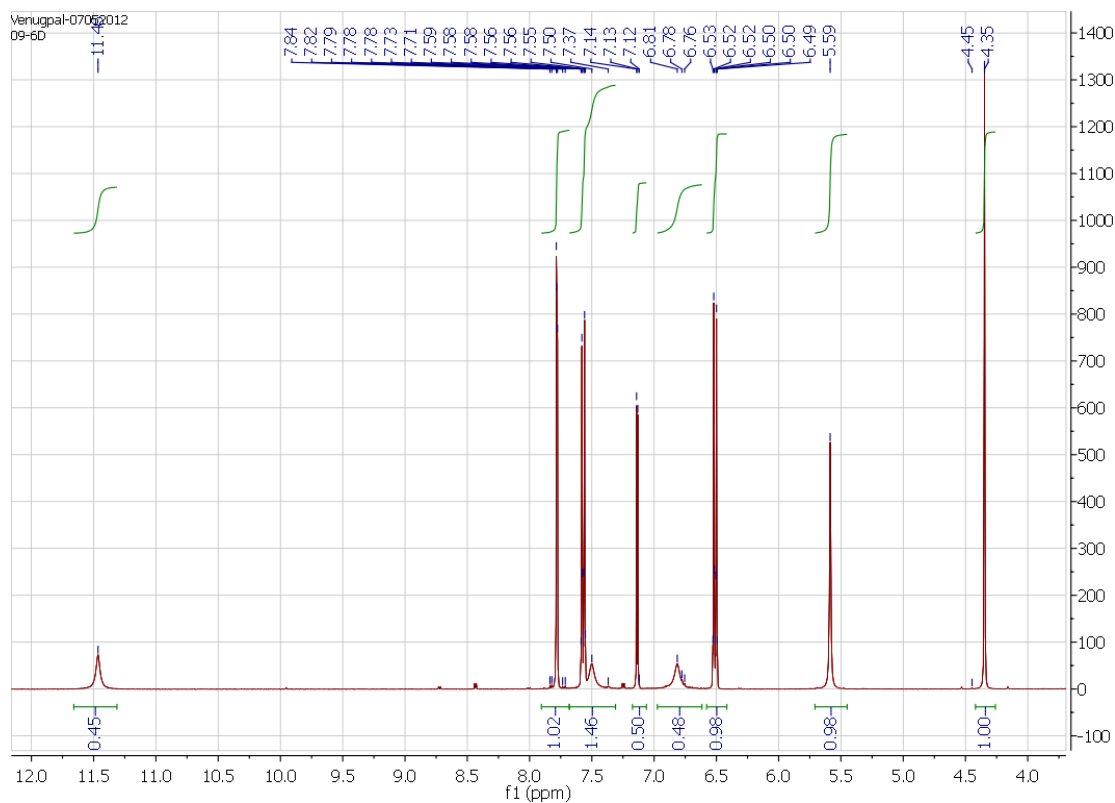


Fig. S8 ^1H NMR spectra of a dehydrated NF-4ABM-ACN at 90 °C in a vacuum oven (~10 mbar pressure) for two days. Notice the chemical shifts in δ ppm at 4.3 (2H), 7.1 (1H), 7.8 (2H) and 11.4 (1H) for NF and at 5.5 (2H), 6.5 (2H), 6.8 (1H), 7.5 (1H) and 7.6 (2H) for 4ABM and an integration indicated for a 1:1 stoichiometry for a co-crystal, NF-4ABM.

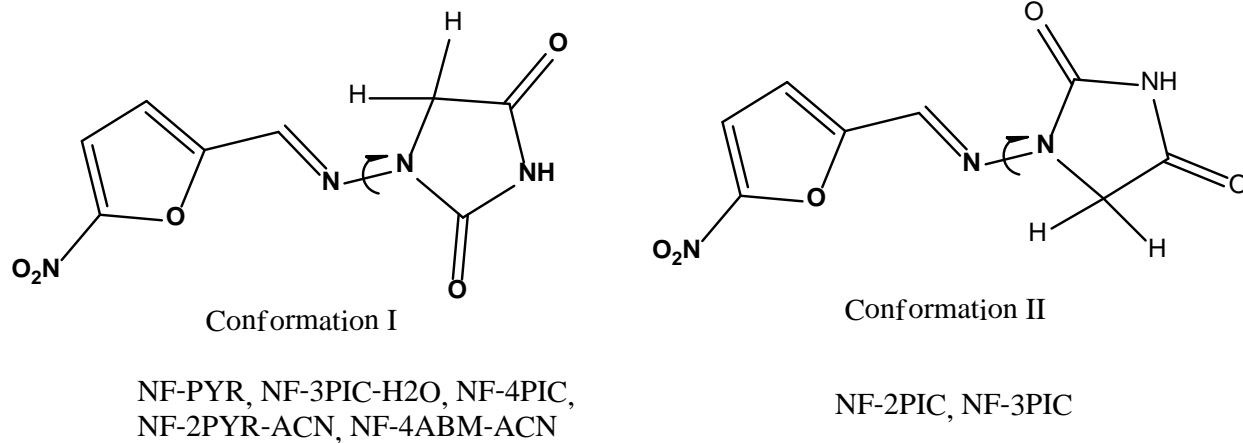


Fig. S9. All the molecular complexes adopt conformation I except for NF-2PIC and NF-3PIC (conformation II).

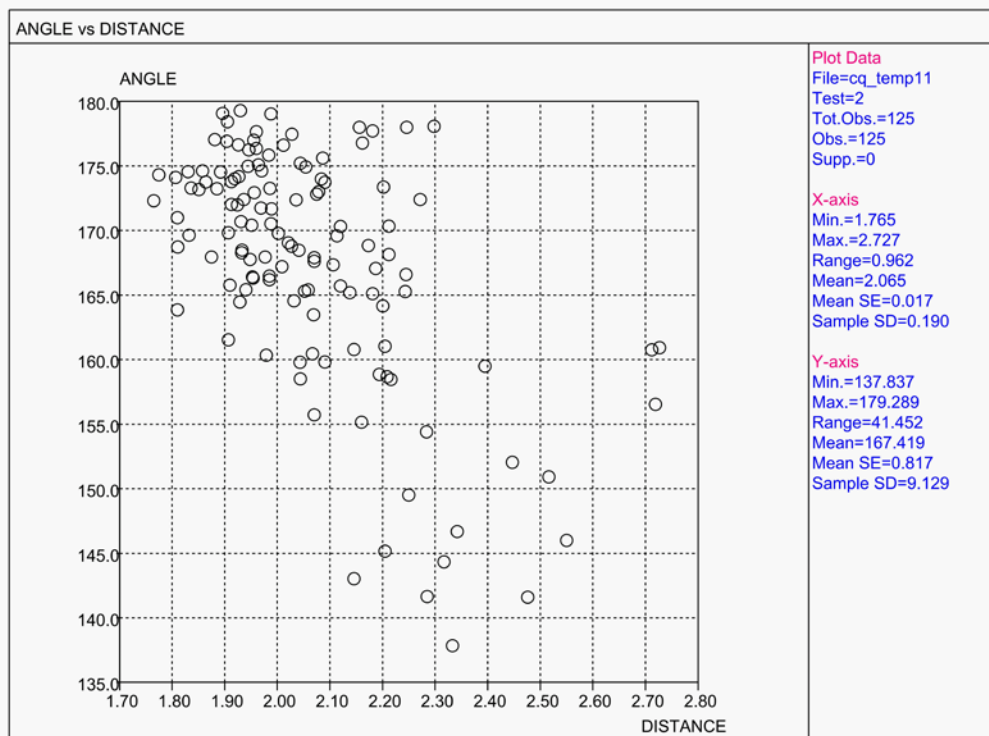


Fig. S10 A scatter plot of N–H···N interactions between imide N–H and pyridyl–N retrieved from CSD. It reveals that in ~37.5% crystal structures N–H···N synthon was observed with the mean of bond distance 2.065 Å and bond angle 167.4°.