Electronic Supplementary Material (ESI) for CrystEngComm

An NMR crystallography approach to analyse the role of intermolecular hydrogen bonding and π–π interactions in driving co-crystallisation of indomethacin and nicotinamide

Dmytro V. Dudenko, Jonathan R. Yates, Kenneth D. M. Harris, Steven P. Brown

S1. NICS Map for IND in the IND-NIC 1:1 Cocrystal

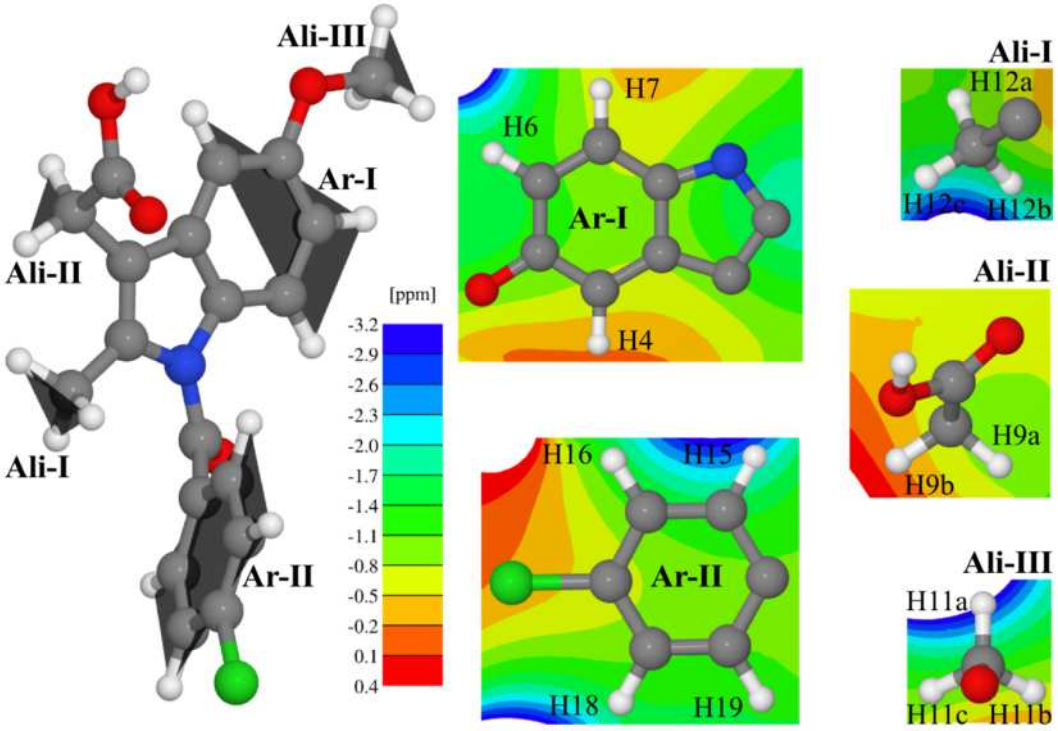

Fig. S1. NICS map for IND in the IND-NIC 1:1 cocrystal showing the effect of aromatic ring currents on the NMR chemical shifts

S2. Molecular Fragments Used for Calculating Interaction Energies

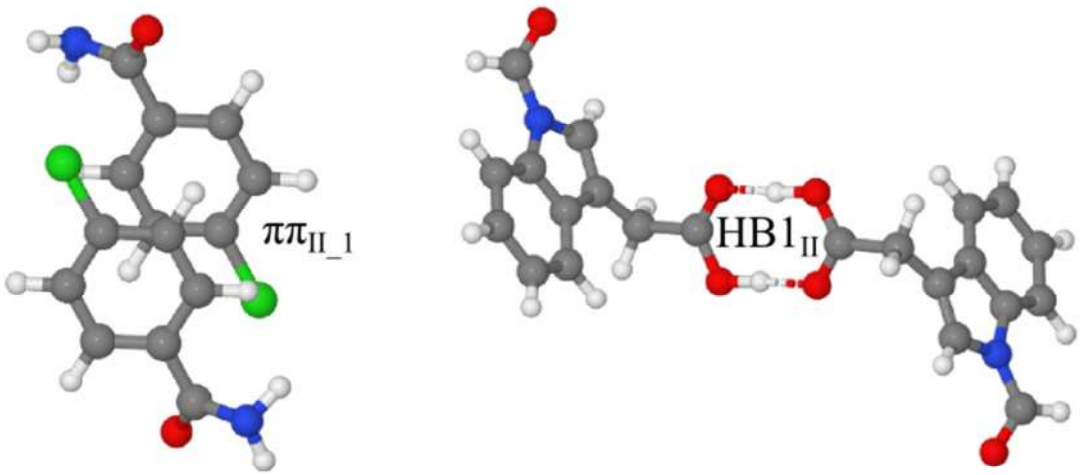

Fig. S2. The molecular fragments used to construct the dimer models employed in the calculation of intermolecular hydrogen bonding and π–π interactions for the IND-γ crystal structure (see Fig. 4 in the main text).

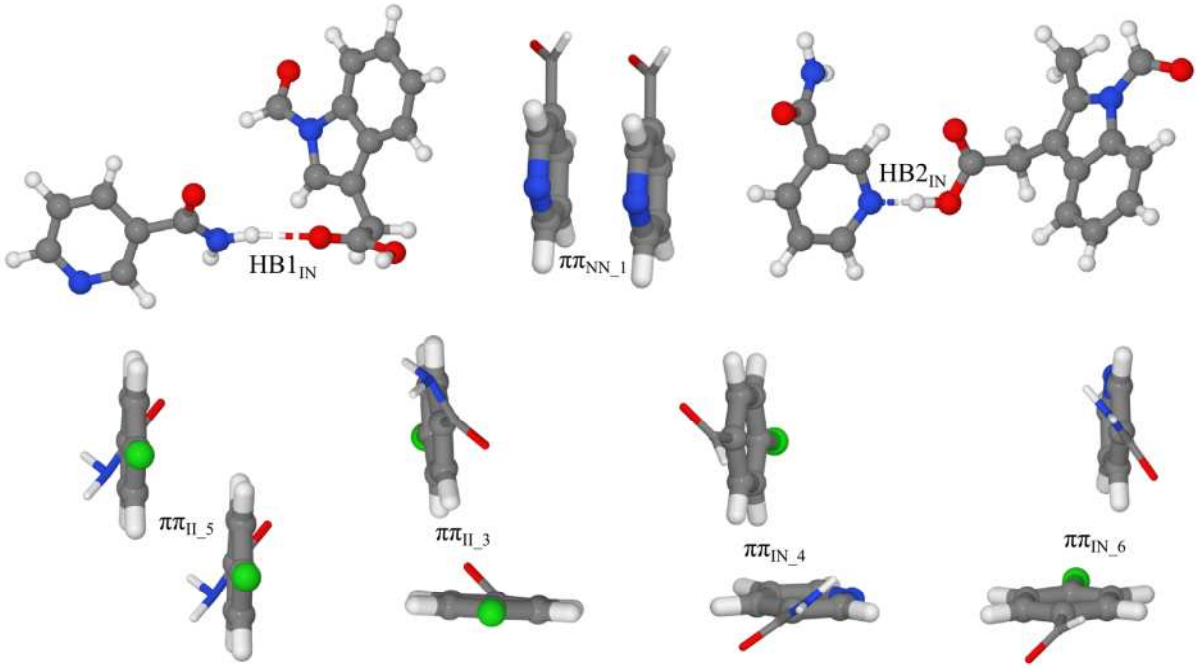

Fig. S3. The molecular fragments used to construct the dimer models employed in the calculation of intermolecular hydrogen bonding and π–π interactions for the IND-NIC crystal structure (see Fig. 6 in the main text)

S3. Comparison Calculations for Energetic Contributions

Table S1. Test comparisons of DFT method with Grimme energy dispersion correction scheme against corresponding MP2 calculations. Energies are in kcal/mol

method	$\pi\pi_{\_II\_1}$ (IND)	$\pi\pi_{\_NN\_1}$ (NIC)	$HB2_{\_NN}$ (NIC)	$HB3_{\_NN}$ (NIC)
B97D/6-311+G*	6.1	2.8	9.0	8.1
MP2/6-311+G*	6.6	2.8	7.7	7.7