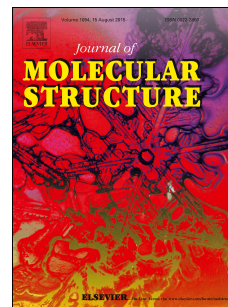


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The Hirshfeld surface of three new isonicotinyldiazine co-crystals: Comparison of hydrogen bonds and crystal structures

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Abstract: The influence of the change of aromatic acids ligand in the interactions with isonicotinyldiazine (ISO) molecule in three new co-crystals has been investigated as well as a study of the hydrogen bonds formed between the ligands through Hirshfeld surface analysis and fingerprint plots. These analyses are extremely sensitive to the chemical environment of the molecule and are unique to a particular molecule so they can identify the differences between the crystal packing in the solid state. Although the conformation of ISO molecule being practically identical in all three compounds and the interactions mainly involve the N – H···O and O – H···N type, the fingerprint plots only for ISO molecule in the three compounds are different and exhibit the influence in this molecule due to the modification of the functional groups of ligands.

Keywords: Hirshfeld surface, fingerprint plots, co-crystals, isonicotinyldiazine, hydrogen bonds.

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