MS35-P29 | INSIGHTS INTO THE MOLECULAR ARRANGEMENTS OF SUBSTITUTED HYDROXYPYRIDINE CARBOXYLIC ACIDS

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Exploring the secondary interactions is important to the development of new pharmaceutical therapies by understanding the interactions at drug binding site, in protein-protein interactions and also in drug encapsulation and targeted release mechanism. Hydroxypyridinecarboxylic acids (HPC) have been proposed recently as potential chelating agents for Fe(III) and Al(III) due to their favourable properties which include low toxicity, no redox activity and high complex stability. A series of mono- and dimethyl, hydroxy-ethyl and carboxy-ethyl substituted HPCs have been crystallized and the crystal structures have been determined by single crystal X-ray diffraction. The non-covalent interactions and molecular arrangements have been studied to investigate the electrostatic and steric effect of H-donor and –acceptor substituents to the molecular self-assembly. The position of the hydroxyl proton involved in an intramolecular hydrogen bond with the carboxylate oxygen inform us about the electrondistribution on the oxygen donor atoms and about the aromaticity of the pyridine ring. This is important because this proton is replaced by the metal ion during the action of chelation therapy. The main secondary interactions (π...π, C-O…π, C-H…O, N-H…O) have been identified with which synthon arrangements are preserved in the crystals of different substituents.

These results could give a deeper understanding of intermolecular interactions and their effect on the arrangement of molecules in the solid phase influenced by addition of H-donor and acceptor substituents.

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