Poster Presentation

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Pharmaceutical Drug Polymorphism: A Case Study of Three Novel Drugs

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Polymorphism is more widespread in pharmaceutical solids, with estimates of 30-50% in drug-like molecules, compared to 4-5% polymorphic crystals in the Cambridge Structural Database (Nangia, 2007). Most of the drug molecules are formulated and marketed in crystalline form and many of these are highly functionalized and can self-organize in several ways in the solid state with nearly the same lattice energies. Though a lot of work is going on in the field of pharmaceutical drug polymorphism and its possible application in the field of crystal engineering, yet there are difficulties in getting polymorphs of many important molecules. The present work deals with a comparative crystallographic study on the existing polymorphic forms of three medicinally important molecules, Aspirin, Paracetamol and Norfloxacin which are known to have a wide spectrum of medicinal activities. Broadly, the present study accounts for the following observations: (i) Choice of the solvent system, its purity and its reaction mechanism with solute under ideal condition of growth/crystallization. (ii) The interaction of grown material with X-rays should be very healthy in the sense that maximum number of planes in a given crystal should diffract the incoming X-ray beam. This aspect is once again related to quality single crystal growth. Fairly good interaction of a compound with X-rays leads to better refined structure, yielding a very high level of confidence between the chemical and computed structure. (iii) Analysis of a molecule's ability to exhibit biological activities by employing some suitable empirical and clinical modes. (iv) Most of physical properties of a grown material depend on how the molecules have been packed in the unit cell and how the derived knowledge of intra and intermolecular interactions is applied for engineering a crystal of choice.

Keywords: Polymorphism, Hydrogen bonding, Preparation of Single crystals