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Crystallographic Perspective of Pharmaceutical Co-crystals: Intermolecular H-Bonding between Heterocyclic Nitrogen Compounds and Carboxylic Acids. Dedong Wu, James A. Osborn, Craig D. Collins, Jean M. Surian, AstraZeneca PLP, Wilmington, DE 19850 USA.

Pharmaceutical co-crystals refer molecular complexes of active pharmaceutical ingredients (APIs) with other molecules. The technique of co-crystal formation is an important alternative method for pharmaceutical form selection. Intermolecular hydrogen bonding plays a key role in co-crystal formation in a pharmaceutical co-crystal. Thus, the study of molecular assembly to form co-crystals in the molecular level can be applied in understanding and designing new crystalline forms of pharmaceutical co-crystals. For the purpose of the study, we have employed heterocyclic aromatic compounds containing basic nitrogen and investigated their occurrence as co-crystals in the Cambridge Structural Database (CSD). Carboxylic acids have been selected as co-crystal agents. The presentation will demonstrate intermolecular bonding modes in crystal structures of co-crystals between heterocyclic nitrogen compounds and carboxylic acids. The tendency to form pharmaceutical co-crystals will also be discussed.