MS32-05 | Supramolecular Synthons Orientation Rule in the Crystals of Benzodiazepines, Quinoxalines and Benzimidazoles as a Predictive Tool in the Material Design

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Creation of new materials and pharmaceuticals based on heterocyclic compounds require the development of the predictive aspect in the description of their structure in the crystalline state. An empirical rule connecting the type and dimension of supramolecular structures (arising due to non-covalent interactions) with their orientation in the unit cell of the crystal has been first formulated. The latter based on the analysis of new series of benzodiazepines, benzimidazoles and quinoxalines with a wide variation of the substituents. According to the rule, the one-dimensional supramolecular structures are oriented predominantly in the crystals along the smallest unit cell parameter, and two-dimensional layers – along two smallest parameters. The analysis of structural data from CSD for all known titled compounds confirm the versatility of the founded rule, which is associated with the orienting effect of the most pronounced structure-forming interactions in the unit cells. This rule of thumb is also observed in the case of the absence of classical hydrogen bonds in the crystal, as well as in crystals of racemic and enantiopure samples, and various polymorphic modifications, and, probably, is of a more general character, not limited only to the classes of compounds studied by us. This makes it possible not only to predict the supramolecular structure and crystal packing of the benzodiazepines and benzimidazoles, and also to expand the opportunities for targeted design of new nitrogen-containing heterocyclic compounds with desired properties.

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