and co-crystal former.
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Keywords: pharmaceutical co-crystal, polymorph, phase transformations

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New crystal forms of gabapentin

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Gabapentin (GBP) is an API used against epilepsy, neuropathic pain and in the treatment of limb tremor[1]. Several polymorphs of GBP have been reported and characterized, but only SCX of Form II was known until very recently. Our group managed to obtain two new SCX structures of different polymorphs[2,3]. These new forms are not as stable as Form II, proved by several experiments. Form IV can even be considered a disappearing polymorph [3] because it readily transforms into another form. New crystal forms of GBP were obtained on acidifying the solution. We obtained GBP chloride hemihydrate, an ethyl ester of GBP and a co-crystal of GBP-lactam and benzoic acid [Fig.1] in different crystallization conditions. All these structures were determined by SCXRD, presenting different physicochemical properties and supramolecular arrangements [5]. Intramolecular interactions are only observed in Form IV and GBP Cl hemi-hydrate.

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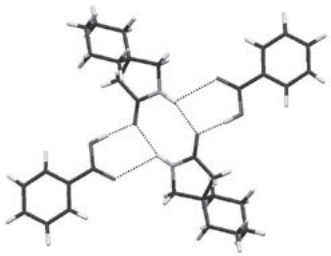

Keywords: crystal engineering, cocrystal, polymorphism

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Molecular cocrystals of peganole with peganine

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Earlier we studied solid solutions of biologically active derivatives of tricyclic quinazolines, the peganole (**1**) with the 6-bromopeganole (**2**) in different stoichiometry [1] using by single crystal X-ray diffraction methods. In all solid solutions, centrosymmetrical hydrogen-bonding interactions are found between the molecules of **1** and **2**, which forms dimers, by O-H...N hydrogen bonding associations. Recently have been prepared of cocrystal of peganole (**1**) and peganine (**3**) in the ratio of 1:1 which similar dimers connected with hydrogen bonds O-H...N. Individual **1** crystallizes as racemate. As against it **3** crystallizes in enantiomorfic forms, that confirm X-ray analysis of single crystals of **3** received by us and the literature [2]. In the unit cell of cocrystals both enantiomorphic forms of each substance (**1** and **3**) are located. Thus, individually peganine crystallizes in enantiomorph form, but in cocrystal take part both enantiomorfic forms. Probably, racemat peganole promote to cocrystallization of racemate peganine.

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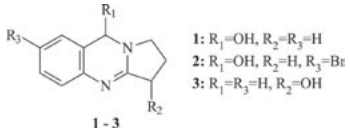

Keywords: cocrystals, solid solutions, hydrogen bonds

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Subtle relationships between the structures of some aspirin derivatives

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Prompted by the identification of a second polymorph of the simple analgesic molecule aspirin, we have made a structural systematics study of some simple derivatives of aspirin. The main aim of this was to see how robust are the packing features in the two phases of the parent molecule, which have 2D similarity, in view of the small changes in the molecular shape and the possibility that the substituent groups may themselves have some involvement in defining intermolecular interactions. Compounds selected were those in which one aromatic ring proton was replaced by a small substituent group. Two relevant structures were already known - 3-methyl aspirin and 6-methyl aspirin. Further examples, namely 4-Me, 5-Me, 5-F, 5-Cl, 5-Br, 5-I, and 5-NO_2 aspirin were synthesised from substituted salicylic acid derivatives. Structure determinations of the new compounds, and detailed comparisons of all structures using the XPac method (Gelbrich and Hursthouse (2005) CrystEngComm 7: 324-336.) revealed that the family contained two isostructural sets − the 5-Cl-, 5-Br- and 5-I- derivatives, and the 5-F-, 5-O_2N- and 5-Me derivatives. A number of lower dimensional similarities were also identified. The poster will describe the relationships found between the structures.

Keywords: aspirin derivatives, systematics of crystal structures, structural motifs

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The influence of hydrogen bonding on generation and stabilization of self-assembled layer structure

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