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Co-crystals of leucyl-alanine

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Although the ability of different molecules to crystallize in a single solid has been known for a long time [1], some of these materials became a subject of intense studies in the last decade due to pharmaceutical and other applications [2]. Short peptides may become a very useful class of co-crystallization agents due to their wide diversity, eco-friendliness and biocompatibility [3]. In this work, we screened the dipeptide leucyl-alanine (LA, see Figure) for the ability to form co-crystals with a variety of solid bioactive compounds. Solvent-assisted grinding of two compounds was followed by a powder X-ray diffraction test. The tested bioactive compounds were found to co-crystallize successfully with the peptide when they possessed both a hydrophobic part and strong hydrogen-bonding functionality. They were primarily derivatives of benzene, phenol, pyridine, pyrazine, quinoline and isoquinoline. Nearly all compounds with an amine or amide group formed a co-crystal, whereas most carboxylic acids did not form a new phase. For the successful combinations, single crystals were obtained when possible and studied using the single-crystal X-ray diffraction analysis. To our surprise, many of the co-crystals formed contained more than the two intended components due to the incorporation of the organic solvent and/or water. For example, one of the co-crystals studied displayed a complex hydrogen bonding framework built by four types of molecules: LA, 8-quinolinecarboxylic acid, ethanol and water in a 1:0.5:0.5:0.5:0.5 ratio.

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