Solid-state characterization and solubility of a genistein-caffeine cocrystal.

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Streszczenie

Combination of genistein and caffeine leads to a 1:1 cocrystalline phase, which was identified by means of a solvent-drop grinding experiment and isolated afterwards in a solution-evaporation approach. Obtained cocrystal was characterized by X-ray single-crystal and powder diffraction as well as investigated in terms of thermal stability and Hirshfeld surfaces. A scale-up procedure was provided by slurry technique, enabling solubility determination. Neutral forms of both compounds cocrystallize in a common $P2_1/c$ space group of the monoclinic crystal system. Analysis of packing and interactions in the crystal lattice reveals formation of molecular layers, formed by O–H···O, O–H···N and C–H···O-type contacts between genistein and caffeine molecules, whereas stabilization of the three-dimensional crystal lattice is provided by π···π interactions. Dissolution studies in a 50:50 v/v ethanol–water medium revealed that the maximum solubility of the cocrystalline phase reached 0.861 mg/mL after 8 h, revealing some degree of enhancement as compared to parent genistein, maximum solubility of which was also reached after 8 h and equalled 0.588 mg/mL.

Słowa kluczowe

Genistein, Caffeine, Cocrystals, Solubility, X-ray crystallography

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