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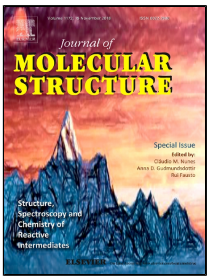


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# Preparation of a 1:1.5 cocrystal of kaempferol with 4,4'-bipyridine based on analyzing intermolecular interaction of building units

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**Abstract:** Based on analyzing intermolecular interaction in building unit of cocrystal of quercetin with 4,4'-bipyridine (**QUE·BPY**) reported by us on before, a new cocrystal of kaempferol with 4,4'-bipyridine (**KAE·BPY**) has been designed and synthesized. Within the reported **QUE·BPY**, 3'-OH was neither involved in the formation of the building unit nor played a big role in the 2D layer. Consequently, we boldly speculate kaempferol without 3'-OH might crystallize with 4,4'-bipyridine to form similar structure to **QUE·BPY**. Just as expected, structural analysis shows kaempferol molecules and 4,4'-bipyridine molecules alternate connect to form the building units through 7-OH and 4'-OH hydrogen bonds, the structure of **KAE·BPY** is similar to **QUE·BPY**. This work proves that new cocrystals could be designed and synthetized by analyzing the intermolecular interaction in building unit and seeking right structure of Active Pharmaceutical Ingredients (APIs). Additionally, the cocrystal of kaempferol with 4,4'-bipyridine shows advantages in terms of hygroscopic stability in comparison to pure kaempferol.

**Key words**: Kaempferol; 4,4'-bipyridine; Cocrystal; Hirshfeld surfaces; Hygroscopic stability