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Prediction of Polymorphism and Crystallographic Properties of Cinnamic Acid using CSD-Materials

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1. Introduction
   Cinnamic acid (2-phenylacrylic acid) is a naturally occurring aromatic fatty acid with known cytotoxic activity towards different cancer cell lines [1]. The activity of this important molecule can be attributed to potential substitution reactions on the phenyl ring, the reducing ability of the C=C double bond and the ability of the -COOH group to donate an H+ to scavenge free radicals [2]. A search in the Cambridge Structural Database (CSD) shows that nine polymorphs of cinnamic acid have been deposited in the database with seven of the entries crystallizing in the P21/n space group and P21/a and P21/c for the remaining two polymorphs. Other entries involving cocrystals of cinnamic acid were also found in the database. These crystals are usually grown in order to investigate the solid state stability and physicochemical properties of the resulting products [3]. Polymorphism, the occurrence of different crystal forms of the same compound under different crystallizing conditions is an important phenomenon in the pharmaceutical industry since two polymorphs of the same compound may have different therapeutic effects [4].
2. Results
   Recently, we crystallized a new polymorph of cinnamic acid which has been deposited in the webCSD with refcode; CINMAC12. It has the following cell parameters; a = 6.0098(2), b = 3.941(2), c = 31.5336(14); α = 90o, β = 90.349(4)o, γ = 90o with a P21/c space group.
   This presentation will demonstrate the prediction of polymorphism and other crystallographic structural parameters using the CSD-Materials functionality in the program Mercury. Parameters such as full interaction maps, hydrogen bond statistics and aromatics analyzer will be accessed. This work will be of interest to crystallographers, crystal engineers, pharmacists and chemists.
3. References

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