



Contribution ID: 122

Type: **not specified**

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

Thursday, 16 November 2023 11:15 (15 minutes)

### 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<sup>+</sup> 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;  $a = 6.0098(2)$ ,  $b = 3.941(2)$ ,  $c = 31.5336(14)$ ;  $\alpha = 90^\circ$ ,  $\beta = 90.349(4)^\circ$ ,  $\gamma = 90^\circ$  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

- Feng, L.S., et al., Cinnamic acid hybrids as anticancer agents: A mini-review. *Archiv der Pharmazie*, 2022. 355(7): p. 2200052.
- De, P., M. Baltas, and F. Bedos-Belval, Cinnamic acid derivatives as anticancer agents-a review. *Current medicinal chemistry*, 2011. 18(11): p. 1672-1703.
- Khushaim, M.S., et al., Experimental and computational simulations of nematogenic liquid crystals based on cinnamic acid in pure and mixed state. *Liquid Crystals*, 2021. 48(11): p. 1493-1504.
- Chistyakov, D. and G. Sergeev, The polymorphism of drugs: New approaches to the synthesis of nanostructured polymorphs. *Pharmaceutics*, 2020. 12(1): p. 34.

**Primary author:** TETTEH, Samuel (University of Cape Coast, Ghana)

**Presenter:** TETTEH, Samuel (University of Cape Coast, Ghana)

**Session Classification:** Partner

**Track Classification:** Partner