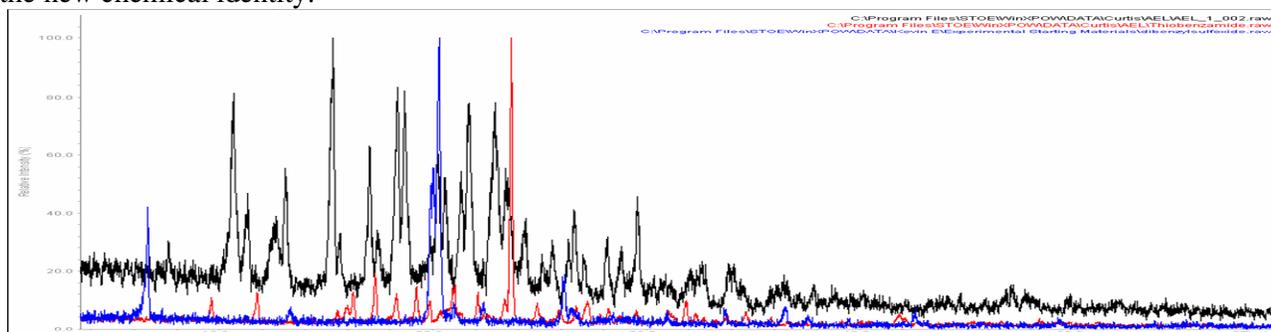


## **Title: Co-crystallization**

There is great interest in co-crystals in recent years, especially within the pharmaceutical arena. This is primarily because co-crystals have the potential to alter and optimize physical properties such as crystalline form, solubility, and stability of an active pharmaceutical ingredient (API) without detrimentally affecting its activity.<sup>1</sup> The design of co-crystals requires knowledge of robust supramolecular synthons. Sulfur functional groups can contain potent hydrogen bond donors and acceptors, and therefore, attracted our attention as powerful co-crystal formers.

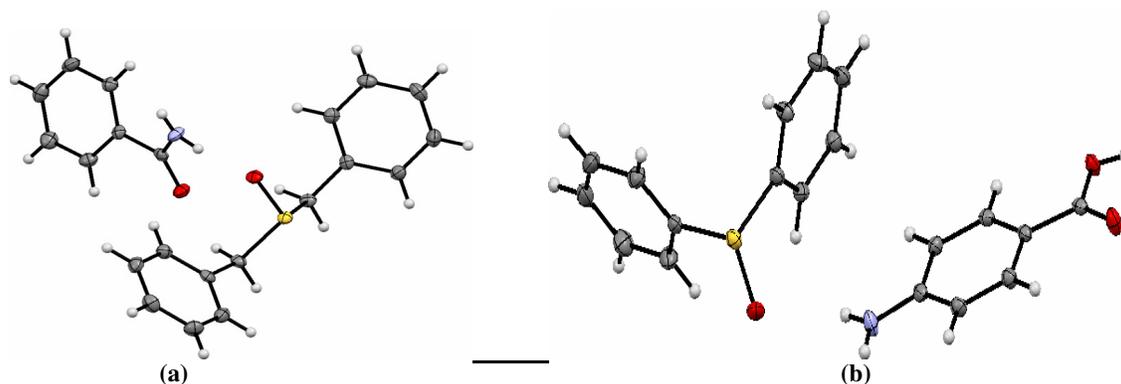
## **Co-crystal Screening:**

An extensive screening process was undertaken, to investigate the formation of co-crystals with sulfur functional groups with a variety of potential co-crystal formers. Co-crystals were prepared using the following techniques: solution crystallisation predominately slow evaporation, melt crystallisation, neat grinding and liquid assisted grinding. Materials was analysed using IR, DSC and PXRD for the formation of the new chemical identity.



**Figure 1:** The PXRD of co-crystal obtained by grinding (black) against starting material sulfoxide (blue) & amide (red)

## **Co-crystal Structures:**



**Figure 2:** The asymmetric unit of (a) dibenzyl sulfoxide benzamide<sup>2</sup> & (b) diphenyl sulfoxide 4-aminobenzoic acid co-crystal<sup>2</sup>

## **Results & Discussion:**

A large variety of sulfur functional group co-crystals have been synthesised and X-ray crystal structures have been obtained. Understanding of intermolecular interactions has lead to the formation of novel solid material.

## **Future Work:**

Co-crystallisation of API molecules and to investigate the physical properties of these novel solids. Investigation of intermolecular interactions between racemic and enantiopure co-crystals.

## **Reference:**

- McNamara, D. P.; Childs, S. L.; Giordano, J.; Iarriccio, A.; Cassidy, J.; Shet, M. S.; Mannion, R.; O'Donnell E.; Park A., *Pharmaceutical co-crystals*. *Pharmaceut. Res.*, **2006**, *23*, 1888-1897.
- Eccles, K. S.; Elcoate, C. J.; Stokes, S. P.; Maguire, A. R.; Lawrence, S., E., *Sulfoxides: Potent Co-Crystal Formers*. *Crystal Growth and Design*, Accepted.