

Oral Contributions

[MS10-02] Evaluation of molecular crystal structures using Full Interaction Maps

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The specific crystalline form of a compound has a significant impact on its solid state properties. A key requirement for chemists developing crystalline materials is therefore to understand and evaluate the crystal form under investigation.

Using a technique already established for identifying favourable interaction sites in protein pockets we calculate molecular interaction maps within the context of a crystal structure.

Using three industrially-relevant compounds – sulfathiazole, anastrozole and cipamfylline – we illustrate how the molecular interaction maps can be used to evaluate the stability of polymorphic structures, assess multiple types of non-covalent interactions and provide a platform for crystal morphology analysis.