MS34-P06 | A Combined Theoretical and Experimental Investigation into the High Throughput Screening of Cocrystal Coformers

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The CrystalPredictor [1,2] and CrystalOptimizer [3] codes have explored crystallographic space successfully in several CSP investigations in recent years, including in CCDC [4] blind tests. Recent advances in CrystalPredictor [5], give significant increases in global search stage efficiency, whilst the capacity of LAM databases to reuse quantum mechanical calculations for the same molecule, allows for QM accuracy in conformation, intramolecular energy and molecular electrostatics, at forcefield cost.

Exploiting these advances, we present a high throughput cocrystallisation study into 4 API's, combined with 10 coformers. Having performed a standard, neat, CSP study on each of the molecules, assessing the energy of potential cocrystals of the API and any of the coformers becomes an almost trivial task, through judicious use of LAM databases. Comparing the energies of the cocrystals, versus the combined single crystal energies, allows the user to predict which coformer can crystallise with the API.

Cocrystallisation experiments were also performed between the API's and coformers; comparisons will be made to assess the accuracy, as well as demonstrate the capacity for the technique to be taken up into standard pharmaceutical development workflows.

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[4] A. M. Reilly, *et. al.*, Acta Crystallogr B **72**, 439 (2016).
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