This work was financially supported by the Russian Science Foundation (grant No 17-13-01209).

References:

[1] Lodochnikova, O.A., Zaripova, A.R., Fayzullin, R.R. et al (2018). CrystEngComm, DOI: 10.1039/C8CE00369.
[2] Lodochnikova, O.A., Dobrynin, A.B., Andreeva, O.V. et al (2014). CrystEngComm, 16, 6234-6243.
[3] Lodochnikova, O.A., Startseva, V.A., Nikitina, L.E. et al (2014). CrystEngComm, 16, 4314-4321.

Keywords: supramolecular synthon, polymorphism, intermolecular interactions

MS31-P11

Combining crystal structure prediction and structural comparison with experimental screening: a potential route to more polymorphs, including a 2-for-the-price-of-1 special

Riccardo Montis[1], Michael Hursthouse[2], John Kendrick[3]

1. School of Chemical Engineering and Analytical Science - The University of Manchester, Manchester, United Kingdom
2. Chemistry - University of Southampton, Southampton, United Kingdom
3. Department of Chemistry and Forensic Science - University of Bradford, Bradford, United Kingdom

email: riccardo.montis@manchester.ac.uk

Although our current knowledge on polymorphism has been advancing significantly in recent years, this fascinating topic still represents a challenging aspect of structural crystallography and solid-state chemistry. Despite the major enhancements in experimental and computational methods, the highly successful computational studies invariably predict far more feasible structures than are experimentally found, even when further extensive experimental screenings are made. Possible reasons for this discrepancy have been previously suggested but still questions such as *Why don't we find more polymorphs?* remain open. [1]

In this work we explore the idea that detailed comparative analyses of predicted and experimental polymorphs may represent a further useful tool for polymorph screening. The identification of structural similarities and differences might help in discriminating which structure, within the crystal energy landscape, would seem likely to be experimentally isolated.[2] This information might be also used to identify whether pairs or groups of structures are so closely related that they may convert one into the other, during the nucleation/crystal growth stages or by proper solid-solid phase transitions, preventing the observation of some potential metastable forms. To follow these objectives, we compared experimental and predicted structures from the previous results of a CSP study by Asmadi et al. [3] on a group of three rigid, planar small molecules of known crystal structures, 2-methyl-, 3-methyl- and 2,3-dimethyl-benzo[b]thiophene 1,1-dioxide.

The results of the crystal structure comparison of the ten lowest energy predictions from the CSP calculations for each derivative with the known, unique experimental crystal structures are discussed. A short experimental screening leading to the discovery of three new polymorphs is also presented.

References:

1. Price, S. L. (2013). Acta Cryst. B69, 313–328
2. Price, S. L. et al (2016) Chem. Commun. 52, 7065-7077
3. Asmadi, A. et al. (2010). Chem. Eur. J. 16, 12701–12709

Keywords: Polymorphism,