



Contribution ID: 52

Type: **Oral contribution**

Chaperone Compounds for Co-crystallization of Organics

Monday 15 March 2021 14:45 (20 minutes)

Modern instrumentation and processing techniques for single crystal X-ray diffraction enable high-quality 3D structure analysis –including absolute structure determination –often in less than an hour, faster and more comprehensively than many spectroscopic methods can even start to achieve. However, large numbers of small or highly flexible organic molecules remain intractable to even the most sophisticated crystallization methods. Our new set of chemical chaperones for co-crystallization ¹ offers a new alternative to other methods, such as the crystal-sponge approach ^{2, 3}, can significantly increase the probability of successful crystallization and provides faster access to the absolute 3D structure of an organic analyte:

- The chaperone method is fast and easy to use
- Structures in hours rather than weeks
- Small quantities of analyte required
- Excellent quality crystals
- 88% diffraction-quality crystals from a 52 organic compounds test screen
- The chaperone compounds are highly stable
- 100% analyte occupancy in the crystal guarantees reliable determination of the absolute configuration.

We will discuss and demonstrate the features in detail along the diastereomers of Limonene including a demonstration of the crystal growth.

1 Richert, et.al, Angew. Chem. Int. Ed. 2020, 59, 15875–15879, doi.org/10.1002/anie.202004992.

2 Fujita et al, IUCrJ 2016, 3, 139-151, doi.org/10.1107/S2052252515024379.

3 Clardy, et.al, Acta Cryst. (2015), A71, 46–58 <https://doi.org/10.1107/S2053273314019573>.

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Session Classification: Organic and metal-organic crystal structures

Track Classification: Organic and metal-organic crystal structures