

Chaperone Compounds for Co-crystallization of Organics

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Modern instrumentation and processing techniques 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, developed by the University of Stuttgart^[1] offers a new alternative to other methods, such as the crystal-sponge approach^[2] and can significantly increase the probability of successful crystallization and provide 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
- Sample screen of 52 organic compounds
 - Diffraction-quality crystals in 88% of cases
 - High resolution X-ray structures in 77% of cases
 - 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] Krupp, F.; Frey, W.; Richert, C. *Angew. Chem. Int. Ed.* (2020), **59**, 15875–15879.

[2] Patent pending.

Keywords: chaperone, organic molecule, co-crystal, high-quality structure, crystal sponge