

## MS03-P06 | CRYSTAL PRODUCTION AND STRUCTURE SOLUTION THANKS TO THE NUCLEATING AND PHASING AGENT, CRYSTALLOPHORE.

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Obtaining crystals and solving the phase problem remain major hurdles encountered by bio-crystallographers in their race to get new high-quality structures.

The crystallophore, Tb-Xo<sub>4</sub>, is a lanthanide complex formed from a molecular cage chelating a terbium atom [2]. We will present the results obtained on about fifteen proteins which show that Xo<sub>4</sub> induces unique crystallization conditions and promotes new crystal packing showing that Tb-Xo<sub>4</sub> acts an efficient nucleating agent. The crystalline forms promoted by the crystallophore bypass crystal defects often encountered by crystallographers such as low-resolution diffracting samples or crystals with twinning.

We will also present few examples of Tb-Xo<sub>4</sub> phasing properties [1,2,4], showing, in particular that the crystallophore is compatible with serial crystallography approaches.

Finally, the versatility of the interactions between Xo<sub>4</sub> and the surface of proteins explains its exceptional properties [3] making this molecule a unique tool for simultaneously solving the two major locks of biocrystallography.

[1] Bernhardsgrütter, I., et al. (2018). *Nature Chemical Biology*. 14, 1127–1132.

[2] Engilberge, S., et al. (2017). *Chem. Sci*. 8, 5909–5917.

[3] Engilberge, S., et al. (2018). *Chemistry*. 24, 9739–9746.

[4] Vögeli, B., et al. (2018). *Proceedings of the National Academy of Sciences*. 115, 3380–3385.