

Crystallophore, an efficient additive to facilitate crystal structure determination

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Crystallophore (Tb-Xo4) is a lanthanide complex [1] that overcomes the two bottlenecks of macromolecular crystallography, i.e. getting single crystals and solving the phase problem.

Tb-Xo4 is a nucleating agent: added to the protein solution, it allows promoting a larger number of crystallization hits, in particular unique conditions that are not observed for the native protein. The crystallophore is highly water-soluble and is perfectly compatible with automatic crystallization platforms. Moreover, the crystals resulting from this process can be easily detected under UV light thanks to the luminescent properties of Tb^{III}.

Tb-Xo4 is a phasing agent: thanks to the use of the unique anomalous signal provided by the lanthanide atom, it highly facilitates the structure determination process.

We will present nucleation and phasing results obtained on a dozen of proteins - including original targets that have resisted to classical approaches - as well as preliminary results on the crystallization reproducibility.

References

[1] - S. Engilberge, F. Riobé, S. Di Pietro, L. Lassalle, N. Coquelle, C.-A. Arnaud, D. Pitrat, J.-C. Mulatier, D. Madern, C. Breyton, et al., Chem. Sci. **9**, 1621 (2017).