MS03 Crystallization and biophysical characterization

MS3-05
Nucleation and reproducibility in protein crystallization assisted by the crystallophore
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Abstract
Obtaining crystals remains the major hurdle encountered by bio-crystallographers in their race to get new high-quality structures. The crystallophore, Xo4, is a family of nucleating and phasing molecules based on lanthanide complexes. Tb-Xo4 was the first molecule of this family to be described [1].

Tb-Xo4 crystallization properties will be first described through results obtained on more than fifteen proteins and will show that Tb-Xo4 is an efficient tool as:
(i) Tb-Xo4 increases the number of crystallization conditions by promoting unique ones [1,2]
(ii) The crystalline forms promoted by the crystallophore bypass crystal defects often encountered by crystallographers such as low-resolution diffracting samples or crystals with twinning [3]
(iii) Crystals can be obtained from enriched fractions containing several proteins, contrary to the dogma that crystallization can only be promoted from pure protein sample [3] leading to the structure determination of a protein complex [4].
(iv) Even more unexpected, the crystallophore is able to induce nucleation directly from the protein solution, as exemplified by the crystallization of hen egg white lysozyme in water [5].

Then, we will focus on the crystallization reproducibility, a prerequisite and particular issue in structure-based drug design. Reproducibility is largely improved with the crystallophore. This will be illustrated by results with three different proteins obtained in the framework of a collaborative project with the High throughput Crystallization Platform (HTX-lab) at EMBL-Grenoble, the Polyvalan startup (https://crystallophore.fr) and Edelris company (https://www.edelris.com).

Altogether, crystallophore is an efficient solution for protein crystallization and structure determination in the bio-crystallographer toolbox.

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