Posters - Crystal to Beam

P6-1

FROM THE CRYSTAL TO THE STRUCTURE THANKS TO AN ALL IN ONE LANTHANIDE COMPLEX

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Since 2000, we developed lanthanide complexes for structure determination of macromolecules, exploiting the high-phasing power of lanthanide elements . Recently, we produced a new complex with luminescent properties. Unexpectedly, this complex ([Ln]) showed promising nucleant properties making it *the first nucleant, luminescent and phasing agent*.

We will present the results of the crystallization properties obtained on 8 proteins including not only commercial ones but also proteins of unknown structures. Potential crystallization hits have been determined using high-throughput crystallization (HTXlab, EMBL, Grenoble) through screening of 576 conventional conditions. We systematically compared the native protein with the one in presence of [Ln]. Results showed that, in most cases, the presence of [Ln] induces a major increase of potential hits and provides new crystallization conditions for all tested proteins. As illustrated in Figure 1, the crystals obtained in presence of [Ln] are better.

The luminescent property of [Ln] allows to facilitate crystal detection in crystallization drops as well as to facilitate crystal centring at synchrotron beamlines.

Finally, using crystals obtained with [Ln], the structures of the 8 proteins (including the two unknown ones) have been determined by means of anomalous-based methods.

In conclusion, this new *all in one lanthanide complex* overcomes *the two major bottlenecks* in protein crystallography: crystallization and phase determination.

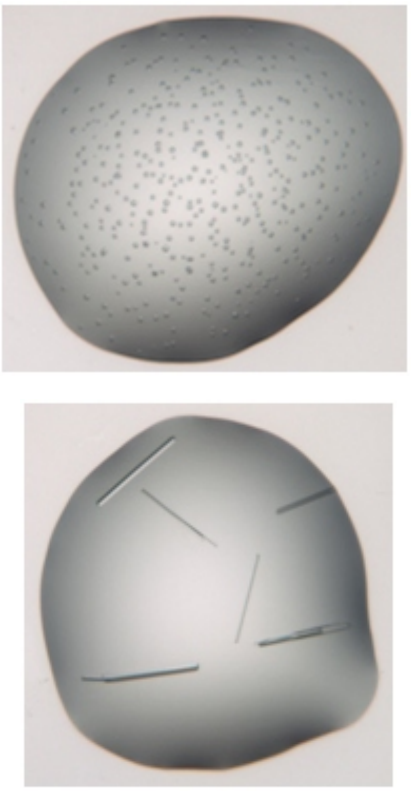

Figure 1. Crystallization drops obtained for the same protein without (top) and with the all in one lanthanide complex (bottom).

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P6-2

TIME-RESOLVED CRYSTALLOGRAPHY OF PROTEINS AT THE FEMTOSECOND X-RAY PLASMA SOURCE IN ELI BEAMLINES

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The advances in designing novel X-ray sources will allow for time resolved X-ray scattering and diffraction on a femtosecond to millisecond time scale. Unlike large scale facilities such as synchrotrons, intensive lasers can be used for the generation of short X-rays pulses in a setup similar in size to the commercially available laboratory X-ray sources. The femtosecond laser driven emission of X-ray pulses from plasma (XPS) offers higher time resolution for fast kinetic measurements than continuously emitting sources. The ELI beamlines facility is planned to start operation by the end of 2016 in Dolni Brezany, Czech Republic. It will give a unique advantage for time resolved crystallography and wide angle scattering for a crystalline samples, including proteins. The generated pulses will span approx. 100 fs with a repetition rate of 1 kHz. The scattered and diffracted by the protein crystal X-rays will be counted using a DECTRIS Eiger 1M area detector which operates at the same frame rate as the source, i.e. 1 kHz. Such setup can be combined with several pump probe lasers to study the fast kinetics for example in proteins relevant to plant photosystems or vision in animals. Because of the interdisciplinary nature of the fields and of the ELI beamlines facility regular discussions between experts in the field of high power laser-matter interaction and potential users, as well as young scientists, are organized.

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Posters - Chemistry of Crystallization

P7-1

A NEW DESIGN OF PLATE GEOMETRY FOR EFFICIENT PROTEIN CRYSTALLIZATION SCREENING

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We propose in this report a new design of geometry for protein crystallization plates. Each plate comprises 96 units corresponding to the 96 conditions of commercial crystallization screening kits. Each unit consists of 4 wells in which four different volume ratios of protein solution to precipitant solution can be set up. Based on the geometry we manufactured two types of crystallization plates: 1) Microbatch plate (M plate): the 96 units are separately sealed but the 4 wells in each unit are sealed to share the same common space; 2) Cross-diffusion microbatch [1] plate (CDM plate): all 96 4 wells are sealed to share the same common space, so that all volatile components in the droplets can freely diffuse in the common space. Figure 1 shows schematically the geometry of these two crystallization plates.

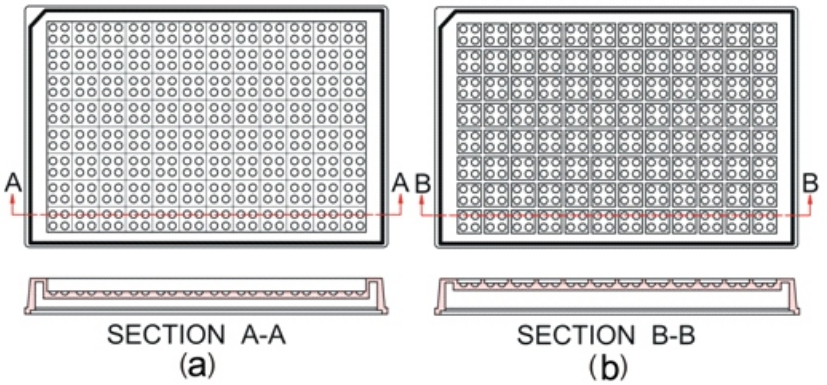

Figure 1. Two types of crystallization plates used in this study. (a) CDM plate; (b) M plate [1].