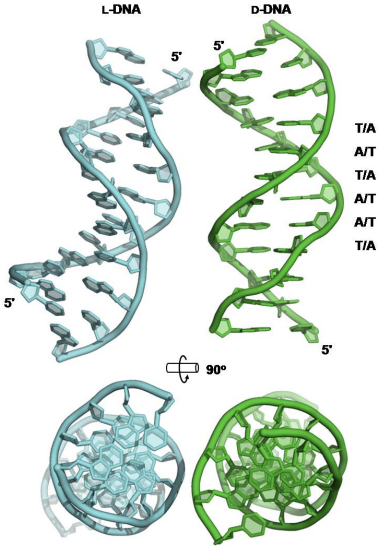

Figure 1. Crystal structure (in space group *P*bca, resolution 1.65 Å) of a DNA duplex containing the Pribnow box consensus promoter sequence 5'–TATAAT–3' with its complementary strand. Right: asymmetric unit, containing one complete D-DNA duplex (green). Left: L-DNA symmetry mate (cyan).

Keywords: Racemic crystallography, DNA, X-ray diffraction, DNA crystallography

MS12-O5 An all-in-one lanthanide complex to overcome the two major bottlenecks in protein crystallography.

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Protein crystallography remains the major technique for protein structure determination. Among 117438 structures deposited on the protein data bank (April 2016), 89 % had been solved using X-ray crystallography. However, protein crystallography is still limited by two major bottlenecks: Obtaining protein crystals and solving the phase problem.

Since 2000, we developed lanthanide complexes for structure determination of macromolecules, exploiting the high-phasing power of lanthanide elements [1-7]. Recently, we produced a new complex with luminescent properties. Unexpectedly, this lanthanide complex ([Ln]) showed nucleant properties making it the first nucleant, luminescent and phasing agent.

To demonstrate the effects of this new molecule, we selected 8 proteins with different molecular weights and different oligomeric states. Among these 8 proteins, two were of unknown structure including one with an unknown fold.

We performed comparative crystallization screening at the HTX lab crystallization plate form (EMBL – Grenoble) with and without [Ln]. We showed that [Ln] significantly increases the number of crystal hits and more importantly, it provides unique crystallization conditions. In many cases the incorporation of [Ln] significantly increases the crystal quality as shown in Figure 1.

The luminescence properties of [Ln] have been used for crystals detection and may be exploited for crystal centering on synchrotron beam line.

The structures of the 8 proteins have been determined using anomalous based phasing methods.

In conclusion, this new all-in-one lanthanide complex allows to overcome the two majors bottlenecks in protein crystallography.

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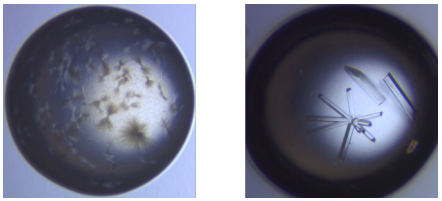

Figure 1. Crystallization drops obtained for the same protein without (left) and with the all in one lanthanide complex (right).

Keywords: Crystallization, Nucleation, Phasing, Anomalous, Luminescence, Lanthanide complex

MS13 Hot structures in biology

Chairs: Mariusz Jaskolski, Udo Heinemann

MS13-O1 Bacterial Resistance to Silver: The Role of SilE Protein

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Silver has been used for hundreds of years for its antimicrobial properties. Since the emergence of many multi-resistant bacterial strains against classical antibiotics, the research of new silver compounds is now at its apogee. While these drugs have been shown to be highly able to kill bacteria, some of these pathogens have developed a resistance to high concentrations of Ag^+. This resistance is provided by the plasmid pMG101, which encodes for eight proteins that act together in an efflux pump system to deal with silver ions. Among these, the SilE protein is the only one of which its mode of action is actually unknown.

To identify the role of SilE in this bacterial machinery, two approaches have been intended in our group. While one way is to study the interaction of the whole protein with silver ions, the other is based on a bottom-up approach, investigating the interaction of silver ions with short peptide sequences of this protein. By NMR studies of these peptide models, we were able to highlight a potential methionine participation in the complexation of Ag^+ by SilE.

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S. Eckhardt, P. S. Brunetto, J. Gagnon, M. Priebe, B. Giese, K. M. Fromm, *Chem. Rev.* **2013**, 113, 4708-4754.

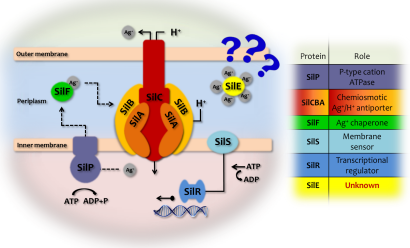

Figure 1. Proteins products of pMG101 silver resistance genes.

Keywords: Bacterial resistance, Silver(I), Metalloprotein, Methionine