Czech Society for Structural Biology

21th Structural Biology Club online on **29 May 2024, 13:00**
with the following scientific talks kindly delivered by our guests

Genuine co-factor identification by intracellular protein crystallization

Presented by **Lars Redecke, Institute of Biochemistry, University of Lübeck, Lübeck, and Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany**

During the past decades, protein crystallization in living cells has been observed surprisingly often in all domains of life as a native assembly process, and emerging evidence indicates that this phenomenon is also accessible for recombinant proteins [1]. The advent of high-brilliance synchrotron sources, X-ray free-electron lasers, and improved serial data collection strategies has allowed the use of these micrometer-sized crystals for structural biology [2-7]. Thus, *in cellulo* crystallization offers exciting new possibilities for proteins, complementing conventional crystallization approaches.
Our efforts to systematically exploit living insect cells as protein crystallization chambers and to streamline this process for structural biology resulted in the establishment of a pipeline to elucidate the structural information of *in cellulo* crystallized target proteins in short time, denoted as 'InCellCryst' pipeline [8]. Due to the quasi-native environment of the proteins in the living cell, the intracellular crystallization approach offers the possibility to identify naturally bound ligands and their conformations, as demonstrated for inosine-5'-monophosphate dehydrogenase (IMPDH) and guanosine monophosphate reductase (GMPR). This unique feature of intracellular protein crystallization cannot be replaced by *in silico* protein folding predictions like AlphaFold.
This talk will present an overview of the InCellCryst approach and its benefits, but also the remaining challenges.

[1] Schönherr R, Rudolph JM, Redecke L, Biol Chem 399, 751-772 (2018). [2] Koopmann R, et al., Nat Methods 9, 259-262 (2012). [3] Redecke L, et al., Science 339, 227-231 (2013). [4] Gati C, et al., IUCrJ 1, 87-94 (2014). [5] Schönherr R, et al., Struct Dyn 2, 041712 (2015). [6] Nass KN, Redecke L, et al., Nat Commun 11, 620 (2020). [7] Lahey-Rudolph JM, et al., IUCrJ 8, 665-677 (2021). [8] Schönherr R, Boger J, Lahey-Rudolph JM, et al., Nat Commun. 15, 1709 (2024).

Structural determinants of juvenile hormone receptor-ligand interactions

Presented by **Roman Tůma, Faculty of Science, University of South Bohemia, České Budějovice and Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds, UK**

Juvenile hormones (JH) are lipophilic signaling molecules that are specific to arthropods and coordinate postembryonic development from larvae to adults. JH receptor has been target of insect-specific endocrine disruptors, i.e. synthetic agonists that serve as effective insecticides. However, molecular basis for their action was unknown until recently. In this presentation, we will illustrate how molecular modelling combined with high-throughput, quantitative ligand activity screening and mutagenesis provided insight into the molecular basis of ligand recognition. The role of receptor dynamics in the recognition process will be discussed.

Moderator: **Barbora Karaffová**, University of South Bohemia, České Budějovice, Czech Republic

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Please, join us on this Zoom link (join 5-10 minutes before the beginning)
https://cesnet.zoom.us/j/92170333913

Barbora Karaffová and Jan Dohnálek
on behalf of the Czech Society for Structural Biology
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