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X-ray free electron laser: Opportunities for drug discovery

Past decades have shown the impact of structural information derived from complexes of drug candidates with their protein targets to facilitate the discovery of safe and effective medicines. Despite recent developments in single particle cryo-electron microscopy, x-ray crystallography has been the main method to derive structural information. The unique properties of x-ray free electron laser (XFEL) with unmet peak brilliance and beam focus allow X-ray diffraction data recording and successful structure determination from smaller and weaker diffracting crystals. This shortens timelines in crystal optimization. To best capitalize on the XFEL advantage, innovations in crystal sample delivery for the x-ray experiment, data collection and processing methods are required. This leads to the development of serial crystallography which allows structure determination at more physiologically relevant room temperature. Together with using the time resolution provided by the femtosecond x-ray pulse, this will enable monitoring and capturing of dynamic processes of ligand binding and associated conformational changes with great impact to the design of candidate drug compounds.

Recent Publications

1. Weinert T, et al. (2017) Serial millisecond crystallography for routine room-temperature structure determination at synchrotrons. Nature Communication 8:542.
2. Huber S, Casagrande F, Hug M N, Wang L, Heine P, Kummer L, Plückthun A and Hennig M (2017) SPR-based fragment screening with neurotensin 1 generates novel small molecule ligands. PLOS One 2017
3. Renaud J P, Chung C W, Danielson U H, Egner U, Hennig M, Hubbard R E and Nar H (2016) Biophysics in drug discovery: impact, challenges and opportunities. Nature Reviews Drug Discovery 15:679-698.
4. Bocquet N, Kohler J, Hug M N, Kusznir E, Rufer A C, Dawson R J, Hennig M, Ruf A, Huber W and Huber S (2015) Real time monitoring of binding events on a thermostabilized human A2A receptor embedded in a lipid bilayer by surface plasmon resonance. BBA- Biomembranes, 2015, Biochim. Biophys Acta 1848(5):1224-1233.

Biography

Michael Hennig studied Physics and Biochemistry and received PhD in Structural Biology at EMBL Hamburg, and the Charité, Humboldt University Berlin, Germany. He followed two years Postdoc work at the Biozentrum, University of Basel, Switzerland. He is author of more than 75 scientific peer reviewed paper and, since 2011, he is a Guest Professor in Structural Biology at the University of Basel. From 1995 he worked for 20 years in pharmaceutical industry at Roche, Basel, Switzerland in various positions and finally Global Head. He is a Principle Leader of discovery technologies with responsibility for structure-based drug discovery, protein science, assay development and HTS, corporate compound library, stem cell platform analytical methods. In 2015, he co-founded and is now CEO of LeadXpro AG, a company dedicated to structure-based drug discovery of membrane protein targets.