## International Symposium on Structure Biology for Drug Discovery@SwissFEL

## Paul Scherrer Institute, Auditorium, 5232 Villigen, Switzerland June 25<sup>th</sup> -27<sup>th</sup> 2019

| AGENDA   |   |   |  |  |
|--|---|---|--|--|
| Tuesday, June, 25th  |   |   |  |  |
| 09.00-10.30  | Registration  |   |  |  |
| 10.30  | Opening/Welcome words from Thierry Strässle (Director of PSI) |   |  |  |
| Session 1 – Structures and Function at FELS (Chair: Michael Hennig, leadXpro AG)       |   |   |  |  |
| 10.45-11.30  | Introduction Keynote: Time resolved serial                    | Petra Fromme                              |  |  |
|  | fs crystallography towards molecular                          | (Arizona State University)                |  |  |
|  | movies of biomolecules "in action"                            |   |  |  |
| 11.30-12.00  | Exploring GPCR and Membrane Protein                           | Gebhard Schertler                         |  |  |
|  | Dynamics with X-ray Free-Electron Lasers                      | (ETHZ/PSI)                                |  |  |
|  | and cryo-EM   |   |  |  |
| 12.00-13.30  | LUNCH   |   |  |  |
| Session 1 – Structures and Function at FELS (Chair: Herbert Nar, Boehringer Ingelheim) |   |   |  |  |
| 13.30-14.15  | Perspectives of using serial femtosecond                      | Vadim Cherezov                            |  |  |
|  | crystallography in drug discovery                             | (University of Southern California)       |  |  |
| 14.15-14.45  | Emerging opportunities for structural                         | Stephen Soisson                           |  |  |
|  | biology in drug discovery                                     | (Merck and Co., Inc. West Point, PA, USA) |  |  |
| 14.45-15.15  | COFFEE BREAK  |   |  |  |
| Session 1 – Structures and Function at FELS (Chair: Matthias Frech, Merck KGaA)        |   |   |  |  |
| 15.15-16.00  | Time resolved structural biology -                            | Tobias Weinert                            |  |  |
|  | Bacteriorhodopsin paves the way to a                          | (PSI)                                     |  |  |
|  | dynamic future  |   |  |  |
| 16.00-16.30  | Observation of conformational switching by                    | Ji-Hye Lee                                |  |  |
|  | laser-induced pH jump using time-resolved                     | (University of Korea)                     |  |  |
|  | serial femtosecond crystallography                            |   |  |  |
| 16.30-17.00  | Costs and benefits of experimentally                          | Jan Pieter Abrahams                       |  |  |
|  | phasing the diffracted electron wave                          | (University of Basel/ PSI)                |  |  |

| Wednesday, June, 26th   |   |                                       |  |  |
|---|---|---------------------------------------|--|--|
| Session 2 – Drug Discovery with EM & X-ray (Chair: Sandra Jacob-Cowan, Novartis Pharma) |   |                                       |  |  |
| 09.00-09.45   | Keynote: Cryo-EM: A (new) tool for drug       | Christian Wiesmann                    |  |  |
|   | discovery at Novartis                         | (Novartis Pharma)                     |  |  |
| 09.45-10.15   | An embarrassment of riches in the Golden      | Jim Kiefer                            |  |  |
|   | Age of Structure Based Drug Design            | (Genentech)                           |  |  |
| 10.15-10.45   | Structures of G protein coupled receptor      | Javier Garcia-Nafria                  |  |  |
|   | (GPCR) complexes by electron cryo-            | (MCR Laboratory of Molecular Biology) |  |  |
|   | microscopy                                    |                                       |  |  |
| 10.45-11.15   | COFFEE BREAK                                  |                                       |  |  |
| Session 2 – Structure based Drug Discovery enabled by x-ray Crystallography on GPCR's   |   |                                       |  |  |
| (Chair: Roger Benoit, PSI)  |   |                                       |  |  |
| 11.15-11.45   | Uncovering the MOA of GPCR ligands            | Rob Cooke                             |  |  |
|   | through structural and biophysical studies    | (Heptares)                            |  |  |
| 11.45-12.15   | Serial crystallography enables the            | Robert Cheng                          |  |  |
|   | structure determination of membrane           | (leadXpro AG)                         |  |  |
|   | protein drug target                           |                                       |  |  |
| 12.15-13.45   | LUNCH   |                                       |  |  |
| Session 2 – Electr  | on Diffraction (Chair: Michel Steinmetz, PSI) |                                       |  |  |
| 13.45-14.15   | Microfluidic Sample Preparation for EM:       | Thomas Braun                          |  |  |
|   | Protein Isolation, High-Resolution cryo-      | (University of Basel)                 |  |  |
|   | EM, and 'Differential Visual Proteomics'      |                                       |  |  |
| 14.15-14.45   | Electron Diffraction of organic molecules     | Gustavo Santiso-Quiñones              |  |  |
|   | Electron Dimaction of organic molecules       | (Crystallise! AG)                     |  |  |
| 14.45- 15.15  | Novel accelerators for X-ray generation       | Rasmus Ischebeck (PSI)                |  |  |
|   | and electron diffraction                      |                                       |  |  |
| 15.30-17.30   | VISIT TO SWISSFEL AND SLS (OPTIONAL)          |                                       |  |  |
| 17.30-18.30   | Special Talk: Life science studies using      | Richard Neutze                        |  |  |
|   | XFEL radiation: an historical overview and    | (University of Gothenburg)            |  |  |
|   | future outlook                                |                                       |  |  |
| 19.00   | DINNER  |                                       |  |  |

| Thursday, June, 27th   |  |                                    |  |  |
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| Session 3 – Method & Instrumentation Developments (Chair: Rafael Abela, leadXpro AG) |  |                                    |  |  |
| 09.00-09.45  | Keynote: Serial crystallography and      | Henry Chapman                      |  |  |
|  | diffraction with X-ray FELs              | (CFEL)                             |  |  |
| 09.45-10.15  | SPIND-TC: First Auto-Indexer for Two     | Xuanxuan Li (Beijing Computational |  |  |
|  | Color Diffraction Patterns               | Science Research Center)           |  |  |
| 10.15-10.45  | SwissMX: Efficient Fixed Target          | Isabelle Martiel                   |  |  |
|  | Femtosecond Macromolecular               | (PSI)                              |  |  |
|  | Crystallography at SwissFEL              |                                    |  |  |
| 10.45-11.15  | COFFEE BREAK                             |                                    |  |  |
| Session 3 – Method & Instrumentation Developments (Chair: Oliver Bunk, PSI)          |  |                                    |  |  |
| 11.15-11.45  | Detectors for XFELs                      | Bernd Schmitt                      |  |  |
|  |  | (PSI)                              |  |  |
| 11.45-12.15  | Serial Crystallography – Methods         | Dominik Oberthuer                  |  |  |
|  | development for time resolved            | (DESY)                             |  |  |
|  | Structural Biology and Drug Discovery    |                                    |  |  |
| 12.15-12.45  | Time-resolved SFX of metalloenzymes      | Allen Orville                      |  |  |
|  |  | (MX – Diamond Light Source)        |  |  |
| 12.45  | Closing remarks and end of the Symposium |                                    |  |  |