Programme LINXS Time-Resolved Structural Biology workshop Oct 2022

Wednesday October 26 (at LINXS)

12:00 Lunch at LINXS

13:00 Introduction

13:10 **Kresten Lindorff-Larsen**, University of Copenhagen
Combining biomolecular simulations with time-dependent and time-resolved experiments

13:40 **Magnus Andersson**, Umeå University
Tracking ATP-dependent membrane protein regulation in real time

14:00 **James Fraser**, University of California San Francisco, USA
Finding new inhibitors for SARS CoV 2 Macrodomain with X-ray fragment screening, neutrons, and entropy

14:30 Coffee Break

15:00 **Kristine Steen Jensen**, Lund University
Early events in SOD1 amyloid formation

15:30 **Angus Robertson**, Lund University
Pressure-Jump NMR investigations of aggregating systems

15:50 **Volha Chukhutsina**, Vrije Universiteit Amsterdam, the Netherlands
Cryotrapping photocycle intermediates to resolve how lazy photoreceptors work

16:20 Coffee Break

16:40 **Thomas Barends**, Max-Planck Institute for Medical Research, Heidelberg, Germany
Time-resolved serial femtosecond crystallography of a photoenzyme: pitfalls and progress

17:10 **Discussion** (moderated by Allen Orville, Diamond Light Source)

18:00 **Poster session**

19:00 End of 1st day

Thursday October 27 (morning at LINXS)

09:00 **Jörg Standfuss**, Paul Scherrer Institute, Switzerland
Release of a photopharmacological drug from tubulin over eleven orders of magnitude in time

09:30 **Martin Weik**, Institut de Biologie Structurale, Grenoble, France
Photoswitchable fluorescent proteins: what we have learnt through time-resolved serial crystallography

10:00 **Jacques-Philippe Colletier**, Institut de Biologie Structurale, Grenoble, France
Use of short X-ray pulses to probe the structural dynamics of the orange carotenoid protein (OCP)

10:30 Coffee Break

10:50 **Ulf Ryde**, Lund University
Improving and interpreting crystal structures with quantum refinement

11:20 **Discussion** (moderated by Allen Orville, Diamond Light Source)

12:00 Lunch at LINXS and transport to MAX IV Laboratory

Thursday October 27 (afternoon at MAX IV Laboratory)

14:00 **Gisela Brändén**, University of Gothenburg
XFEL- and synchrotron-based serial crystallography studies of the membrane-bound proton pump cytochrome c oxidase

14:30 **Sam Horrell**, Diamond Light Source, UK
Time-resolved X-ray Crystallography at Diamond Light Source

14:50 **Michal Kepa**, Paul Scherrer Institute, Switzerland
Towards automation of serial crystallography using a multi-reservoir high viscosity extruder

15:10 Introduction to MicroMAX

15:20 **Discussion** (moderated by Allen Orville, Diamond Light Source)

15:50 Coffee Break

16:10 **Visit of MAX IV & MicroMAX**

17:00 Break before dinner

19:00 **Dinner in Lund**

Friday October 28 (at LINXS)

09:00 **Manuel Maestre-Reyna**, National Taiwan University (remote presentation)
Watching DNA repair via time-resolved serial femtosecond crystallography

09:30 **Alessandra Henkel**, CFEL/DESY, Hamburg, Germany
CFEL TapeDrive 2.0: Conveyor belt-based sample delivery system for multi-dimensional serial crystallography

09:50 Coffee Break

10:20 **Stephen Muench**, University of Leeds, UK
The development and application of time-resolved single particle cryoEM

10:50 **Gergely Katona**, University of Gothenburg
Deformation networks in protein crystals revealed by steady state and THz pump - X-ray probe crystallography

11:20 **Discussion** (moderated by Allen Orville, Diamond Light Source)

12:00 Lunch

13:00 End of Meeting

LINXS

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