

# EARLY CAREER DIFFRACTION METHODS SEMINAR 2024

21st-22nd July 2024

## SUNDAY 21ST JULY

11:00-13:00	Arrival and Registration
13:00-14:00	Light Welcome Lunch
14:00-14:10	Welcome from the Chairs
<b>14:10-15:30</b>	<b>Keynote Session</b> Discussion Leader: <b>Louise Dunnett</b> (Diamond Light Source, UK)
14:10-14:30	Introduction by Discussion Leader "I04-1, XChem and Diamond"
14:30-15:30	<b>Marcus Fischer</b> (St. Jude Children's Research Hospital, USA) "Protein Bikram Yoga"
15:30	Break
<b>16:00-18:00</b>	<b>Serial and Time-Resolved Crystallography</b> Discussion Leader: <b>Yelyzaveta Pulnova</b> (ELI ERIC, Czechia)
16:00-16:20	<b>Nicolas Caramello</b> (ESRF, France) "The in crystallo optical spectroscopy toolbox: easy correction and analysis of spectroscopic data recorded in crystals"
16:20-16:40	<b>Anaïs Chretien</b> (XFEL, Germany) "Time-resolved structural analysis of the BLUF photoreceptor OaPAC"
16:40-17:00	<b>Caitlin Hatton</b> (University of Hamburg, Germany) "Using ultrahigh-resolution and time-resolved crystallography to investigate allostery in enzymes"
17:00-17:20	<b>Jake Hill</b> (University of Leeds, UK) "Investigating UV damage in cataract formation with serial crystallography"
17:20-17:40	<b>Maria Spiliopoulou</b> (UKE, Germany) "T4 lysozyme, a model system for ligand binding using integrative temperature-dependent, time-resolved crystallography"
17:40-18:00	<b>General Discussion</b>
18:30	Dinner
<b>20:00-21:30</b>	<b>Posters &amp; Discussion</b>

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## MONDAY 22ND JULY

<b>9:00-11:00</b>	<b>Computational Advances in Structural Biology</b> Discussion Leader: <b>Mahmoud Rizk</b>
9:00-9:20	<b>Virginia Apostolopoulou</b> (CFEL, Germany) "Mathematically deriving loop mobility for single protein structures"
9:20-9:40	<b>Maggie Klureza</b> (Harvard University, USA) "Data processing methods for Hadamard time-resolved X-ray crystallography"
9:40-10:00	<b>Katie O'Flynn</b> (DESY, Germany) "Mapping protein conformational changes using torsion angles"
10:00-10:20	<b>Amy Thompson</b> (Diamond Light Source, UK) "New clustering methods to identify dynamics in multi-crystal datasets"
10:20-10:40	<b>Conor Wild</b> (Diamond Light Source, UK) "PanDDA 2: leveraging large scale diffraction data to accelerate fragment screens"
10:40-11:00	<b>General Discussion</b>
11:00	Break
<b>11:30-13:00</b>	<b>Posters &amp; Discussion</b>
13:00	Lunch
<b>14:00-15:30</b>	<b>Crystallographic Methods and Analysis</b> Discussion Leader: <b>Mikael Londen</b> (Åbo Akademi University, Finland)
14:00-14:20	<b>Liliana Guerrero Porras</b> (CUNY ASRC, USA) "Unveiling the dynamic world of STEP: structural analysis in response to temperature, pressure, ligand binding, and dehydration"
14:20-14:40	<b>Laura Pacoste</b> (Stockholm University, Sweden) "Refinement of 3D ED data reveals organic ligands, not metal ions, as primary influencers in iron(III) acetyl acetonate charge distribution"
14:40-15:00	<b>Dimitrios Triantafyllidis</b> (University of Hamburg, Germany) "Emergence of order from proteins under nucleation"
15:00-15:20	<b>Eta Isiorho</b> (CUNY ASRC, USA) "Seeding success: practical insights for nucleating a crystallization facility"
15:20-15:30	<b>General Discussion</b>

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15:30	Break
<b>15:40-17:10</b>	<b>Panel discussion:</b> Navigating your career in structural biology Discussion Leader: <b>Karin Kühnel</b> (Structure, Cell Press)
15:40-16:00	Introduction by Discussion Leader "Navigating your career in structural biology - my journey"
16:00-17:00	Panel members: <b>Louise Dunnett</b> (Diamond light source, UK) <b>Marcus Fischer</b> (St. Jude Children's Research Hospital, USA) <b>Helen Ginn</b> (DESY, Germany) <b>Nicholas Pearce</b> (Linköping University, Sweden)
17:00-17:10	<b>General Discussion</b>
<b>17:10-17:30</b>	<b>Evaluation Period</b> <b>Election of Future Chair(s)</b>
<b>17:30</b>	<b>Seminar Concludes</b>