

Programme

Wednesday November 13, 2019

13:00 Registration

13:45 Welcome Address

Session 1: Recent Advances in FBDD

Session Chair

Dr Mike HANN
(GSK MEDICINES RESEARCH CENTRE, Stevenage, United Kingdom)

14:00 PhABits – Shining New Light on Fragments Approaches for Assessing Targets Tractability (IL01)

Dr Mike HANN
(GSK MEDICINES RESEARCH CENTRE, Stevenage, United Kingdom)

14:30 Fast Molecular Interaction Screening and Affinity Determination in Biophysical Drug Discovery Projects with Dianthus NT.23 and Tycho NT.6 (OC01)

Mr Andreas LANGER
(NANOTEMPER TECHNOLOGIES GMBH, Munich, Germany)

14:45 Targeting TIR Domain Assemblies in TLR Signaling Pathways to Design Anti-Inflammatory Compounds (OC02)

Mr Md Habibur RAHAMAN
(UNIVERSITY OF QUEENSLAND, Brisbane, Australia)

15:00 Ligand-Based Fluorine NMR Screening in Drug Discovery (IL02)

Dr Anna VULPETTI
(NOVARTIS, Basel, Switzerland)

15:30 Coffee Break & Exhibition

**16:05 Exhibitor Short Presentation: Crelux – A WuXi AppTec company
A Fragment-Based Approach to Leverage Challenging Targets: Human STING**

16:15 ¹⁹F NMR Screening Applied to Multiple Cancer Target (OC03)

Dr Kenneth CAMERON
(CRUK BEATSON INSTITUTE, Glasgow, United Kingdom)

16:30 Enabling Drug Discovery with Crude Reaction Mixture Screening (IL03)

Dr Ben DAVIS
(VERNALIS RESEARCH, Cambridge, United Kingdom)

Academia Keynote Lecture

Session Chair

17:00 Structure-biophysics Driven PROTAC Design for Degrading Undruggable Cancer Targets (KL01)

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Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

18:00 **Welcome Reception**

19:30 **End of the Day**

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Thursday November 14, 2019

09:00 Registration

Session 2: Challenging Targets (GPCRs, Ion Channels...)

Session Chair

Dr Junichi SAITO
(KYOWA KIRIN CO., LTD., Shizuoka, Japan)

09:30 Structural Biology of Seven-Transmembrane Receptors Toward Drug Discovery (IL04)

Prof. Shigeyuki YOKOYAMA
(RIKEN, Yokohama City, Japan)

10:00 Venturing into the Untapped: Discovery of Small-Molecule Drugs Targeting Messenger RNAs Using Biophysical and Computational Methods (OC04)

Dr Ella MORISHITA
(VERITAS IN SILICO, Tokyo, Japan)

10:15 Coffee Break & Exhibition

10:45 Cryo-EM Structures Capturing the Transport Cycle of the P4-ATPase Flippase (OC05)

Mr Masahiro HIRAIZUMI (MITSUBISHI TANABE PHARMA CORPORATION, Yokohama, Japan)

11:00 Advancing Cryo-EM for Determination of G Protein-Coupled Receptor Structure (IL05)

Prof. Patrick M. SEXTON
(MONASH UNIVERSITY, Parkville, Australia)

11:30 Poster Session

12:30 Lunch Break, Exhibition & Networking

Session 3: Cryo-EM in Drug Discovery

Session Chair

Dr Midori KAMIMURA
(TEIJIN PHARMA LIMITED, Tokyo, Japan)

14:00 Cryo-EM Structural Studies of The Human TRPV4 Ion-Channel: Insights and Characterization of a Novel Open-Conformation (OC06)

Dr Simon HOLTON
(BAYER, Berlin, Germany)

14:15 Cryo-EM Application for Drug Discovery (OC07)

Dr Wen-ti LIU
(NOVALIX, Illkirch, France)

14:30 Advancing Drug Discovery in Pharma Using Cryo-EM (IL06)

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Dr Claudio CIFERRI
(GENENTECH, South San Francisco, United States)

15:00 **Exhibitor Short Presentation: Thermo Fisher Scientific
Cryo-EM Single Particle Analysis Productivity: the State of the Art**

15:10 **Coffee Break & Exhibition**

Session 4: X-ray Crystallography / Cryo-EM Complementarity

Session Chair

Dr Denis ZEYER
(NOVALIX, Illkirch, France)

15:45 **Increased Performance in High-Throughput Compound and Fragment Screening Campaigns by the Use of
"Club Class" Data Collection (IL07)**

Dr Gerard BRICOGNE
(GLOBAL PHASING LTD., Cambridge, United Kingdom)

16:15 **Discovery of a Regulatory Subunit of the Yeast Fatty Acid Synthase (IL08)**

Prof. Holger STARK
(MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)

16:45 **Applying Hybrid Biophysical and Structural Methods to Study Allosteric Regulation of GTP Cyclohydrolase I -
A Target for Treating Inflammatory and Neuropathic Pain (IL09)**

Dr Herbert NAR
(BOEHRINGER INGELHEIM, Biberach, Germany)

17:15 **Posters & Drinks**

18:30 **End of the Day**

20:00 **Conference Dinner**

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Friday November 15, 2019

08:30 Registration

Session 5: Hot Topics

Session Chair

Dr Herbert NAR
(BOEHRINGER INGELHEIM, Biberach, Germany)

09:00 Re-energizing Small Molecule Drug Discovery by Centaur Chemist™ (IL10)

Dr Daisuke TANAKA
(EXSCIENTIA, Osaka, Japan)

Industry Keynote Lecture

Session Chair

Dr Mike HANN
(GSK MEDICINES RESEARCH CENTRE, Stevenage, United Kingdom)

09:30 From Fragments to Pharmaceuticals (KL02)

Dr Harren JHOTI
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

Session 5: Hot Topics (continued)

Session Chair

10:30 Coffee Break & Exhibition

**11:00 Exhibitor Short Presentation: NanoTemper Technologies
Biophysical Tools for Measuring Binding Affinity, Protein Stability or Protein Quality with just a Tiny Amount of Sample**

**11:10 Exhibitor Short Presentation: NovAliX
Single Particle Cryo-EM a Cutting Edge Service for Drug Discovery**

11:20 Uncovering a Ligand-Induced Twisted State of a Homodimeric Enzyme by Pulsed Electron-Electron Double Resonance (OC08)

Dr Dzung NGUYEN
(PHILIPPS-UNIVERSITÄT MARBURG, Marburg, Germany)

11:35 Structural Mechanisms of and Drug Discovery Targeting Substrate of Gamma-Secretase in Alzheimer's Disease (OC09)

Prof. Chunyu WANG
(RENSSELAER POLYTECHNIC INSTITUTE, Latham, United States)

11:50 Poster Prize and Closing Remarks

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12:05 **End of the Conference**