

### 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 <sup>19</sup>F 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)

# 7th NovAliX Conference

## Programme

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

**18:00**    **Welcome Reception**

**19:30**    **End of the Day**

### 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  
(RENSELAER POLYTECHNIC INSTITUTE, Latham, United States)

**11:50 Poster Prize and Closing Remarks**

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12:05    End of the Conference