

## 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 <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

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

**18:00**      **Welcome Reception**

**19:30**      **End of the Day**

## Programme

### 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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## Programme

### 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