

### Wednesday 13/06/2018

12:30 **Registration**

13:45 **Welcome Address**

#### Session 1: Hot Topics

##### Session Chair

Dr Chaohong SUN  
(ABBVIE, North Chicago, United States)

14:00 **OC01 - Making Off-Rate Screening in FBDD More Amenable For Fast Dissociating Compounds**

Dr Menachem GUNZBURG  
(MONASH UNIVERSITY, Parkville, Australia)

14:15 **OC02 - Novel Active Site and Allosteric Site Binders Identified for FPPS Of T. cruzi**

Ms Joy PETRICK  
(NOVARTIS, Basel, Switzerland)

14:30 **OC03 - Dynamic Single-Molecule Approaches to Accelerate the Development of More Efficient Drugs**

Dr Gerrit SITTERS  
(LUMICKS, Amsterdam, The Netherlands)

14:45 **OC04 - Quantitative Irreversible Tethering (QIT) for Covalent Ligand Discovery**

Dr Gregory CRAVEN  
(IMPERIAL COLLEGE LONDON, London, United Kingdom)

15:00 **OC05 - Large Protein Conformational Changes in Pi3kgamma Linked to the Binding of a New Class of Highly Selective Inhibitors**

Dr Göran DAHL  
(ASTRAZENECA, Mölndal, Sweden)

15:15 **IL01 - Binding Kinetics and Thermodynamics in Drug Discovery**

Dr Chaohong SUN  
(ABBVIE, North Chicago, United States)

15:45 **Coffee Break**

#### Session 2 : Target Engagement

##### Session Chair

Dr Daniel WYSS  
(MERCK, Kenilworth, United States)

16:25 **IL02 - Chemical Probes for Epigenetic Targets**

Prof. Masoud VEDADI  
(STRUCTURAL GENOMICS CONSORTIUM, Toronto, Canada)

# 5th NovAliX Conference

## Programme

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- 16:55**     **Exhibitor Short Presentation: Bruker**  
**Development and Proof-of-Concept of a New Flow-through System for High Resolution NMR to Evaluate Biologics-producing Cell Lines and Their Growth Environments**  
Dr Jason S. WOOD  
(BRUKER BIOSPIN, Billerica, United States)
- 17:05**     **Exhibitor Short Presentation: Creoptix**  
**The Wave of the Future in Kinetics**  
Dr Matyas VEGH  
(CREOPTIX AG, Wädenswil, Switzerland)
- 17:15**     **OC06 - Quantification of Target Occupancy in Cells and Tumor Tissue Using FCCS**  
Dr Frank BECKER  
(INTANA BIOSCIENCE GMBH, Planegg, Germany)
- 17:30**     **IL03 - How to Be Selectively Promiscuous**  
Prof. Jack TAUNTON  
(UNIVERSITY OF CALIFORNIA, San Francisco, United States)
- Keynote Lecture**
- Session Chair**  
Dr Daniel WYSS  
(MERCK, Kenilworth, United States)
- 18:00**     **KL01 - From Simulations of Biomolecules to Fighting Diseases**  
Prof. Martin KARPLUS  
(UNIVERSITY OF STRASBOURG, FRANCE & HARVARD UNIVERSITY, Cambridge, United States)
- 19:00**     **Welcome Reception**
- 20:30**     **End of the Day**

### Thursday 14/06/2018

**08:30 Registration**

#### Session 3 : Cryo-EM

##### Session Chair

Dr Bridget CARRAGHER  
(NEW YORK STRUCTURAL BIOLOGY CENTER, New York, United States)

**09:00 IL04 - How Low Can You Go? Size and Resolution Limits Using Conventional Cryo-EM**

Dr Gabriel LANDER  
(THE SCRIPPS RESEARCH INSTITUTE, San Diego, United States)

**09:30 IL05 - Cryo-EM for Characterization and Structure Based Drug Design**

Dr Bridget CARRAGHER  
(NEW YORK STRUCTURAL BIOLOGY CENTER, New York, United States)

**10:00 Coffee Break**

#### Session 3 (continued) : Cryo-EM

**10:30 OC07 - Cryo-EM to Address Intractable Targets in Drug Discovery**

Dr Hervé REMIGY  
(THERMO FISHER SCIENTIFIC, Eindhoven, The Netherlands)

**10:45 OC08 - Strength of Cryo-EM in Drug Discovery: One Could Always See Something**

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

**11:00 IL06 - Single Particle Cryo-EM Structure of the Insulin Receptor:Insulin Complex**

Dr Giovanna SCAPIN  
(MERCK & CO. INC (MSD), Whitehouse Station, United States)

**11:30 Poster Session**

**12:30 Lunch & Networking**

#### Session 4 : Membrane Proteins

##### Session Chair

Dr Dan ERLANSON  
(CARMOT THERAPEUTICS, South San Francisco, United States)

**14:00 IL07 - New Tools Reveal Mechanisms of Allosteric Coupling in Human GPCRs**

Dr Matthew EDDY  
(UNIVERSITY OF SOUTHERN CALIFORNIA, Los Angeles, United States)

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- 14:30**     **Exhibitor Short Presentation: Pall ForteBio**  
**Dissecting Biomolecular Interactions - Pall ForteBio's Next Gen SPR and BLI Label-Free Platforms: Providing Faster and Easier Solutions to Your Emerging Applications**  
Mr Bob DASS  
(PALL FORTEBIO, Menlo Park, United States)
- 14:40**     **OC09 - Enabling NMR-Based Fragment Screening Using Stabilized Native GPCR: Case Study of Adenosine Receptor**  
Dr Anass JAWHARI  
(CALIXAR, Lyon, France)
- 14:55**     **OC10 - Crystal Structures of Human Glycine Receptor Alpha3 Bound to a Novel Class of Analgesic Potentiators**  
Dr Xin HUANG  
(AMGEN, Cambridge, United States)
- 15:10**     **IL08 - Structural Insight into Allosteric Modulation of GPCRs**  
Dr Miles CONGREVE  
(HEPTARES, Welwyn Garden City, United Kingdom)
- 15:40**     **Coffee Break**
- Session 5 : Protein-Protein Interactions**
- Session Chair**  
Dr MariJean EGGEN  
(ELI LILLY, Indianapolis, United States)
- 16:20**     **IL09 - Design Considerations for Synthetic Macrocycles in Drug Discovery**  
Prof. Adrian WHITTY  
(BOSTON UNIVERSITY, Boston, United States)
- 16:45**     **OC11 - Use of Complementary Biophysical Methods to Characterize Ligand Binding to IL-17A**  
Dr Parag SAHASRABUDHE  
(PFIZER, Groton, United States)
- 17:00**     **OC12 - Systematic Development of Small Molecules to Inhibit Specific Microscopic Steps of  $\alpha$ -Synuclein Aggregation in Parkinson's Disease**  
Ms Roxine STAATS  
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)
- 17:15**     **IL10 - Design of the First-in-Class, Highly Potent Irreversible Inhibitor Targeting the Menin-MLL Protein-Protein Interaction**  
Dr Shilin XU  
(UNIVERSITY OF MICHIGAN, Michigan, United States)
- 18:00**     **Posters & Drinks**
- 19:30**     **End of the Day**
- 20:00**     **Conference Dinner**

# 5th NovAliX Conference

## Programme

**Friday 15/06/2018**

**08:30 Registration**

**Session 6 : Biotherapeutics**

**Session Chair**

Dr Jim BRYSON  
(BRISTOL-MYERS-SQUIBB, Princeton, United States)

**09:00 IL11 - Attacking the Cancer Cell Surface-ome with Recombinant Antibodies**

Prof. Jim WELLS  
(UCSF, San Francisco, United States)

**09:30 Exhibitor Short Presentation: Sierra Sensors  
Controlling Throughput for SPR**

Dr Christopher WHALEN  
(SIERRA SENSORS, Greenville, United States)

**09:40 IL12 - Multi-Specific Designer Proteins for Tumor Therapeutics**

Dr Karyn T. O'NEIL  
(AR? BIOTHERAPEUTICS, Philadelphia, United States)

**10:10 Coffee Break**

**Session 6 (continued) : Biotherapeutics**

**10:40 Exhibitor Short Presentation: WuXi AppTec  
Crelux – A Fully Integrated Offering, from Protein to Screen, Through Crystallography Confirmation and Beyond.**

Dr Thomas WALDMANN  
(CRELUX, A WUXI APPTEC COMPANY, Martinsried, Germany)

**10:50 IL13 - Emerging Higher Order Structure Techniques in Biotherapeutics Development**

Dr Tapan K. DAS  
(BRISTOL-MYERS SQUIBB, New York, United States)

**11:20 Poster Prizes and Closing Remarks**

**11:45 Farewell Lunch & Networking**

**13:00 End of the Conference**