# 5th NovAliX Conference

## Programme

### Wednesday June 13, 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 & CO., INC., Morristown, United States)

**16:25** **IL02 - Chemical Probes for Epigenetic Targets**
Prof. Masoud VEDADI
(STRUCTURAL GENOMICS CONSORTIUM, Toronto, Canada)

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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 & CO., INC., Morristown, 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**

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### Thursday June 14, 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 ?-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

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### Friday June 15, 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**