

5th NovAliX Conference

Programme

Wednesday June 13, 2018

12:30 **Registration**

13:45 **Welcome Address**

Session 1: Hot Topics

14:00 **OC01 - Title to be announced**

14:15 **OC02 - Dynamic Single-Molecule Approaches to Accelerate the Development of More Efficient Drugs**

Dr Gerrit SITTERS
(LUMICKS, Amsterdam, The Netherlands)

14:30 **OC03 - Quantitative Irreversible Tethering (QIT) for Covalent Ligand Discovery**

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

14:45 **OC04 - Systematic Development of Small Molecules to Inhibit Specific Microscopic Steps of α -Synuclein Aggregation in Parkinson's Disease**

Ms Roxine STAATS
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

15:00 **OC05 - Large Protein Conformational Changes in $\text{Pi3k}\gamma$ Linked to the Binding of a New Class of Highly Selective Inhibitors**

Dr Göran DAHL
(ASTRAZENECA, Mölndal, Sweden)

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

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

15:45 **Coffee Break**

Session 2 : Target Engagement

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

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

16:55 **Exhibitor Short Presentation**

17:05 **Exhibitor Short Presentation**

17:15 **OC06 - Quantification of Target Occupancy in Cells and Tumor Tissue Using FCCs**

Dr Frank BECKER
(INTANA BIOSCIENCE GMBH, Planegg, Germany)

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17:30 IL03 - Title to be announced

Prof. Jack TAUNTON
(UNIVERSITY OF CALIFORNIA, San Francisco, United States)

Keynote Lecture

18:00 KL01 - From Simulations of Biomolecules to Fighting Diseases

Prof. Martin KARPLUS
(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

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 - CryoEM for Small Molecules Discovery, Design, Understanding and Application

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

10:00 Coffee Break

Session 3 (continued) : Cryo-EM

10:30 OC07 - Title to be announced

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

10:45 OC08 - Title to be announced

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

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

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

14:30 Exhibitor Short Presentation

14:40 OC09 - Enabling NMR-Based Fragment Screening Using Stabilized Native GPCR: Case Study of Adenosine Receptor

Dr Anass JAWHARI
(CALIXAR, LYON , France)

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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

16:20 **IL09 - Design Considerations for Synthetic Macrocycles in Drug Discovery**

Prof. Adrian WHITTY
(BOSTON UNIVERSITY, Boston, United States)

16:45 **Exhibitor Short Presentation**

16:55 **OC11 - Use of Complementary Biophysical Methods to Characterize Ligand Binding to IL-17A**

Dr Parag SAHASRABUDHE
(PFIZER, Groton, United States)

17:10 **OC12 - Oral Communication to be selected from submitted abstracts**

17:25 **IL10 - Title to be announced**

Prof. Shaomeng WANG
(UNIVERSITY OF MICHIGAN, Michigan, United States)

18:10 **Posters & Drinks**

19:30 **End of the Day**

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Session 6 : Biotherapeutics

09:00 IL11 - Title to be announced
Prof. Jim WELLS
(UCSF, San Francisco, United States)

09:30 Exhibitor Short Presentation

09:40 IL12 - Centyrin Designer Proteins for Targeted Delivery
Dr Karyn T. O'NEIL
(AR? BIOTHERAPEUTICS, Philadelphia, United States)

10:10 Coffee Break

Session 6 (continued) : Biotherapeutics

10:40 OC13 - Oral Communication to be selected from submitted abstracts

10:55 Exhibitor Short Presentation

11:05 IL13 - Emerging Higher Order Structure Techniques in Biotherapeutics Development
Dr Tapan K. DAS
(BRISTOL-MYERS SQUIBB, New York, United States)

11:35 Poster Prizes and Closing Remarks

12:00 Departure