

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 α -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**

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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