

2nd NovAliX Conference - Biophysics in Drug Discovery 2015

Scientific Programme

Tuesday June 9, 2015

11:00 Registration

13:30 Welcome Address

SESSION 1: Method Development & Emerging Technologies

Session Chair

Dr Johannes OTTL
(NOVARTIS INSTITUTE OF BIOMEDICAL RESEARCH, Basel, Switzerland)

13:45 Monitoring Drug Target Engagement in Cells and Tissues Using the Cellular Thermal Shift Assay

Dr Pär NORDLUND
(KAROLINSKA INSTITUTE & NANYANG TECHNOLOGICAL UNIVERSITY, Singapore, Singapore)

14:30 No Crystal, No Problem: Hydrogen Deuterium Exchange Mass Spectrometry in Drug Discovery

Dr Nino CAMPOBASSO
(GLAXOSMITHKLINE, Collegeville, United States)

15:15 Strategies to Target Protein-Protein Interactions

Dr Marta WESTWOOD
(UCB, Slough, United Kingdom)

15:40 Coffe break & exhibition

16:10 Characterization of IL17A Inhibitors by Hydrogen/Deuterium Exchange Mass Spectrometry (HDX-MS)

Mr Alfonso ESPADA
(ELI LILLY, ALCOBENDAS, Spain)

16:35 Second-Harmonic Generation (SHG) Measures and Resolves Protein Conformations: High-Throughput Structural Drug Discovery

Dr Joshua SALAFSKY
(BIODESY, South San Francisco, United States)

KEYNOTE LECTURE

Chair

Dr Ursula EGNER
(BAYER, Berlin, Germany)

17:20 Molecular Recognition in Protein-Ligand Complexes

Prof. Gerhard KLEBE
(PHILIPPS-UNIVERSITY MARBURG, Marburg, Germany)

18:20 Welcome Reception

19:35 End of Day 1

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Wednesday June 10, 2015

08:30 **Registration**

SESSION 2: Biophysics for Integral Membrane Proteins

Session Chair

Dr Vincent MIKOL
(SANOFI, Vitry-sur-Seine, France)

09:00 **Improving the Biophysical Properties of GPCRs for Drug Screening and Structural Biology**

Prof. Andreas PLÜCKTHUN
(UNIVERSITY OF ZÜRICH, Zurich, Switzerland)

09:45 **Fluorine NMR Screening: Principles and Application to a Membrane Protein**

Dr Claudio DALVIT
(UNIVERSITY OF NEUCHÂTEL, Neuchâtel, Switzerland)

10:30 **Coffee break & exhibition**

11:00 **Drug Discovery at the Single Molecule Level**

Dr Anders GUNNARSSON
(ASTRAZENECA, Mölndal, Sweden)

11:25 **First Crystal Structure of Transmembrane Domain of G-Protein-Coupled Receptor MGLU5 Provides Insight Into Efficient New Drugs Design**

Dr Krzysztof OKRASA
(HEPTARES THERAPEUTICS, Welwyn Garden City, United Kingdom)

SESSION 4 (anticipated): The Use of Kinetics in Drug Discovery

Session Chair

Dr Geoff HOLDGATE
(ASTRAZENECA, Macclesfield, United Kingdom)

11:50 **Towards a Better Understanding of the Structural Mechanisms of Kinase Inhibitor Binding Kinetics**

Prof. Stefan KNAPP
(OXFORD UNIVERSITY, Oxford, United Kingdom)

12:35 **Lunch, exhibition & networking**

SESSION 3: Impact of Biophysics on Drug Discovery Projects

Session Chair

Dr Herbert NAR
(BOEHRINGER INGELHEIM, Biberach, Germany)

14:15 **Some Examples of Biophysics Helping Drug Discovery**

Prof. Rod HUBBARD
(UNIVERSITY OF YORK & VERNALIS, Cambridge, United Kingdom)

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- 15:00** **Making Every Interaction Count: Impact of Biophysical Methods Across the AstraZeneca Small-Molecule Portfolio**
Dr Stefan GESCHWINDNER
(ASTRAZENECA, Mölndal, Sweden)
- 15:45** **Coffee break & exhibition**
- 16:15** **Biophysical Approaches for Hit Finding and Evaluation at Bayer**
Dr Ursula EGNER
(BAYER, Berlin, Germany)
- 17:00** **Biophysics and Structural Biology Enabling the Discovery of Therapeutic Solutions: from Small Molecule Inhibitors to Vaccine Design**
Dr Vincent MIKOL
(SANOFI, Vitry-sur-Seine, France)
- 17:45** **End of Day 2**

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Thursday June 11, 2015

SESSION 4: The Use of Kinetics in Drug Discovery

Session Chair

Dr Geoff HOLDGATE
(ASTRAZENECA, Macclesfield, United Kingdom)

- 09:15 CCR2 Antagonists: From Structure-Kinetics Relationships to in vivo Efficacy**
Prof. Laura HEITMAN
(UNIVERSITY OF LEIDEN, Leiden, The Netherlands)
- 10:00 A Universal Homogeneous Assay for High-Throughput Determination of Binding Kinetics**
Dr Amaury FERNANDEZ MONTALVAN
(BAYER, Biberach an der Riss, Germany)
- 10:25 Coffee break & exhibition**
- 10:55 CDK8 Inhibitors with Long Residence Time Emerging from a Retro-Design Approach: New Opportunities for Cancer Treatment**
Dr Anita WEGERT
(MERCACHEM-SYNCOM, Nijmegen, The Netherlands)
- 11:20 Analysis of Binding Kinetics and Thermodynamics of DPP-4 Inhibitors and their Relationship to Structure**
Dr Herbert NAR
(BOEHRINGER INGELHEIM, Biberach, Germany)
- 12:05 Lunch, exhibition & networking**
- 13:45 Poster Session**
- 16:00 Coffee break & exhibition**
- 16:30 Round Table Discussion**
The Round Table will sum up the topics discussed in the first four Sessions of this Conference
- Chair**
Prof. Rod HUBBARD
(UNIVERSITY OF YORK & VERNALIS, Cambridge, United Kingdom)
- 17:15 Poster Prizes**
- 17:25 End of Day 3**
- 20:00 Conference Dinner at the Restaurant Maison Kammerzell**
(optional, subject to prior booking)

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Friday June 12, 2015

SESSION 5: Special Focus on Epigenetics

Session Chair

Prof. Helena DANIELSON
(UPPSALA UNIVERSITY, Uppsala, Sweden)

- 09:15 Interrogating the Bromodomain Family Through Chemical Biology**
Dr Richard CUMMINGS
(CONSTELLATION PHARMACEUTICALS, Cambridge, United States)
- 10:00 When to get Biophysical with Readers, Writers and Erasers**
Dr Chun-wa CHUNG
(GLAXOSMITHKLINE, Stevenage, United Kingdom)
- 10:45 Coffee break & exhibition**
- 11:15 Protein Methyltransferase Inhibitors as Personalised Cancer Therapeutics**
Dr Robert A. COPELAND
(EPIZYME, Cambridge, United States)
- 12:00 Closing Remarks**
- 12:15 End of Day 4**
- 14:15 Guided tour of the Cathedral of Strasbourg**
(subject to prior registration)