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

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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 Relatiosnhips 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 **Coffe 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)**