# 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)

## Scientific Programme

**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**

## Scientific Programme

### 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)**