

# 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, MADRID, 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 HEALTHCARE, 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 HEALTHCARE, 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**  
Dr Laura HEITMAN  
(UNIVERSITY OF LEIDEN, Leiden, The Netherlands)
- 10:00 A Universal Homogeneous Assay for High-Throughput Determination of Binding Kinetics**  
Dr Amaury Ernesto FERNANDEZ MONTALVAN  
(BAYER, Berlin, 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, 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)