

## Scientific Programme

**Tuesday 06/06/2017**

**13:00 Registration**

**14:00 Welcome Address**

### **Session 1: Biophysical Techniques for the Study of Integral Membrane Proteins**

#### **Session Chair**

Dr Ursula EGNER  
(BAYER, Berlin, Germany)

**14:15 Use of Mini-G Proteins to Study the Activate State of G Protein-Coupled Receptors (PL01)**

Dr Chris TATE  
(MRC LABORATORY OF MOLECULAR BIOLOGY, Cambridge, United Kingdom)

**15:00 Biophysical Analysis to Aid and Complement Structure Based Drug Design for GPCRS (OC01)**

Dr Carmen DREGGER  
(HEPTARES THERAPEUTICS, Welwyn Garden City, United Kingdom)

**15:25 Method for Rapid Optimization of Recombinant GPCR Protein Expression and Stability Using Virus-Like Particles (OC02)**

Dr Kathleen AERTGEERTS  
(DART NEUROSCIENCE, San Diego, United States)

**15:50 Coffee Break**

**16:20 Enabling Biophysics on Membrane Proteins Targets : Example of a Human Nucleoside Transporter (PL02)**

Dr Nicolas BOCQUET  
(LEADXPAG, Villigen, Switzerland)

**17:05 Exhibitor Short Presentation: Creoptix  
The Wave of the Future in Kinetics**

Dr Matyas VEGH  
(CREOPTIX AG, Wädenswil, Switzerland)

**17:15 Exhibitor Short Presentation: Synthelis  
Cell-free technology, expertise and services for your project in structural biology**

Mrs Safia EZZINE  
(SYNTHELIS, La Tronche, France)

#### **Keynote Lecture**

#### **Chair**

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

**17:25 Allosteric Mechanisms of Signal Transduction Investigated with Pentameric Ligand Gated Ion Channels: Consequences for Drug Design (KL01)**

Prof. Jean-Pierre CHANGEUX  
(COLLÈGE DE FRANCE & INSTITUT PASTEUR, Paris, France)

# 4th NovAliX Conference

Scientific Programme

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18:25      Welcome Reception

20:00      End of the Day

## Scientific Programme

### Wednesday 07/06/2017

**08:30 Registration**

#### **Session 2: Recent Advances in NMR**

##### **Session Chair**

Dr Chun-wa CHUNG  
(GLAXOSMITHKLINE, Stevenage, United Kingdom)

**09:00 Study of Protein Folding and Ligand Binding by Pressure Jump NMR (PL03)**

Prof. Ad BAX  
(NATIONAL INSTITUTES OF HEALTH, Bethesda, United States)

**09:45 NMR as a Powerful Tool for Identifying Natural Compounds Able to Interfere with ELAV-mRNA Complexes (OC03)**

Dr Francesca VASILE  
(UNIVERSITY OF MILANO, Milano, Italy)

**10:10 Coffee Break**

**10:40 New NMR Tools for Drug Discovery : From Validation to Structure Determination (PL04)**

Dr Alvar GOSSERT  
(ETH ZÜRICH, Zürich, Switzerland)

#### **Session 3: Hot Topics**

##### **Session Chair**

Dr Sandra JACOB  
(NOVARTIS, Basel, Switzerland)

**11:25 Biophysical Assays to Answer Evolving Questions in Drug Discovery (OC04)**

Dr Derrick MEINHOLD  
(GLAXOSMITHKLINE, Berwyn, United States)

**11:50 Exhibitor Short Presentation: Sierra Sensors  
High-Throughput SPR Screening in Drug Discovery**

Dr Sven MALIK  
(SIERRA SENSORS, Champs sur Marne, France)

**12:00 Exhibitor Short Presentation: Biodesy  
Screening with Structural Insight: High Throughput Measurement of Protein Conformational Change**

Dr Tad GEORGE  
(BIODESY, San Francisco, United States)

#### **Session 5: Detecting Allosteric Effectors (advanced)**

##### **Session Chair**

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

## Scientific Programme

**12:10      Surface Plasmon Resonance Based Method to Discriminate Direct Competition and Allosteric Effects in Ternary Systems (OC10)**

Dr Armin RUF  
(F. HOFFMANN - LA ROCHE, Basel, Switzerland)

**12:35      Lunch & Networking**

**Session 4: Recent Advances in FBDD**

**Session Chair**

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

**14:00      FBLD and Biophysics: Better Together (KL02)**

Dr Dan ERLANSON  
(CARMOT THERAPEUTICS, South San Francisco, United States)

**15:00      XCHEM: A High Throughput in Crystallo Fragment Screening Platform (OC06)**

Dr Alexandre DIAS  
(DIAMOND LIGHT SOURCE LTD, Didcot, Oxon, United Kingdom)

**15:25      Fragment Screening against DC-SIGN Identifies Multiple Druggable Secondary Sites (OC07)**

Mr Hannes BAUKMANN  
(MAX PLANCK INSTITUTE OF COLLOIDS AND INTERFACES, Potsdam-Golm, Germany)

**15:50      Coffee Break**

**16:20      Fragment Based Lead Generation – What Drives Success? (PL05)**

Dr Jenny SANDMARK  
(ASTRAZENECA, Gothenburg, Sweden)

**17:05      A New Heuristic to Predict 3D Ligand Bound Conformation by Mining PDB Subpockets (OC08)**

Mr Olivier BEQUIGNON  
(JANSSEN R&D, Val de Reuil Cedex, France)

**17:30      Exhibitor Short Presentation: Domainex  
The MST Approach to Fragment Screening**

Prof. Trevor PERRIOR  
(DOMAINEX LIMITED, Cambridge, United Kingdom)

**17:40      Navigating Biophysical Space in Search of Medicines (PL06)**

Dr Glyn WILLIAMS  
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

### Thursday 08/06/2017

#### Session 5: Detecting Allosteric Effectors

##### Session Chair

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

**09:00 Large Scale Protein Conformational Motions : From Fundamental Biophysics to Functional Dynamics (PL07)**

Prof. Martin BLACKLEDGE  
(INSTITUT DE BIOLOGIE STRUCTURALE (IBS), Grenoble, France)

**09:45 Identifying Allosteric Modifiers of K-RAS Using Second Harmonic Generation (OC09)**

Dr Elizabeth VO  
(UCSF, San Francisco, United States)

**10:10 Coffee Break**

**10:40 Analysis of Allosteric Modulators with Kinetic Fret (OC11)**

Dr Martin REDHEAD  
(UCB, Slough, United Kingdom)

**11:05 Spectroscopic Adventures in Orthosteric and Allosteric Inhibition (PL08)**

Dr Richard TAYLOR  
(UCB, Slough, United Kingdom)

#### Session 3: Hot Topics (continued)

##### Session Chair

Dr Sandra JACOB  
(NOVARTIS, Basel, Switzerland)

**11:50 Precision of Biophysical Techniques that Determine Protein? Compound Dissociation Constants, Lessons from our Database of over 700 Ligand Kds Determined by ITC, FTSA(DSF), SPR, and SFA (OC05)**

Prof. Daumantas MATULIS  
(INSTITUTE OF BIOTECHNOLOGY, Vilnius, Lithuania)

**12:15 Lunch & Networking**

**13:15 Poster Session**

#### Session 6: IDPs and the Dark Proteome

##### Session Chair

Dr Geoff HOLDGATE  
(ASTRAZENECA, Macclesfield, United Kingdom)

**14:30 Mechanistic Insights into TSPO and IDPs through NMR (PL09)**

Prof. Markus ZWECKSTETTER  
(MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)

## Scientific Programme

### Roundtable Discussion

**15:15**      **Increasing Success in Science by Increasing Diversity: From Methods to Gender**

### Session 6: IDPs and the Dark Proteome (continued)

#### Session Chair

Dr Geoff HOLDGATE  
(ASTRAZENECA, Macclesfield, United Kingdom)

**16:00**      **Finding Small-Molecules Inhibitors of the Interaction between the Intrinsically Disordered Androgen Receptor N-Terminal Domain and its Globular Partner RAP74 C-Terminal Domain (OC12)**

Dr Marta FRIGOLE-VIVAS  
(INSTITUTE FOR RESEARCH IN BIOMEDICINE (IRB BARCELONA), Dresden, Germany)

**16:25**      **Coffee Break**

**16:55**      **Systematic Development of Small Molecules Against A $\beta$  Aggregation (PL10)**

Prof. Michele VENDRUSCOLO  
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

**17:40**      **Poster Prizes**

**17:50**      **End of the Day**

**20:00**      **Conference Dinner**

### Friday 09/06/2017

#### Session 7: Antibodies and Relatives

##### Session Chair

Dr Jim BRYSON  
(BRISTOL-MYERS-SQUIBB, Princeton, United States)

- 09:00**     **Cutting-Edge Mass Spectrometry Methods for the Multi-Level Structural Characterization of mAbs and ADCs (KL03)**  
Dr Alain BECK  
(PIERRE FABRE, St Julien-en-Genevois, France)
- 10:00**     **Adnectin Bioconjugates for PET Imaging and Targeted Drug Conjugates (PL11)**  
Dr Jim BRYSON  
(BRISTOL-MYERS-SQUIBB, Princeton, United States)
- 10:45**     **Coffee Break**
- 11:15**     **Exhibitor Short Presentation: Pall ForteBio**  
**Our Label-Free, Real-Time Kinetics Technologies with Microplate Sampling Allow for High-Throughput in Screening & Characterisation of Drug Candidates Including Challenging Matrixes Like Crude Biologicals or Fragments in DMSO**  
Mr Attila ARANYOS  
(SARTORIUS, France)
- 11:25**     **Thermal Stabilization and Conformational Trapping of Membrane Transporters by in Vitro Selected Synthetic Nanobodies (PL12)**  
Prof. Markus SEEGER  
(UNIVERSITY OF ZURICH, Zürich, Switzerland)
- 12:10**     **Closing Remarks and Departure**