

Tuesday June 6, 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 HEALTHCARE, 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

18:25 **Welcome Reception**

20:00 **End of the Day**

Wednesday June 7, 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 INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

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

Dr Derrick MEINHOLD
(GLAXOSMITHKLINE, Conshohocken, United States)

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

Dr Sven MALIK
(SIERRA SENSORS, Hamburg, Germany)

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, 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 June 8, 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
(IBS - INSTITUT DE BIOLOGIE STRUCTURALE, 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 INSTITUTES FOR BIOMEDICAL RESEARCH, 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)

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)**

Mrs Marta FRIGOLÉ-VIVAS
(INSTITUTE FOR RESEARCH IN BIOMEDICINE (IRB BARCELONA), Barcelona, Spain)

16:25 **Coffee Break**

16:55 **Systematic Development of Small Molecules Against A β 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 June 9, 2017

Session 7: Antibodies and Relatives

Session Chair

Dr Jim BRYSON
(BRISTOL-MYERS-SQUIBB R&D, New York, 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 R&D, New York, 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
(PALL CORPORATION, Saint-Germain-en-Laye, 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