4th NovAliX Conference

Scientific Programme

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, 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
(LEADXPRO AG, 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)

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18:25 **Welcome Reception**

20:00 **End of the Day**

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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, 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)

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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)

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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
(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)

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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? 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**

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Friday June 9, 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**