

Wednesday 20/03/2019

12:00 Registration

13:15 Welcome Address

Dr Jean-Paul RENAUD
(NOVALIX & RIBOSTRUCT, Illkirch, France)

Session 1: Hot Topics

Session Chair

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

13:30 The Way Home: Molecular Recognition Path of L-TRP to IDO1 (OC01)

Prof. Antonio MACCHIARULO
(UNIVERSITY OF PERUGIA, Perugia, Italy)

13:45 Fragment Based Screening: Critical Aspects of its Performance and Evaluation Screening a Diverse Set of Cancer Target Classes (OC02)

Dr Andrea GOHLKE
(BEATSON INSTITUTE FOR CANCER RESEARCH, Glasgow, United Kingdom)

14:00 High-Throughput, Automated Crystallography Pipelines for Drug Discovery (OC03)

Dr Irina CORNACIU
(EMBL GRENOBLE, Grenoble, France)

14:15 Exhibitor Short Presentation: ForteBio Integrated Solutions for Early Stage Biologics Discovery

14:25 Structure of an Essential Inner Membrane Protein-LPS Complex (OC04)

Dr Thomas CLAIRFEUILLE
(GENENTECH, INC., South San Francisco, United States)

14:40 Fragment Based Target Screening to Prioritise Novel Antimicrobial Targets (OC05)

Dr Peter CANNING
(LIFEARC, Stevenage, United Kingdom)

14:55 Biophysics as a Key Element in the Early Phase of Drug Discovery (IL01)

Dr Matthias FRECH
(MERCK, Darmstadt, Germany)

15:25 Coffee Break & Exhibition

Session 2: X-ray Crystallography ? Cryo-EM Complementarity

Session Chair

Dr Michael HENNIG
(LEADXP, Villigen, Switzerland)

15:55 High-Resolution Structure Determination of Dynamic Macromolecular Complexes by Cryo-EM (IL02)

Scientific Programme

Prof. Holger STARK
(MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)

16:25 Using X-ray and Cryo-EM Approaches to Study Allosteric Regulation of GTP Cyclohydrolase I (OC06)

Dr Rebecca EBENHOCH
(BOEHRINGER INGELHEIM, Biberach, Germany)

16:40 Structural Studies of Chromatin Remodellers by Cryo-EM: Challenges and Opportunities for Drug Development (IL03)

Prof. Karl-Peter HOPFNER
(LUDWIG-MAXIMILIANS UNIVERSITY, München, Germany)

**17:10 Exhibitor Short Presentation: ThermoFisher Scientific
New Optical Modes to Improve Cryo-EM Throughput**

17:20 Cryo-EM, a New Tool for Drug Discovery at Novartis (IL04)

Dr Christian WIESMANN
(NOVARTIS, Basel, Switzerland)

Keynote Lecture

Chair

Dr Herbert NAR
(BOEHRINGER INGELHEIM, Biberach, Germany)

17:50 Integrative Structural Biology of GPCRs (KL01)

Prof. Kurt WÜTHRICH
(THE SCRIPPS RESEARCH INSTITUTE, USA & ETH ZÜRICH, Zurich, Switzerland)

18:50 Welcome Reception

20:00 End of the Day

Thursday 21/03/2019

08:30 Registration

Session 3: Chemical Biology Meets Biophysics for Drug Discovery

Session Chair

Dr Sandra JACOB
(NOVARTIS, Basel, Switzerland)

09:00 **Illuminating the Path to New E3-Ligases for Targeted Protein Degradation (IL05)**

Ms Hannah LITHGOW (UNIVERSITY OF STRATHCLYDE & GSK, Glasgow, United Kingdom)
(BIOIB,RICA)

09:30 **The Development and Biophysical Characterisation of Click-Tagged, Reversible Probes to Measure Target Occupancy of ERK1/2 Kinase Inhibitors (OC07)**

Dr Chiara Rosa VALENZANO
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

09:45 **Biophysical and Structural Principles of PROTAC Mechanism of Action (IL06)**

Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

10:15 Coffee Break & Exhibition

10:45 **The PROTAC Design Toolbox: Biophysically Enabling the Optimisation of a Potent SMARCA Degradator (OC08)**

Dr David ZOLLMAN
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

11:00 **Exhibitor Short Presentation: Creoptix Pushing Boundaries in Kinetics Analysis**

11:10 **Rational Design of Kinase Inhibitors Using Structure and Biophysical Data (IL07)**

Prof. Stefan KNAPP
(GOETHE UNIVERSITY FRANKFURT, Frankfurt am Main, Germany)

11:40 **Poster Session**

12:40 **Lunch, Exhibition & Networking**

Session 4: MS-Based Methods

Session Chair

Dr Stefan GESCHWINDNER
(ASTRAZENECA, Mölndal, Sweden)

14:00 **Advances in Structural Mass Spectrometry for Drug Discovery and Therapeutic Protein Characterization (IL08)**

Scientific Programme

Dr Sarah CIANFERANI
(UNIVERSITY OF STRASBOURG, Strasbourg, France)

14:30 Identifying an Escape Route from Adverse Effects of the Liver X Receptor Ligands Using HDX-MS (OC09)

Dr Anna BELORUSOVA
(ASTRAZENECA, Molndal, Sweden)

14:45 Sugars in the Gas Phase? Novel Techniques to Unravel the Glycocode (IL09)

Prof. Kevin PAGEL
(FREIE UNIVERSITÄT BERLIN, Berlin, Germany)

**15:15 Exhibitor Short Presentation: Bruker Daltonics
High-Throughput SPR Screening in Drug Discovery**

15:25 Use of Mass Spectrometry in Small Molecule Lead Discovery (IL10)

Dr Jörg HOERNSCHEMEYER
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

15:55 Coffee Break & Exhibition

Session 5: Characterisation of Small Molecules Binding to RNA

Session Chair

Dr Ursula EGNER
(BAYER, Berlin, Germany)

16:25 Hit Discovery for Riboswitch Ligands (IL11)

Prof. Ruth BRENK
(UNIVERSITY OF BERGEN, Bergen, Norway)

16:55 Detection of Ligand-Induced Conformational Changes in Oligonucleotides by Second-Harmonic Generation (OC10)

Dr Margaret BUTKO
(BIODESY, South San Francisco, United States)

17:10 Structural Basis for Gene-Specific RNA Splicing Correction Induced by a Small Molecule (IL12)

Prof. Frédéric ALLAIN
(ETH ZURICH, Zurich, Switzerland)

**17:40 Exhibitor Short Presentation: 2bind
Work with the Experts in Biophysics – A Quick Dive into 2bind's Tailor-made Services for Drug Discovery**

17:50 Ribosomal Translation and Human Diseases (IL13)

Prof. Eric WESTHOF
(INSTITUT DE BIOLOGIE MOLÉCULAIRE ET CELLULAIRE, Strasbourg, France)

18:20 Poster Session & Drinks

19:20 End of the Day

20:00 Conference Dinner

6th NovAliX Conference

Scientific Programme

Friday 22/03/2019

Session 6: Enabling Tools for Biophysical and Structural Studies

Session Chair

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

- 09:00** **Innovating Drug Discovery by Locking GPCRs in Functional Conformations (IL14)**
Dr Christel MENET
(CONFO THERAPEUTICS, Brussels, Belgium)
- 09:30** **New Biophysical Approaches to Study IRES RNA/Ribosomes Interactions (OC11)**
Dr Eric ENNIFAR
(CNRS, Strasbourg, France)
- 09:45** **Exhibitor Short Presentation: Synthelis From Gene to Structure (FGTS)**
- 09:55** **Strategies to Enable Challenging Biophysical and Structural Studies (IL15)**
Dr Stefan GESCHWINDNER
(ASTRAZENECA, Mölndal, Sweden)
- 10:25** **Coffee Break & Exhibition**
- 10:55** **SPR-Based Approaches to Enable Direct Binding Assays for Membrane Proteins (IL16)**
Dr Sylwia HUBER
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)
- 11:25** **Impact of Mechanistic Enzymology and Bio-Structural Mass Spectrometry on the Progression of a Serine Hydrolase Inhibitor Discovery Project (OC12)**
Dr Mathias ANTOINE
(INSTITUT DE RECHERCHES SERVIER, Croissy-Sur-Seine, France)
- 11:40** **An Integrated Molecular-Scale Biophysics Approach to Drug Discovery: the Contribution of the ARBRE-MOBIEU European Network (IL17)**
Dr Patrick ENGLAND
(INSTITUT PASTEUR, Paris, France)
- 12:10** **Exhibitor Short Presentation: Crelux
Crelox – A Fully Integrated Offering, from Protein to Screen, Through Crystallography Confirmation and Beyond**
- 12:20** **Wave-Guided Interferometry and Biophysical Methods Enabling Structure-Based Drug Discovery on Membrane Protein Targets (IL18)**
Dr Nicolas BOCQUET
(LEADXPOR AG, Villigen, Switzerland)
- 12:50** **Poster Prizes and Closing Remarks**
- 13:00** **Departure**