

2nd NovAliX Virtual Conference

Program

Tuesday March 9, 2021

Session Opening

19:00 Opening Address by Conference Chairman

Dr Jean-Paul RENAUD
(URANIA THERAPEUTICS, Ostwald, France)

Session Session 1: Hot Topic - COVID-19

19:10 Introduction by the Session Chair

Dr Chaohong SUN
(ABBVIE, North Chicago, United States)

19:15 Structural and Functional Analysis of the D614G SARS-CoV-2 Spike Protein Variant (OC01)

Dr Xue WANG
(THERMO FISHER SCIENTIFIC, Eindhoven, The Netherlands)

19:30 SARS-CoV-2 3CL protease: Structure-Based Virtual Screening, Crystallographic Fragment Screening and Assay Implementation to Identify Novel Starting Points for Inhibition (OC02)

Dr Alexander METZ
(IDORSIA PHARMACEUTICALS LTD, Allschwil, Switzerland)

Session Session 2: Induced-Proximity Drug Discovery : Selective Protein Degraders, PPI Stabilizers, etc.

19:45 Introduction by the Session Chair

Dr Matthias FRECH
(MERCK, Darmstadt, Germany)

19:50 The Structural Basis of Indisulam-Mediated Recruitment of RBM39 to the DCAF15-DDB1-DDA1 E3 Ligase Complex (IL01)

Dr Dirksen BUSSIERE
(ELI LILLY, San Diego, United States)

**20:20 Exhibitor Short Presentation - Nanomaging Services
Leading the Revolution: CryoEM-Enabled Drug Discovery**

Dr Melanie ADAMS-CIOABA
(NANOIMAGING SERVICES, San Diego, United States)

20:30 Targeting a Cryptic Binding Pocket by Disulfide-Induced Rupture of a Homodimeric Protein-Protein Interface (OC03)

Dr Dzung NGUYEN
(PHILIPPS-UNIVERSITÄT MARBURG, Marburg, Germany)

**20:45 Exhibitor Short Presentation - Crelux, a WuXi AppTec company
Target To Hit Solutions: Drug Discovery Of Bifunctional Molecules**

Dr Thomas WALDMANN
(CRELUX, A WUXI APPTEC COMPANY, Martinsried, Germany)

20:55 Dissecting Protein-Protein Interaction Networks (KL01)

Prof. Michelle ARKIN
(UNIVERSITY OF CALIFORNIA, San Francisco, United States)

Session Networking

21:40 Networking, Exhibition & Posters

23:00 End of the day

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Wednesday March 10, 2021

Session Networking

18:00 **Networking, Exhibition & Posters**

Session Session 3: Integrative Structural Biology & Biophysics

19:00 **Introduction by the Session Chair**

Dr MariJean EGGEN
(ELI LILLY, Indianapolis, United States)

19:05 **Hijacking Molecular Plasticity to Fine Tune Nuclear Receptor Signaling: Structural Proteomics and Precision Therapeutics (IL02)**

Prof. Patrick GRIFFIN
(THE SCRIPPS RESEARCH INSTITUTE, Jupiter, United States)

19:35 **Exhibitor Short Presentation - NovAliX
NovAliX: Drug Discovery fueled with Biophysics**

Dr James TARVER
(NOVALIX, Philadelphia, United States)

19:45 **Synergistic Use of Ligand Based NMR and Crystallography to Elucidate Small Molecules Interactions with Challenging Targets (OC04)**

Dr Ariele VIACAVA FOLLIS
(EMD SERONO R&D INSTITUTE INC, Stow, United States)

20:00 **Exhibitor Short Presentation - Wuxi Biortus Biosciences Co., Ltd.
Your Partner for Proteins and Structures**

Dr Yujian YOU
(WUXI BIORTUS BIOSCIENCES CO., LTD., Jiangyin, China)

20:10 **Fragment Screening Reveals a Novel Pocket in Cysteine Protease ATG4B (OC05)**

Dr Troy JOHNSON
(UNIVERSITY OF TEXAS MD ANDERSON CANCER CENTER, Houston, United States)

20:25 **Exhibitor Short Presentation - Bruker
An Introduction to Bruker SPR Technology**

Mr Cameron PARAST
(BRUKER SCIENTIFIC, Billerica, United States)

20:35 **Inhibition of the Cysteine Desulfurase in the SUF Pathway of Iron-Sulfur Cluster Biogenesis Towards Development of Novel Antibacterials (OC06)**

Dr Amy BONCELLA
(COLORADO SCHOOL OF MINES, Golden, United States)

20:50 **Identification, Characterization and Conformational Assessment of STING Modulators (IL03)**

Dr Daniel WYSS
(MERCK, Morristown, United States)

Session Networking

21:20 **Networking, Exhibition & Posters**

23:00 **End of the day**

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Thursday March 11, 2021

Session Networking

18:00 **Networking, Exhibition & Posters**

Session Session 4: Cryo-EM in Drug Discovery - Accelerating Drug Design for Intractable Targets
a full day session organized by Thermo Fisher Scientific, Platinum Sponsor of the NovAliX Conference

Introduction by the Session Chair

Dr Jeffrey LENGYEL
(THERMO FISHER SCIENTIFIC, New York, United States)

19:15 **From Concept to Reality: CryoEM as an Integral Part of Drug Discovery and Development (IL04)**

Dr Corey STRICKLAND
(MERCK, Kenilworth, United States)

19:45 **Structural Characterization of Different TRPA1 Inhibitors (IL05)**

Dr Lionel ROUGÉ
(GENENTECH, San Francisco, United States)

20:15 **Improving Protein-Ligand Modeling into Cryo-EM Data and the use of those Models in Drug Discovery Efforts (IL06)**

Dr Kenneth BORRELLI
(SCHRÖDINGER, INC., New York, United States)

20:45 **Using Cryo-EM for GPCR Drug Discovery and Development (IL07)**

Prof. Patrick M. SEXTON
(MONASH UNIVERSITY, Parkville, Australia)

21:15 **Break**

Session Panel Discussion: Cryo-EM in Drug Discovery - Accelerating Drug Design for Intractable Targets

21:20 **Moderator**

Dr Jeffrey LENGYEL
(THERMO FISHER SCIENTIFIC, New York, United States)

Speakers

Mr Benjamin APKER
(MITEGEN, Ithaca, United States)

Dr Corey STRICKLAND
(MERCK, Kenilworth, United States)

Dr Denis ZEYER
(NOVALIX, Illkirch, France)

Session Networking

22:05 **Networking, Exhibition & Posters**

23:00 **End of the day**

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Friday March 12, 2021

Session Networking

18:00 Networking, Exhibition & Posters

Session Session 5: Advances in Biophysical Techniques : Single-Molecule Techniques, Label-Free Technologies, Surface-Immobilized Techniques beyond SPR, etc.

19:00 Introduction by the Session Chair

Dr Daniel WYSS
(MERCK, Morristown, United States)

19:05 Ligand-Dependent Structural Plasticity of TrkA Kinase Studied by NMR Spectroscopy (IL08)

Dr Reto HORST
(PFIZER, INC., Grotton, United States)

19:35 Exhibitor Short Presentation - Dynamic Biosensors
heliX® biosensor – your structure-based drug discovery tool

Dr Joanna DEEK
(DYNAMIC BIOSENSORS, Martinsried/Planegg, Germany)

19:45 Real-Time Single-Molecule Detection of Drug-Protein Interactions Using a Novel DNA-Based Nanoscale Actuator (OC07)

Prof. Terence STRICK
(ECOLE NORMALE SUPERIEURE, Paris, France)

20:00 Exhibitor Short Presentation - MiTeGen
Crystallography and Cryo-EM - Sample Preparation Technology Developments

Mr Benjamin APKER (MITEGEN, Ithaca, United States)
(BIOIBÉRICA)

20:10 Development of a Microscale Thermophoresis-Based Method for Screening Inhibitors of the Methyl-Lysine Reader Protein MRG15 (OC08)

Dr Alessandra FEOLI
(UNIVERSITÀ DEGLI STUDI DI SALERNO, Fisciano (Salerno), Italy)

20:25 SAR by 19F NMR: Using Protein-Observed Fluorine NMR for Targeting Protein Complexes (IL09)

Prof. William POMERANTZ
(UNIVERSITY OF MINNESOTA, Minneapolis, United States)

20:55 Focal Molography - A New Bioanalytical Tool to Eliminate Guess Work in Pharma Research (OC09)

Dr Volker GATTERDAM
(LINO BIOTECH AG, Zurich, Switzerland)

21:10 Exhibitor Short Presentation - Biosensing Instruments
Cell-based SPR Introduction

Mrs Akemi UEKI
(BIOSENSING INSTRUMENT, Tempe, United States)

21:20 Too Weak for Biophysics: Concentration-Dependent Crystallographic Soaking as Tool for Fragment Hit Prioritisation (OC10)

Ms Yuliya DUBIANOK
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

21:35 Microcrystal Electron Diffraction (MicroED): Methodology and Applications (KL02)

Prof. Brent NANNENGA
(ARIZONA STATE UNIVERSITY, Tempe, United States)

22:20 Closing Remarks

Dr Jean-Paul RENAUD
(URANIA THERAPEUTICS, Ostwald, France)

22:30 End of the Conference