### **Program**

### Tuesday March 9, 2021

#### **Session Opening**

07:00 Opening Address by Conference Chairman

pm

Dr Jean-Paul RENAUD

(URANIA THERAPEUTICS, Ostwald, France)

Session Session 1: Hot Topic - COVID-19

07:10 Introduction by the Session Chair

pm

Dr Chaohong SUN

(ABBVIE, North Chicago, United States)

07:15 Structural and Functional Analysis of the D614G SARS-CoV-2 Spike Protein Variant (OC01)

pm

Dr Xue WANG

(THERMO FISHER SCIENTIFIC, Eindhoven, The Netherlands)

07:30 SARS-CoV-2 3CL protease: Structure-Based Virtual Screening, Crystallographic Fragment Screening and

pm 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.

07:45 Introduction by the Session Chair

pm

Dr Matthias FRECH

(MERCK, Darmstadt, Germany)

07:50 The Structural Basis of Indisulam-Mediated Recruitment of RBM39 to the DCAF15-DDB1-DDA1 E3 Ligase

pm Complex (IL01)

Dr Dirksen BUSSIERE

(ELI LILLY, Indianapolis, United States)

08:20 Exhibitor Short Presentation - NanoImaging Services

pm Leading the Revolution: CryoEM-Enabled Drug Discovery

Dr Melanie ADAMS-CIOABA

(NANOIMAGING SERVICES, San Diego, United States)

08:30 Targeting a Cryptic Binding Pocket by Disulfide-Induced Rupture of a Homodimeric Protein-Protein Interface

pm (OC03)

Dr Dzung NGUYEN

(PHILIPPS-UNIVERSITÄT MARBURG, Marburg, Germany)

08:45 Exhibitor Short Presentation - Crelux, a WuXi AppTec company pm Target To Hit Solutions: Drug Discovery Of Bifunctional Molecules

Target 10 The Coldions. Drug Discovery Of Bhancaonar molec

(CRELUX, A WUXI APPTEC COMPANY, Martinsried, Germany)

08:55 Dissecting Protein-Protein Interaction Networks (KL01)

pm

Prof. Michelle ARKIN

(UNIVERSITY OF CALIFORNIA, San Francisco, CA, United States)

#### **Session Networking**

09:40 Networking, Exhibition & Posters

pm

11:00 End of the day

pm

### **Program**

### Wednesday March 10, 2021

#### **Session Networking**

06:00 Networking, Exhibition & Posters

pm

#### Session Session 3: Integrative Structural Biology & Biophysics

07:00 Introduction by the Session Chair

pm

Dr MariJean EGGEN

(ELI LILLY, Indianapolis, United States)

07:05 Hijacking Molecular Plasticity to Fine Tune Nuclear Receptor Signaling: Stuctural Proteomics and Precision

pm Therapeutics (IL02)

Prof. Patrick GRIFFIN

(THE SCRIPPS RESEARCH INSTITUTE, Jupiter, United States)

07:35 Exhibitor Short Presentation - NovAliX

pm NovAliX: Drug Discovery fueled with Biophysics

Dr James TARVER

(NOVALIX, Philadelphia, United States)

07:45 Synergistic Use of Ligand Based NMR and Crystallography to Elucidate Small Molecules Interactions with

pm Challenging Targets (OC04)

Dr Ariele VIACAVA FOLLIS

(EMD SERONO R&D INSTITUTE INC, Stow, United States)

08:00 Exhibitor Short Presentation - Wuxi Biortus Biosciences Co., Ltd.

pm Your Partner for Proteins and Structures

Dr Yujian YOU

(WUXI BIORTUS BIOSCIENCES CO., LTD., Jiangyin, China)

08:10 Fragment Screening Reveals a Novel Pocket in Cysteine Protease ATG4B (OC05)

pm

Dr Troy JOHNSON

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

08:25 Exhibitor Short Presentation - Bruker

pm An Introduction to Bruker SPR Technology

Mr Cameron PARAST

(BRUKER SCIENTIFIC, Billerica, United States)

08:35 Inhibition of the Cysteine Desulfurase in the SUF Pathway of Iron-Sulfur Cluster Biogenesis Towards

pm Development of Novel Antibacterials (OC06)

Dr Amy BONCELLA

(COLORADO SCHOOL OF MINES, Golden, United States)

08:50 Identification, Characterization and Conformational Assessment of STING Modulators (IL03)

pm

Dr Daniel WYSS

(MERCK & CO., INC., Morristown, United States)

#### Session Networking

09:20 Networking, Exhibition & Posters

pm

11:00 End of the day

pm

### **Program**

### Thursday March 11, 2021

#### **Session Networking**

06:00 Networking, Exhibition & Posters

pm

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)

07:15 From Concept to Reality: CryoEM as an Integral Part of Drug Discovery and Development (IL04)

pm

Dr Corey STRICKLAND

(MERCK, Kenilworth, United States)

07:45 Structural Characterization of Different TRPA1 Inhibitors (IL05)

pm

Dr Lionel ROUGÉ

(GENENTECH, San Francisco, United States)

08:15 Improving Protein-Ligand Modeling into Cryo-EM Data and the use of those Models in Drug Discovery Efforts

m (IL06)

Dr Kenneth BORRELLI

(SCHRÖDINGER, INC., New York, United States)

08:45 Using Cryo-EM for GPCR Drug Discovery and Development (IL07)

pm

Prof. Patrick M. SEXTON

(MONASH UNIVERSITY, Parkville, Australia)

09:15 Break

pm

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

09:20 Moderator

pm

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**

10:05 Networking, Exhibition & Posters

pm

11:00 End of the day

pm

### **Program**

### Friday March 12, 2021

#### **Session Networking**

06:00 Networking, Exhibition & Posters

pm

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

07:00 Introduction by the Session Chair

pm

Dr Daniel WYSS

(MERCK & CO., INC., Morristown, United States)

07:05 Ligand-Dependent Structural Plasticity of TrkA Kinase Studied by NMR Spectroscopy (IL08)

pm

Dr Reto HORST

(PFIZER, INC., Grotton, United States)

07:35 Exhibitor Short Presentation - Dynamic Biosensors

pm heliX® biosensor – your structure-based drug discovery tool

Dr Joanna DEEK

(DYNAMIC BIOSENSORS, Martinsried/Planegg, Germany)

07:45 Real-Time Single-Molecule Detection of Drug-Protein Interactions Using a Novel DNA-Based Nanoscale

pm Actuator (OC07)

Prof. Terence STRICK

(ECOLE NORMALE SUPERIEURE, Paris, France)

08:00 Exhibitor Short Presentation - MiTeGen

pm Crystallography and Cryo-EM - Sample Preparation Technology Developments

Mr Benjamin APKER (MITEGEN, Ithaca, United States)

(BIOIBÉRICA)

08:10 Development of a Microscale Thermophoresis-Based Method for Screening Inhibitors of the Methyl-Lysine

pm Reader Protein MRG15 (OC08)

Dr Alessandra FEOLI

(UNIVERSITÀ DEGLI STUDI DI SALERNO, Fisciano (Salerno), Italy)

08:25 SAR by 19F NMR: Using Protein-Observed Fluorine NMR for Targeting Protein Complexes (IL09)

pm

Prof. William POMERANTZ

(UNIVERSITY OF MINNESOTA, Minneapolis, United States)

08:55 Focal Molography - A New Bioanalytical Tool to Eliminate Guess Work in Pharma Research (OC09)

pm

Dr Volker GATTERDAM

(LINO BIOTECH AG, Zurich, Switzerland)

09:10 Exhibitor Short Presentation - Biosensing Instruments

pm Cell-based SPR Introduction

Mrs Akemi UEKI

(BIOSENSING INSTRUMENT, Tempe, United States)

09:20 Too Weak for Biophysics: Concentration-Dependent Crystallographic Soaking as Tool for Fragment Hit

pm Prioritisation (OC10)

Ms Yuliya DUBIANOK

(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

09:35 Microcrystal Electron Diffraction (MicroED): Methodology and Applications (KL02)

pm

Prof. Brent NANNENGA

(ARIZONA STATE UNIVERSITY, Tempe, United States)

10:20 Closing Remarks

pm

Dr Jean-Paul RENAUD

(URANIA THERAPEUTICS, Ostwald, France)

## Program

10:30 End of the Conference pm