

ACSMEDI-EFMC Medicinal Chemistry Frontiers 2023

Scientific Program

Saturday 10/06/2023

15:00 **Registration**

Opening Session

17:30 **Opening of the Symposium and Welcome address**

Prof. Daniel HARKI
(UNIVERSITY OF MINNESOTA, Minneapolis, MN, United States)

17:45 **PL01- Medicinal Chemistry of the Future: Trends, Targets and Technologies**

Dr Klaus URBAHNS
(EMD SERONO, Billerica, MA, United States)

18:30 **Welcome Reception**

Scientific Program

Sunday 11/06/2023

08:00 Registration

Session 1 - Chemical Modulation of RNA

Session chair

Dr Darby SCHMIDT
(SONATA THERAPEUTICS, Cambridge, MA, United States)

09:00 IL01 - Modulating the Conformation and Function of Disease-Relevant RNA with Small Molecules

Prof. Amanda HARGROVE
(DUKE UNIVERSITY, Durham, NC, United States)

09:30 IL02 - Targeting Non-Coding RNAs Using Synthetic Small Molecules: Original Targets for Innovative Therapies

Dr Maria DUCA
(UNIVERSITY OF CÔTE D'AZUR, Nice, France)

10:00 IL03 - Discovery and Development of Selective Splicing Modifiers as Therapeutics

Dr Matthew WOLL
(PTC THERAPEUTICS, South Plainfield, NJ, United States)

10:15 IL04 - Small Molecules Targeting RNA - a Safety Perspective

Dr Helen Louise LIGHTFOOT
(F. HOFFMANN-LA ROCHE AG, BASEL, Switzerland)

10:30 Coffee break & Exhibition

Session 2 - Advances in Targeted Protein Degradation

Session chair

Prof. Terry MOORE
(UNIVERSITY OF ILLINOIS, Chicago, IL, United States)

11:00 IL05 - Ligand Directed Degradation: from Proof-of-Concept Degradation to Clinical Studies

Dr Deborah MORTENSEN
(BRISTOL MYERS SQUIBB, San Diego, CA, United States)

11:30 IL06 - Chemical Approaches to Edit Post-Translational Modification In Cells

Prof. Christina WOO
(HARVARD UNIVERSITY, Cambridge, MA, United States)

12:00 OC01 - Treatment of Pediatric AML Via Protac-Mediated Degradation of CDK9

Ms Alexandria CHAN
(UNIVERSITY OF MARYLAND SCHOOL OF PHARMACY, Baltimore, United States)

12:15 OC02 - Targeting Progerin Degradation as a New Therapeutic Approach for Treating Progeria

Prof. Silvia ORTEGA-GUTIERREZ
(COMPLUTENSE UNIVERSITY, Madrid, Spain)

12:30 Lunch & Exhibition

Scientific Program

- 12:45** **Company Workshop by Pelago Bioscience: CETSA® Enabled Drug Discovery: An Applied Workshop on Target Identification/Validation and Target Engagement-Driven Lead Generation and Optimization**
Dr Fredrik RAHM (PELAGO BIOSCIENCE, Solna, Sweden)
Dr Stina LUNDGREN (PELAGO BIOSCIENCE, Solna, Sweden)
- Session 3 - Proximity-inducing Molecules and their Therapeutic Applications**
- Session chair**
Dr Amit CHOUDHARY
(THE BROAD INSTITUTE, Cambridge, MA, United States)
- 14:00** **IL07 -Chemoproteomic-Enabled Development of Proximity-Inducing Molecules**
Dr Christopher PARKER
(THE SCRIPPS RESEARCH INSTITUTE, La Jolla, CA, United States)
- 14:30** **IL08 - An Intramolecular Bivalent Degradar Glues an Intrinsic BRD4-DCAF16 Interaction**
Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)
- 15:00** **OC03 - Discovery of MRT-2359, an Orally Bioavailable GSPT1 Molecular Glue Degradar, for MYC-Driven Cancers**
Dr Bernhard FASCHING
(MONTE ROSA THERAPEUTICS, Basel, Switzerland)
- 15:15** **OC04 - Integrated Platform Approach for Molecular Degradar Discovery in Proxidrugs**
Dr Johanna HUCHTING
(FRAUNHOFER INSTITUTE FOR TRANSLATIONAL MEDICINE AND PHARMACOLOGY, Hamburg, Germany)
- 15:30** **Coffee break & Exhibition**
- 16:00** **PL02 - RIPTACs: A New 'Hold and Kill'-based Therapeutic Modality**
Prof. Craig CREWS
(YALE UNIVERSITY, New Haven, CT, United States)
- 16:45** **Poster session 1 (odd numbers)**
- 18:00** **End of the scientific programme**
- 18:10** **City Tour**

Scientific Program

Monday 12/06/2023

08:00 **ACMEDI-YMCC | EFMC-YSN Programme for Early Career Researchers**

Chair

Dr Melissa GRENIER-DAVIES
(GLAXOSMITHKLINE, Cambridge, MA, United States)

08:00 **Panel Discussion - "Landing a Job in Industry"**

Dr Chris DE GRAAF (SOSEI HEPTARES, Cambridge, United Kingdom)
Dr Abdellatif EL MARROUNI (MERCK & CO., West Point, United States)
(SANOFI-AVENTIS DEUTSCHLAND GMBH)
Dr Malin LEMURELL (ASTRAZENECA, Gothenburg, Sweden)
Dr Darby SCHMIDT (SONATA THERAPEUTICS, Cambridge, MA, United States)

Session 4 - Drug Targets in GPCR Signaling

Session chair

Prof. György KESERU
(HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)

09:00 **IL09 - New Hot Targets? Medicinal Chemistry of G Protein-Coupled Receptors Involved in Immunity and Cancer**

Prof. Christa MÜLLER
(UNIVERSITY OF BONN, Bonn, Germany)

09:30 **IL10 - Frontier SBDD across the Orthosteric and Allosteric GPCRome**

Dr Chris DE GRAAF
(SOSEI HEPTARES, Cambridge, United Kingdom)

10:00 **OC05 - Best-In-Class Orally Bioavailable CXCR4 Antagonists to Treat Renal Cell Carcinoma**

Dr Eric MILLER
(EMORY UNIVERSITY SCHOOL OF MEDICINE, Atlanta, United States)

10:15 **OC06 - Targeting Sodium Binding Pocket in Mu Opioid Receptor to Design Safer Analgesics**

Dr Susruta MAJUMDAR
(UHSP & WASHINGTON UNIVERSITY, Saint Louis, United States)

10:30 **Coffee break & Exhibition**

Session 5 - Organic Synthesis Impacting Medicinal Chemistry & Chemical Biology

Session chair

Prof. Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)

11:00 **IL11 - Photocatalysis in the Pharmaceutical Industry: Synthesis under a New Light**

Dr Giulia BERGONZINI
(ASTRAZENECA, Gothenburg, Sweden)

11:30 **IL12 - HTE Chemistry to Accelerate Medicinal Chemistry Programs**

Dr Fabio LIMA
(NOVARTIS, Basel, Switzerland)

Scientific Program

- 12:00** **OC07 - New Precision Anti-TB Agents by Allosteric Inhibition of Glutamate-5-Kinase Enzyme**
Prof. Concepcion GONZALEZ-BELLO
(UNIVERSIDADE DE SANTIAGO DE COMPOSTELA - CIQUS, santiago de compostela, Spain)
- 12:15** **OC08 - Impact of gem-Difluoromethylene Group on Physicochemical Properties in Medchem-Relevant Building Blocks**
Dr Sergey RYABUKHIN
(ENAMINE LTD, Kyiv, Ukraine)
- 12:30** **Lunch & Exhibition**
- 12:45** **Company Workshop by Schrödinger: Augmenting Medicinal Chemistry with Digital Chemistry: A Lead Optimization Design Challenge for D-Amino Acid Oxidase Inhibitors**
Mr Wade MILLER
(SCHRÖDINGER, Cambridge, United States)
- Session 6 - Enabling Chemistries for Chemical Biology Research**
- Session chair**
Prof. Daniel HARKI
(UNIVERSITY OF MINNESOTA, Minneapolis, MN, United States)
- 14:00** **IL13 - Chemical Probes Enabling Drug Target Discovery and Validation**
Prof. Edward TATE
(IMPERIAL COLLEGE LONDON, London, United Kingdom)
- 14:30** **IL14 - Generating Stem-Like T Cells with Small-Molecule Modulators for Cancer Immunotherapy**
Prof. Peng WU
(THE SCRIPPS RESEARCH INSTITUTE, La Jolla, CA, United States)
- 15:00** **OC09 - Targeting Receptor Complexes with Therapeutic Peptides**
Prof. Kristian STROMGAARD
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)
- 15:15** **OC10 - Azetidin-2-Ones as Quenched Activity-Based Probes to Profile Human Neutrophil Elastase in Proteomes**
Ms Rita FÉLIX
(IMED.ULISBOA - RESEARCH INSTITUTE FOR MEDICINES, Lisbon, Portugal)
- 15:30** **Coffee break & Exhibition**
- 16:00** **PL03 -Carbohydrates in Health and Disease**
Prof. Laura KIESSLING
(MIT, Cambridge, MA, United States)
- 16:45** **Poster session 2 (even numbers)**
- 18:00** **End of the scientific programme**
- 20:00** **Banquet (optional)**

Tuesday 13/06/2023

Session 7 - A Focus on Early Career Investigators

Session chair

Dr Melissa GRENIER-DAVIES
(GLAXOSMITHKLINE, Cambridge, MA, United States)

09:00 IL15 - E3 Ligase Ligand Discovery for TPD

Dr Benika PINCH
(NOVARTIS, Cambridge, MA, United States)

09:15 IL16 - Chemical Approaches to Enhance Cellular Immunotherapies

Dr Mark P. FARRELL
(UNIVERSITY OF KANSAS, Lawrence, KS, United States)

09:30 IL17 - Machine Learning Tools to Accelerate Chemical Biology Studies

Dr Tiago RODRIGUES
(UNIVERSITY OF LISBON, Lisbon, Portugal)

09:45 OC11 - Chemical Probes for RHO GEF/GTPase Complexes

Ms Mia CALLENS
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

10:00 OC12 - Potent Targeted Activator of Cell Kill Molecules Selectively Eliminate HIV Infected Cells

Dr Abdellatif EL MARROUNI
(MERCK & CO., West Point, United States)

10:15 OC13 - Borrowing Transcriptional Kinases to Activate Apoptosis Using Chemically Induced Proximity

Dr Roman SAROTT
(STANFORD UNIVERSITY, Menlo Park, United States)

10:30 Coffee break & Exhibition

Session 8 - Approaches to Identify and Target Cryptic and Allosteric Pocket

Session chair

Dr Malin LEMURELL
(ASTRAZENECA, Gothenburg, Sweden)

11:00 IL18 - A Computation-First Approach to Drug Challenging Disease Targets

Dr Woody SHERMAN
(PSIVANT THERAPEUTICS, Boston, MA, United States)

11:30 IL19 - X-ray Crystallographic Fragment Screening for the Identification of Allosteric Binding Sites

Dr Andrew WOODHEAD
(ASTEX THERAPEUTICS, Cambridge, United Kingdom)

12:00 IL20 - Exploiting Allostery for Computer-Aided Drug Design of Oncogenes

Dr Zoe COURNIA
(BIOMEDICAL RESEARCH FOUNDATION ACADEMY OF ATHENS, Athens, Greece)

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- 12:30** **OC14 - Structure-Based Drug Discovery and Umbrella Sampling Simulations Identify Novel Potent Troponin Calcium Sensitizers and Elucidate their Function**
Prof. Steffen LINDERT
(OSU, Columbus, United States)
- 12:45** **Lunch & Exhibition**
- 13:00** **Company Workshop by CAS: The Evolution of Science at CAS: Connections Between Multi-disciplinary Data and Capabilities**
Mrs Vee LINDSAY (CAS, Columbus, United States)
Dr Angela ZHOU (CAS, Columbus, United States)
- Session 9 - Getting Out of the Starting Block: New Hit Finding and Chemotype Advancement Methods**
- Session chair**
Dr Carolyn DZIERBA
(BRISTOL-MYERS SQUIBB, Cambridge, MA, United States)
- 14:00** **IL21 - RAPID – a Next-Generation Chemoproteomics Technology Enabling the Discovery of Reversible Binders to Pre-specified Targets in Living Cells**
Dr Justin RETTENMAIER
(JNANA THERAPEUTICS, Boston, MA, United States)
- 14:30** **IL22 - Covalent Fragment-Based Drug Discovery**
Dr Daniel ERLANSON
(FRONTIER MEDICINES, South San Francisco, CA, United States)
- 15:00** **IL23 - Large-scale in Silico Fragment Screening of ~200 Million Fragments Based on Absolute Free Energy Perturbation**
Dr Eric THERRIEN
(SCHRODINGER, New York, NY, United States)
- 15:15** **OC15 - Small Molecule Drug Discovery with Peptide-Encoded Libraries**
Dr Nathalie GROB
(MASSACHUSETTS INSTITUTE OF TECHNOLOGY, Cambridge, United States)
- 16:00** **Closing Ceremony & Poster Prizes Ceremony**
- 16:30** **End of the Symposium**
- 19:10** **Boston Red Sox's game (optional)**