

ACSMEDI-EFMC Medicinal Chemistry Frontiers 2023

Scientific Program

Saturday June 10, 2023

Registration

Opening Session

Opening of the Symposium and Welcome address

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

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

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

Welcome Reception

Scientific Program

Sunday June 11, 2023

Registration

Session 1 - Chemical Modulation of RNA

Session chair

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

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

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

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

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

IL03 - Discovery and Development of Selective Splicing Modifiers as Therapeutics

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

IL04 - Small Molecules Targeting RNA - a Safety Perspective

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

Coffee break & Exhibition

Session 2 - Advances in Targeted Protein Degradation

Session chair

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

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

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

IL06 - Chemical Approaches to Edit Post-Translational Modification In Cells

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

OC01 - Treatment of Pediatric AML Via Protac-Mediated Degradation of CDK9

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

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

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

Lunch & Exhibition

Scientific Program

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)

IL07 -Chemoproteomic-Enabled Development of Proximity-Inducing Molecules

Dr Christopher PARKER
(THE SCRIPPS RESEARCH INSTITUTE, La Jolla, CA, United States)

IL08 - An Intramolecular Bivalent Degradar Glues an Intrinsic BRD4-DCAF16 Interaction

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

OC03 - Discovery of MRT-2359, an Orally Bioavailable GSPT1 Molecular Glue Degradar, for MYC-Driven Cancers

Dr Bernhard FASCHING
(MONTE ROSA THERAPEUTICS, Basel, Switzerland)

OC04 - Integrated Platform Approach for Molecular Degradar Discovery in Proxodrugs

Dr Johanna HUCHTING
(FRAUNHOFER INSTITUTE FOR TRANSLATIONAL MEDICINE AND PHARMACOLOGY, Hamburg, Germany)

Coffee break & Exhibition

PL02 - RIPTACs: A New 'Hold and Kill'-based Therapeutic Modality

Prof. Craig CREWS
(YALE UNIVERSITY, New Haven, CT, United States)

Poster session 1 (odd numbers)

End of the scientific programme

City Tour

Monday June 12, 2023

ACMEDI-YMCC | EFMC-YSN Programme for Early Career Researchers

Chair

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

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)

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

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

IL10 - Frontier SBDD across the Orthosteric and Allosteric GPCRome

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

OC05 - Best-In-Class Orally Bioavailable CXCR4 Antagonists to Treat Renal Cell Carcinoma

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

OC06 - Targeting Sodium Binding Pocket in Mu Opioid Receptor to Design Safer Analgesics

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

Coffee break & Exhibition

Session 5 - Organic Synthesis Impacting Medicinal Chemistry & Chemical Biology

Session chair

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

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

Dr Giulia BERGONZINI
(ASTRAZENECA, Gothenburg, Sweden)

IL12 - HTE Chemistry to Accelerate Medicinal Chemistry Programs

Dr Fabio LIMA
(NOVARTIS, Basel, Switzerland)

Scientific Program

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)

OC08 - Impact of gem-Difluoromethylene Group on Physicochemical Properties in Medchem-Relevant Building Blocks

Dr Sergey RYABUKHIN

(ENAMINE LTD, Kyiv, Ukraine)

Lunch & Exhibition

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)

IL13 - Chemical Probes Enabling Drug Target Discovery and Validation

Prof. Edward TATE

(IMPERIAL COLLEGE LONDON, London, United Kingdom)

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)

OC09 - Targeting Receptor Complexes with Therapeutic Peptides

Prof. Kristian STROMGAARD

(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

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)

Coffee break & Exhibition

PL03 -Carbohydrates in Health and Disease

Prof. Laura KIESSLING

(MIT, Cambridge, MA, United States)

Poster session 2 (even numbers)

End of the scientific programme

Banquet (optional)

Tuesday June 13, 2023

Session 7 - A Focus on Early Career Investigators

Session chair

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

IL15 - E3 Ligase Ligand Discovery for TPD

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

IL16 - Chemical Approaches to Enhance Cellular Immunotherapies

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

IL17 - Machine Learning Tools to Accelerate Chemical Biology Studies

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

OC11 - Chemical Probes for RHO GEF/GTPase Complexes

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

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

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

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

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

Coffee break & Exhibition

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

Session chair

Dr Malin LEMURELL
(ASTRAZENECA, Gothenburg, Sweden)

IL18 - A Computation-First Approach to Drug Challenging Disease Targets

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

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

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

IL20 - Exploiting Allostery for Computer-Aided Drug Design of Oncogenes

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

Scientific Program

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)

Lunch & Exhibition

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)

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)

IL22 - Covalent Fragment-Based Drug Discovery

Dr Daniel ERLANSON
(FRONTIER MEDICINES, South San Francisco, CA, United States)

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)

OC15 - Small Molecule Drug Discovery with Peptide-Encoded Libraries

Dr Nathalie GROB
(MASSACHUSETTS INSTITUTE OF TECHNOLOGY, Cambridge, United States)

Closing Ceremony & Poster Prizes Ceremony

End of the Symposium

Boston Red Sox's game (optional)