

37th ACS National Medicinal Chemistry Symposium

Scientific Program

Sunday June 26, 2022

- 11:00** **Registration**
- 13:00** **Welcome Address by NMCS NYC Co-Chairs**
- 13:00**
Dr Amjad ALI (MERCK & CO. INC., Kenilworth, United States)
Prof. Robert DEVITA (ICAHN SCHOOL OF MEDICINE AT MT. SINAI, New York, NY, United States)
- 13:15** **Session 1: Integrating Novel Chemical Modalities in Hit-to-lead: a New Paradigm for Early Drug Discovery**
Session Sponsored by X-Chem
- 13:15** **Introduction by Session Chair**
Dr Maria-Jesus BLANCO
(ATAVISTIK BIO, Cambridge, MA, United States)
- 13:20** **Integrating DNA-Encoded Library Technologies in Lead Discovery (IL01)**
Dr Lisa MARCAURELLE
(GSK, Cambridge, United States)
- 13:55** **Discovery of IRAKIMiDs: Dual-Mechanism Degraders Targeting IRAK4 and IMiD Substrates for Oncology (IL02)**
Dr Lewis PENNINGTON
(KYMERA THERAPEUTICS INC., Watertown, United States)
- 14:30** **Development and Optimization of Small Molecule RNA Degraders (IL03)**
Prof. Matthew DISNEY
(SCRIPPS RESEARCH INSTITUTE, Jupiter, United States)
- 15:05** **Coffee Break & Exhibition**
- 15:35** **Oral Peptides: Theory and Practice (IL04)**
Dr Lauren MONOVICH
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)
- 16:10** **Structural Approach to Identify Lead Scaffolds for Protein-Protein Interaction Targets (IL05)**
Prof. Kyle HADDEN
(UNIVERSITY OF CONNECTICUT, Storrs, United States)
- 16:45** **Poster Session 1**
- 16:45** **Poster Session (posters with odd numbers)**
Chaired by
Dr Lori FERRINS (NORTHEASTERN UNIVERSITY, Boston, MA, United States)
Prof. Andrii MONASTYRSKYI (MOFFITT CANCER CENTER & RESEARCH INSTITUTE, Tampa, United States)
- 18:15** **Welcome Reception & Networking**
- 20:00** **End of the Day**

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- 08:30** **Session 2: New Directions in Targeting DNA Damage Repair (DDR)**
Session Sponsored by NuChem Sciences
- 08:30** **Introduction by Session Chairs**
Dr Erin DIMAURO (MERCK & CO. INC., Boston, United States)
Dr Srinivasa KARRA (AVILAR THERAPEUTICS, Waltham, United States)
- 08:35** **M3541 and M4076: Discovery and Optimization of Potent and Selective ATM Kinase Inhibitors with Strong Anti-tumor Efficacy in Combination Therapies (IL06)**
Dr Thomas FUCHSS
(MERCK KGAA, HEALTHCARE, Darmstadt, Germany)
- 09:10** **Discovery and Validation of in vitro and in vivo Probes for Human DNA Polymerase Theta (Pol?) (IL07)**
Dr Robert HEALD
(ARTIOS PHARMA LTD, Cambridge, United Kingdom)
- 09:45** **The Modification of Pyrazolopyrimidinones and their Effect on WEE1 Inhibition and the DNA Damage Response (IL08)**
Prof. Phil REIGAN
(UNIVERSITY OF COLORADO, Aurora, United States)
- 10:20** **Coffee Break & Exhibition**
- 10:50** **Discovery of KB-0742, a Potent, Selective, Orally Bioavailable Small Molecule Inhibitor of CDK9/cyclin T1 for MYC-dependent Cancers (IL09)**
Dr David FREEMAN
(KRONOS BIO, INC. , Massachussetts, United States)
- 11:25** **Harnessing CDK12 Inhibition of Transcriptional Machinery to Induce Dimerization between DDB1 and CDK12-cyclinK Complex for Targeted Protein Degradation (IL10)**
Prof. Andrii MONASTYRSKYI
(MOFFITT CANCER CENTER & RESEARCH INSTITUTE, Tampa, United States)
- 12:00** **Lunch & Exhibition until 1:15 PM**
Sponsored by ACS Publications
- 12:20** **Optional Schrödinger Workshop - Augmenting Medicinal Chemistry with Digital Chemistry: A CDK2 Inhibitor Design Challenge**
Mr Wade MILLER
(SCHRÖDINGER, Cambridge, United States)
- 13:15** **Session 3: Hot Targets from NYC Academic and Biotech Scene**
- 13:15** **Introduction by Session Chairs**
Dr Amjad ALI (MERCK & CO. INC., Kenilworth, United States)
Prof. Robert DEVITA (ICAHN SCHOOL OF MEDICINE AT MT. SINAI, New York, NY, United States)
- 13:20** **Rational Design of Inhibitors of Protein-Protein Interactions (IL11)**
Prof. Paramjit ARORA
(NYU, New York, United States)

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- 13:55** **Next Generation Drug Discovery (IL12)**
Dr Steve COLLETTI
(ZYMERGEN INC., New York, United States)
- 14:30** **Optimization of Mycobacterium Tuberculosis (Mtb) Selective Inhibitors of Lipoamide Dehydrogenase (Lpd) (IL13)**
Dr John GINN
(TRI-INSTITUTIONAL THERAPEUTICS DISCOVERY INSTITUTE, New York, United States)
- 15:05** **Coffee Break & Exhibition**
- 15:35** **Therapeutic Potential of the Gut-Brain Axis (IL14)**
Dr Iyassu SEBHAT
(KALLYOPE, New Jersey, United States)
- 16:10** **Designing and Combining Cancer's Off Switches (IL15)**
Dr Karen AKINSANYA
(SCHRODINGER, New York City, United States)
- 16:45** **End of Session 3**
- 16:50** **Optional Iktos Workshop - AI Tools for Medicinal Chemists: Novel Compound Design and Retrosynthesis Prediction**
Dr Rohit ARORA (IKTOS INC, Ashland, United States)
Dr Brian ATWOOD (IKTOS INC, Los Angeles, United States)
- 17:15** **Poster Session 2**
- 17:15** **Poster Session 2 (posters with even numbers)**
Chaired by
Dr Lori FERRINS (NORTHEASTERN UNIVERSITY, Boston, MA, United States)
Prof. Andrii MONASTYRSKYI (MOFFITT CANCER CENTER & RESEARCH INSTITUTE, Tampa, United States)
- 18:45** **End of the Day**

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Tuesday June 28, 2022

- 08:30** **Session 4: Targeting Autophagy for Cancer, Neurodegeneration, or Autoimmune Disease**
- 08:30** **Introduction by Session Chairs**
Dr Erin DIMAURO (MERCK & CO. INC., Boston, United States)
Dr Hongjun David ZHANG (CEREVEL THERAPEUTICS, LLC, Boston, United States)
- 08:35** **Unraveling Autophagy in Cancer Using Chemical Genetics (IL16)**
Prof. Jeff MACKEIGAN
(MICHIGAN STATE UNIVERSITY, East Lansing, United States)
- 09:05** **Small Molecule PINK1 Activators Rescue Parkinson's Disease Pathology (IL17)**
Dr Nicholas HERTZ
(MITOKININ INC, San Francisco, United States)
- 09:35** **Revolutionizing Discovery and Development of ALS Therapeutics using Transformational, AI-powered 'All-in-Human' Platforms (IL18)**
Dr Irene CHOI
(VERGE GENOMICS, South San Francisco, United States)
- 10:05** **Coffee Break & Exhibition**
- 10:35** **Chasing Challenging Targets: Development of Selective Inhibitors of the Autophagy Pathway to Impact Cancer Therapy (IL19)**
Prof. Leslie ALDRICH
(UNIVERISTY OF ILLINOIS AT CHICAGO, Chicago, United States)
- 11:05** **Chemical Activation of Chaperone-Mediated Autophagy for Protection against Neurodegeneration (IL20)**
Prof. Eviropidis GAVATHIOTIS
(ALBERT EINSTEIN COLLEGE OF MEDICINE, Bronx, United States)
- 11:35** **Necessary Complexity: The Discovery of Selective, CNS Penetrant LRRK2 Inhibitors for the Treatment of Parkinson's Disease (IL21)**
Dr Peter FULLER
(MERCK & CO. INC., Boston, United States)
- 12:05** **End of AM Program**
- 13:00** **Social Activities & Free Time**
- 17:45** **Award Session**
- 17:45** **Award Dinner**
- 19:15** **Award Session - Opening Address**
- 19:29** **2022 Division of Medicinal Chemistry Award**

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- 19:30** **Award Ceremony chaired by ACS Medi Division Chair 2022, Prof. Amanda Bryant-Friedrich (Wayne State University, United States)**
- 19:40** **2022 Division of Medicinal Chemistry Award Lecture
A Perspective on the Arc of Innovation in Drug Discovery over Three Decades (AL01)**
Dr Lawrence G. HAMANN
(INTERDICT BIO, San Francisco, United States)
- 20:24** **2022 IUPAC-Richter Prize**
- 20:25** **Prize Ceremony chaired by Dr Janos Eles (Gedeon Richter, Hungary)**
- 20:35** **2022 IUPAC-Richter Prize Lecture
Drug Discovery in Academia: Some Success Stories (AL02)**
Prof. Michael E. JUNG
(UCLA CHEMISTRY & BIOCHEMISTRY, Los Angeles, United States)
- 21:20** **End of the Day**

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Wednesday June 29, 2022

- 08:30** **Session 5: Next Generation Therapies Shaped by Clinical Data**
- 08:30** **Introduction by Session Chair**
Dr Steven MCKERRALL
(SEPTERNA, South San Francisco, United States)
- 08:35** **Discovery of LPA1 antagonists for the treatment of Pulmonary Fibrotic Diseases (IL22)**
Dr Peter CHENG
(BRISTOL-MYERS SQUIBB R & D, Hopewell, United States)
- 09:05** **Discovery of Risdiplam, a Medicine for the Treatment of Spinal Muscular Atrophy (IL23)**
Dr Luke GREEN
(HOFFMANN-LA ROCHE, Basel, Switzerland)
- 09:35** **The Invention of MK-8262, a CETP Inhibitor for the Treatment of Coronary Heart Disease (IL24)**
Dr Petr VACHAL
(MERCK & CO. INC (MSD), Kenilworth, United States)
- 10:05** **Coffee Break & Exhibition**
- 10:35** **Discovery of Inavolisib, a Highly Selective Inhibitor of PI3K- γ that Induces Degradation of Mutant-p110 γ Protein (IL25)**
Dr Marie-Gabrielle BRAUN
(GENENTECH, South San Francisco, United States)
- 11:05** **Discovery of PF-07081532: a Small Molecule GLP-1 Receptor Agonist Suitable for Once-daily Oral Administration (IL26)**
Dr David A. GRIFFITH
(PFIZER INC., Cambridge, United States)
- 11:35** **Discovery of LY3154885, a Second Generation Human Dopamine D1 Receptor Positive Allosteric Modulator with an Improved Drug-Drug Interaction Risk Profile (IL27)**
Dr Erik HEMBRE
(ELI LILLY & CO., Indianapolis, United States)
- 12:05** **Lunch Break & Exhibition until 1:20PM**
Sponsored by Paraza Pharma
- 12:20** **Optional Aseda Sciences Workshop - Drug Discovery Platforms, the Predictive Information Gap, and How to Bridge it**
Dr Andrew BIEBERICH
(ASEDA SCIENCES, West Lafayette, United States)
- 13:20** **Session 6: Lessons from Drug Hunters across Academia, NPOs and the Pharmaceutical Industry**
- 13:20** **Introduction by Session Chair**
Dr Philip KYM
(ABBVIE, North Chicago, United States)
- 13:25** **Small Molecule Drug Discovery in Academia: DYRK1A Inhibitors as Novel beta-Cell Regenerative Drugs for Diabetes (IL28)**

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Prof. Robert DEVITA
(ICAHN SCHOOL OF MEDICINE AT MT. SINAI, New York, NY, United States)

14:00 Discovery of Upadacitinib: a Tricyclic Janus Kinase 1 (JAK1) Inhibitor (IL29)

Dr Kristine E. FRANK
(ABBVIE, North Chicago, United States)

14:35 Anticancer Drug Discovery from Pets to People, the Story of PAC-1 (IL30)

Prof. Paul J. HERGENROTHER
(UNIVERSITY OF ILLINOIS, Urbana, United States)

15:10 Coffee Break & Exhibition

15:40 Discovery of Nix-TB as a Novel Regimen that Significantly Shortens Treatment of Tuberculosis (IL31)

Dr Christopher B. COOPER
(TB ALLIANCE, GLOBAL ALLIANCE FOR TB DRUG DEVELOPMENT, New York, United States)

16:15 Adventures in Drug Hunting (IL32)

Dr Wendy YOUNG
(MPM CAPITAL, Brisbane, CA, United States)

16:50 Closing Remarks

Dr Amjad ALI (MERCK & CO. INC., Kenilworth, United States)
Prof. Robert DEVITA (ICAHN SCHOOL OF MEDICINE AT MT. SINAI, New York, NY, United States)

17:00 Departure