

37th ACS National Medicinal Chemistry Symposium

Scientific Program

Sunday June 26, 2022

11:00 am Registration

01:00 pm Welcome Address by NMCS NYC Co-Chairs

01:00 pm

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

**01:15 pm Session 1: Integrating Novel Chemical Modalities in Hit-to-lead: a New Paradigm for Early Drug Discovery
*Session Sponsored by X-Chem***

01:15 pm Introduction by Session Chair

Dr Maria-Jesus BLANCO
(ATAVISTIK BIO, Cambridge, MA, United States)

01:20 pm Integrating DNA-Encoded Library Technologies in Lead Discovery (IL01)

Dr Lisa MARCAURELLE
(GSK, Cambridge, United States)

01:55 pm Discovery of IRAKIMiDs: Dual-Mechanism Degraders Targeting IRAK4 and IMiD Substrates for Oncology (IL02)

Dr Lewis PENNINGTON
(KYMERA THERAPEUTICS INC., Watertown, United States)

02:30 pm Development and Optimization of Small Molecule RNA Degraders (IL03)

Prof. Matthew DISNEY
(SCRIPPS RESEARCH INSTITUTE, Jupiter, United States)

03:05 pm Coffee Break & Exhibition

03:35 pm Oral Peptides: Theory and Practice (IL04)

Dr Lauren MONOVICH
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)

04:10 pm Structural Approach to Identify Lead Scaffolds for Protein-Protein Interaction Targets (IL05)

Prof. Kyle HADDEN
(UNIVERSITY OF CONNECTICUT, Storrs, United States)

04:45 pm Poster Session 1

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04:45 pm 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)

06:15 pm Welcome Reception & Networking

08:00 pm End of the Day

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Monday June 27, 2022

08:30 am Session 2: New Directions in Targeting DNA Damage Repair (DDR)
Session Sponsored by NuChem Sciences

08:30 am Introduction by Session Chairs

Dr Erin DIMAURO (MERCK & CO. INC., Boston, United States)
Dr Srinivasa KARRA (AVILAR THERAPEUTICS, Waltham, United States)

08:35 am 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 am 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 am 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 am Coffee Break & Exhibition

10:50 am 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 am 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 pm Lunch & Exhibition until 1:15 PM
Sponsored by ACS Publications

12:20 pm Optional Schrödinger Workshop - Augmenting Medicinal Chemistry with Digital Chemistry: A CDK2 Inhibitor Design Challenge

Mr Wade MILLER
(SCHRÖDINGER, Cambridge, United States)

01:15 pm Session 3: Hot Targets from NYC Academic and Biotech Scene

01:15 pm 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)

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01:20 pm Rational Design of Inhibitors of Protein-Protein Interactions (IL11)

Prof. Paramjit ARORA
(NYU, New York, United States)

01:55 pm Next Generation Drug Discovery (IL12)

Dr Steve COLLETTI
(ZYMERGEN INC., New York, United States)

02:30 pm Optimization of Mycobacterium Tuberculosis (Mtb) Selective Inhibitors of Lipoamide Dehydrogenase (Lpd) (IL13)

Dr John GINN
(TRI-INSTITUTIONAL THERAPEUTICS DISCOVERY INSTITUTE, New York, United States)

03:05 pm Coffee Break & Exhibition

03:35 pm Therapeutic Potential of the Gut-Brain Axis (IL14)

Dr Iyassu SEBHAT
(KALLYOPE, New Jersey, United States)

04:10 pm Designing and Combining Cancer's Off Switches (IL15)

Dr Karen AKINSANYA
(SCHRODINGER, New York City, United States)

04:45 pm End of Session 3

04:50 pm 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)

05:15 pm Poster Session 2

05:15 pm 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)

06:45 pm End of the Day

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Tuesday June 28, 2022

08:30 am Session 4: Targeting Autophagy for Cancer, Neurodegeneration, or Autoimmune Disease

08:30 am 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 am Unraveling Autophagy in Cancer Using Chemical Genetics (IL16)

Prof. Jeff MACKEIGAN
(MICHIGAN STATE UNIVERSITY, East Lansing, United States)

09:05 am Small Molecule PINK1 Activators Rescue Parkinson's Disease Pathology (IL17)

Dr Nicholas HERTZ
(MITOKININ INC, San Francisco, United States)

09:35 am 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 am Coffee Break & Exhibition

10:35 am Chasing Challenging Targets: Development of Selective Inhibitors of the Autophagy Pathway to Impact Cancer Therapy (IL19)

Prof. Leslie ALDRICH
(UNIVERSITY OF ILLINOIS AT CHICAGO, Chicago, United States)

11:05 am Chemical Activation of Chaperone-Mediated Autophagy for Protection against Neurodegeneration (IL20)

Prof. Evripidis GAVATHIOTIS
(ALBERT EINSTEIN COLLEGE OF MEDICINE, Bronx, United States)

11:35 am 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 pm End of AM Program

01:00 pm Social Activities & Free Time

05:45 pm Award Session

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05:45 pm Award Dinner

07:15 pm Award Session - Opening Address

07:29 pm 2022 Division of Medicinal Chemistry Award

07:30 pm Award Ceremony chaired by ACS Medi Division Chair 2022, Prof. Amanda Bryant-Friedrich (Wayne State University, United States)

07:40 pm 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)

08:24 pm 2022 IUPAC-Richter Prize

08:25 pm Prize Ceremony chaired by Dr Janos Eles (Gedeon Richter, Hungary)

08:35 pm 2022 IUPAC-Richter Prize Lecture
Drug Discovery in Academia: Some Success Stories (AL02)

Prof. Michael E. JUNG
(UCLA CHEMISTRY & BIOCHEMISTRY, Los Angeles, United States)

09:20 pm End of the Day

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Wednesday June 29, 2022

08:30 am Session 5: Next Generation Therapies Shaped by Clinical Data

08:30 am Introduction by Session Chair

Dr Steven MCKERRALL
(SEPTERNA, South San Francisco, United States)

08:35 am 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 am Discovery of Risdiplam, a Medicine for the Treatment of Spinal Muscular Atrophy (IL23)

Dr Luke GREEN
(HOFFMANN-LA ROCHE, Basel, Switzerland)

09:35 am 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 am Coffee Break & Exhibition

10:35 am Discovery of Inavolisib, a Highly Selective Inhibitor of PI3K- γ that Induces Degradation of Mutant-p110? Protein (IL25)

Dr Marie-Gabrielle BRAUN
(GENENTECH, South San Francisco, United States)

11:05 am 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 am 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 pm Lunch Break & Exhibition until 1:20PM
Sponsored by Paraza Pharma

12:20 pm 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)

01:20 pm Session 6: Lessons from Drug Hunters across Academia, NPOs and the Pharmaceutical Industry

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01:20 pm Introduction by Session Chair

Dr Philip KYM
(ABBVIE, North Chicago, United States)

01:25 pm Small Molecule Drug Discovery in Academia: DYRK1A Inhibitors as Novel beta-Cell Regenerative Drugs for Diabetes (IL28)

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

02:00 pm Discovery of Upadacitinib: a Tricyclic Janus Kinase 1 (JAK1) Inhibitor (IL29)

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

02:35 pm Anticancer Drug Discovery from Pets to People, the Story of PAC-1 (IL30)

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

03:10 pm Coffee Break & Exhibition

03:40 pm 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)

04:15 pm Adventures in Drug Hunting (IL32)

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

04:50 pm 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)

05:00 pm Departure