

# 37th ACS National Medicinal Chemistry Symposium

## Scientific Program

### Sunday 26/06/2022

- 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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### Monday 27/06/2022

- 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 28/06/2022

- 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  
(UNIVERSITY 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 29/06/2022

- 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- $\gamma$  that Induces Degradation of Mutant-p110 $\gamma$  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**