

38th ACS National Medicinal Chemistry Symposium

Program

Sunday 23/06/2024

- 11:00** **Registration**
- 13:00** **Welcome Address by NMCS Co-Chairs**
Dr Patrick BURKE (ENLAZA THERAPEUTICS, San Diego, CA, United States)
Dr Rheem A. TOTAH (UNIVERSITY OF WASHINGTON, Lake Forest Park, WA, United States)
- 13:15** **Plenary Opening Session: Recent Advances and Emerging Opportunities in Medicinal Chemistry**
Sponsored by Gilead
- Session Chair**
Dr Paul SCOLA
(BRISTOL MYERS SQUIBB, Cambridge, MA, United States)
- 13:15** **Introduction**
- 13:20** **A Synopsis of the Impact of Small Molecules on Human Health and Longevity (PL01)**
Dr Nicholas MEANWELL
(BARUCH S. BLUMBERG INSTITUTE AND UNIVERSITY OF MICHIGAN, Wallingford, CT, United States)
- 14:05** **Rediscovering Macrocycles as a Modality in Drug Discovery (PL02)**
Dr Katerina LEFTHERIS
(VILYA, INC., SF Bay Area, CA, United States)
- 14:50** **Coffee Break & Exhibition**
- 15:20** **Inhibition of Protein Aggregation and the Development of AKV9 (formerly NU-9) for Amyotrophic Lateral Sclerosis and Other Neurodegenerative Diseases (PL03)**
Prof. Richard B. SILVERMAN
(NORTHWESTERN UNIVERSITY, Evanston, IL, United States)
- 16:05** **Flash Poster Session 1**
- Session Chair**
Dr Juhienah KHALAF
(INIMMUNE CORPORATION, Missoula, MT, United States)
- 16:05** **Flash Poster presentations**
- 16:35** **Poster Session 1**
- 18:00** **Welcome Reception**
- 19:00** **End of the day**

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Monday 24/06/2024

08:30 **Session 1: Advances in Protein Proximity, Induction and Degradation**

Session Chairs

Dr Timothy HEFFRON (GENENTECH, South San Francisco, CA, United States)
Dr Elisia VILLEMURE (GENENTECH, South San Francisco, CA, United States)

08:30 **Introduction**

08:35 **Ubiquitin Ligases and Molecular Glue Degraders (IL01)**

Prof. Ning ZHENG
(UNIVERSITY OF WASHINGTON, Seattle, WA, United States)

09:05 **Informatics Accelerated CRBN Glue Lead Discovery (IL02)**

Dr Lingling SHEN
(NOVARTIS, Belmont, United States)

09:35 **Design and Optimisation of Molecular Glue Degraders (IL03)**

Dr Magnus WALTER
(MONTE ROSA THERAPEUTICS, Basel, Switzerland)

10:05 **Coffee Break & Exhibition**

10:35 **Stabilization of 14-3-3 Protein-Protein Interactions with Covalent Molecular Glues (IL04)**

Dr Markella KONSTANTINIDOU
(UNIVERSITY OF CALIFORNIA, SAN FRANCISCO, San Francisco, CA, United States)

11:05 **Hold and Kill: RIPTAC™ Therapeutics Present a Novel Mechanism to Conquer Cancer (IL05)**

Dr Kat KAYSER-BRICKER
(HALDA THERAPEUTICS, New Haven, CT, United States)

11:35 **Magnet Biomedicine's TrueGlue Platform: A Systematic Approach Towards the Discovery of Molecular Glues for Therapeutic Intervention (IL06)**

Dr Matthew HAYWARD
(MAGNET BIOMEDICINE, Boston, MA, United States)

12:05 **Lunch & Exhibition**

12:15 **Optional Schrodinger Workshop
Prioritizing DLK Inhibitors for Potency, Selectivity, and Brain-penetration: a Digital Chemistry Design Challenge**

13:20 **Session 2: Chemical Perturbation of Methylation towards Anticancer Drug Discovery**

Session Chairs

Prof. Rong HUANG (PURDUE UNIVERSITY, West Lafayette, IN, United States)
Dr Rheem A. TOTAH (UNIVERSITY OF WASHINGTON, Lake Forest Park, WA, United States)

13:20 **Introduction**

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- 13:25** **Discovery of Novel Small-molecule Degraders for Protein Methyltransferases and Development of New Approaches to Target Undruggable Proteins (IL07)**
Prof. Jian JIN
(ICAHN SCHOOL OF MEDICINE AT MOUNT SINAI, New York, NY, United States)
- 13:55** **Development of Potent and Specific Inhibitors for Methyltransferases (IL08)**
Prof. Rong HUANG
(PURDUE UNIVERSITY, West Lafayette, IN, United States)
- 14:25** **Discovery of MRTX1719, a Synthetic Lethal Approach for the Treatment of MTAP-Deleted Cancers (IL09)**
Dr Matthew MARX
(MIRATI THERAPEUTICS INC, San Diego, United States)
- 14:55** **Coffee Break & Exhibition**
- 15:25** **Session 3: Infectious Disease Drug Discovery**
- Session Chair**
Dr Lori FERRINS
(NORTHEASTERN UNIVERSITY, Boston, MA, United States)
- 15:25** **Introduction**
- 15:30** **Targeting Infectious Diseases with Kinase Inhibitors (IL10)**
Dr David DREWRY
(UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL, Chapel Hill, NC, United States)
- 16:00** **Development of Quinazolin-4-Ones that Show Efficacy in Lethal Murine Models of Venezuelan and Eastern Equine Encephalitis (IL11)**
Dr Jennifer GOLDEN
(UNIVERSITY OF WISCONSIN, Madison, WI, United States)
- 16:30** **Invention of MK-7602: an Antimalarial Drug Discovery Collaboration (IL12)**
Dr John A. MCCAULEY
(MERCK, West Point, United States)
- 17:00** **Flash Poster Session 2**
- Session Chair**
Dr Juhienah KHALAF
(INIMMUNE CORPORATION, Missoula, MT, United States)
- 17:00** **Flash Poster presentations**
- 17:30** **Poster Session 2**
- 19:00** **End of the day**

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Tuesday 25/06/2024

08:30 **Session 4: Targeted Drug Delivery**

Session Chair

Dr Patrick BURKE
(ENLAZA THERAPEUTICS, San Diego, CA, United States)

08:30 **Introduction**

08:35 **Development of a Novel TOPO1 α ADC Platform: from Concept to Pipeline Application (IL13)**

Dr Mark PETERSEN
(ZYMEWORKS, Vancouver, Canada)

09:05 **Harnessing the Power of ADCs by Careful Selection of Target, Linker, Payload, Indication, and Combination Partner (IL14)**

Dr Sharsti SANDALL
(PFIZER, Bothell, WA, United States)

09:35 **Targeted Radionuclide Therapy: the Promise and Challenges of Short-lived Alpha-emitting Actinides (IL15)**

Dr Rebecca ABERGEL
(UNIVERSITY OF CALIFORNIA, Berkeley, CA, United States)

10:05 **Coffee Break & Exhibition**

10:35 **Session 5: Non-catalytic Kinase Function and Pseudokinases as Drug Targets**

Session Chair

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

10:35 **Introduction**

10:40 **Targeting Functional Sites on Pseudokinase Complexes (IL16)**

Dr Arvin DAR
(MEMORIAL SLOAN KETTERING CANCER CENTER, New York, NY, United States)

11:10 **Discovery of the Tyk2 Pseudokinase Domain as a Drug Target (IL17)**

Dr John TOKARSKI
(BRISTOL MYERS SQUIBB, Princeton, United States)

11:40 **Discovery of TAK-279, a Highly Potent and Selective TYK2 Pseudokinase Inhibitor for the Treatment of Autoimmune Diseases, through Structure-based Drug Design (IL18)**

Dr Angela TOMS WEST
(NIMBUS THERAPEUTICS, INC., Franklin, MA, United States)

12:40 **Poster Prizes**

12:50 **End of AM Scientific Program**

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- 13:00** **Optional MilliporeSigma Workshop**
Decoding De Novo Design: Applying Generative Methods to Build Novel Molecule Sets
- 13:00** **Free afternoon & Excursions**
- 17:44** **Award Session**
- 17:45** **Award Dinner**
- 19:15** **Award Session**
- 19:15** **MEDI Division Award Ceremony**
Prof. Gunda GEORG
(UNIVERSITY OF MINNESOTA, Minneapolis, United States)
- 19:25** **MEDI Division Award Lecture**
Unlocking Allostery for Drug Discovery (AL01)
Dr Maria-Jesus BLANCO
(ATAVISTIK BIO, Cambridge, MA, United States)
- 20:10** **Ralph F. Hirschmann Award Lecture**
Rational Design of Protein-Protein Interaction Inhibitors: a Quixotic Quest (AL02)
Prof. Paramjit ARORA
(NYU, New York, United States)
- 21:05** **End of the day**

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Wednesday 26/06/2024

08:30 **Session 6: A Medicinal Chemist's Toolbox**

Session Chair

Dr Nicholas MEANWELL
(BARUCH S. BLUMBERG INSTITUTE AND UNIVERSITY OF MICHIGAN, Wallingford, CT, United States)

08:30 **Introduction**

08:35 **Non-additivity in Drug Design (IL19)**

Dr Bernd KUHN
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

09:05 **The Rise of Targeting Chimeras (TACs): Next-generation Medicines that Preempt Cellular Events (IL20)**

Dr Veerabahu SHANMUGASUNDARAM
(BRISTOL MYERS SQUIBB, Cambridge, MA, United States)

09:35 **Kinetic Selectivity? A Missed Opportunity in Drug Discovery? (IL21)**

Prof. Peter TONGE
(STONY BROOK UNIVERSITY, Stony Brook, NY, United States)

10:05 **Coffee Break & Exhibition**

10:35 **Mechanism-Based Approaches for Targeting Histone Reader Proteins (IL22)**

Prof. Marcey WATERS
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, NC, United States)

11:05 **Lessons in Proteome-Wide Covalent Drug Discovery (IL23)**

Dr Benjamin HORNING
(VIVIDION THERAPEUTICS INC., San Diego, United States)

11:35 **Metabolism-Driven Drug Design: Role of Metabolite Profiling and Identification in Medicinal Chemistry (IL24)**

Dr Deepak DALVIE
(CRINETICS PHARMACEUTICALS, San Diego, CA, United States)

12:05 **Lunch & Exhibition**

12:15 **Optional Enzymologic Workshop
Kinetic Selectivity: a Missed Opportunity in Drug Design?**

13:20 **Session 7: Use of Machine Learning in Drug Discovery**

Session Chair

Dr Katerina LEFOTHERIS
(VILYA, INC., SF Bay Area, CA, United States)

13:20 **Introduction**

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- 13:25 Machine Learning Guided Design of Peptide-based Antibiotics and Antivirals (IL25)**
Dr Gaurav BHARDWAJ
(UNIVERSITY OF WASHINGTON, Seattle, WA, United States)
- 13:55 The Application of AI and ML to Small Molecule Drug Discovery (IL26)**
Dr Gavin HIRST
(ATOMWISE, San Francisco, CA, United States)
- 14:25 Driving Innovation with Machine Learning: Impact on a Pipeline of Drug Discovery Programs (IL27)**
Dr Jennifer KNIGHT
(SCHRÖDINGER, New York, NY, United States)
- 14:55 Coffee Break & Exhibition**
- 15:25 Rapid Identification of HPGD Inhibitors Using Physics-based Machine Learning Methods (IL28)**
Dr Leela Sriram DODDA
(NIMBUS THERAPEUTICS, Boston, United States)
- 15:55 Applying Active Learning in Drug Discovery (IL29)**
Dr Patrick WALTERS
(RELAY THERAPEUTICS, Cambridge, MA, United States)
- 16:25 Generate-make-test: AI-in-the-loop High-throughput Drug Discovery (IL30)**
Dr Matt WELBORN
(IAMBIC THERAPEUTICS, La Jolla, CA, United States)
- 16:55 Closing Remarks**
Dr Patrick BURKE (ENLAZA THERAPEUTICS, San Diego, CA, United States)
Dr Rheem A. TOTAH (UNIVERSITY OF WASHINGTON, Lake Forest Park, WA, United States)
- 17:05 End of NMCS 2024 & Departure**