

ACS Medi 37th National Medicinal Chemistry Symposium

Scientific Program

Sunday June 28, 2020

10:00 am Registration

01:00 pm Welcome Address by NMCS NYC 2020 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, United States)

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

01:15 pm Introduction by Session Chair

Dr Maria-Jesus BLANCO
(SAGE THERAPEUTICS, Cambridge, United States)

01:20 pm Protein Degradation beyond Oncology

Dr Nello MAINOLFI
(KYMERA THERAPEUTICS, Cambridge, United States)

01:50 pm Integrating DNA-Encoded Library Technologies in Lead Discovery

Dr Lisa MARCAURELLE
(GSK, Cambridge, United States)

02:20 pm Translating RNA Sequence into Lead Small Molecule Medicines

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

02:50 pm Coffee Break & Exhibition

03:20 pm Structural Approach to Identify Lead Scaffolds for Protein-Protein Interaction Targets

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

03:50 pm Discovery and Development of Macrocyclic Peptides for the Treatment of Complement-Mediated Disorders

Dr Susan ASHWELL
(RA PHARMA, Cambridge, United States)

04:20 pm Impact of Structure Based Drug Design in GPCR Lead Optimisation Strategies

Dr Miles CONGREVE
(SOSEI HEPTARES, Welwyn Garden City, United Kingdom)

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04:50 pm Free Time

06:00 pm Welcome Reception & Networking

07:00 pm End of the Day

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Monday June 29, 2020

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

08:30 am Introduction by Session Chairs

Dr Erin DIMAURO (MERCK & CO. INC., Boston, United States)
Dr Srinivasa KARRA (NOT EMPLOYED, Pembroke, United States)

08:35 am Damage Incorporated: Discovery of ATR Inhibitor BAY 1895344 with Favorable PK Properties and Promising Anti-Tumor Efficacy in Monotherapy and Combination in Preclinical Tumor Models

Dr Ulrich LÜCKING
(BAYER AG, Berlin, Germany)

09:05 am Discovery and Optimization of Novel PARG Inhibitors

Dr Hilary BECK
(IDEAYA BIOSCIENCES, SOUTH SAN FRANCISCO, United States)

09:35 am The Modification of Pyrazolopyrimidinones and their Effect on WEE1 Inhibition and the DNA Damage Response

Prof. Phil REIGAN
(UNIVERSITY OF COLORADO, Aurora, United States)

10:05 am Coffee Break & Exhibition

10:35 am M3541 and M4076: Discovery and Optimization of Potent and Selective ATM Kinase Inhibitors with Strong Anti-tumor Efficacy in Combination Therapies

Dr Thomas FUCHSS
(MERCK KGAA - MERCK BIOPHARMA, Darmstadt, Germany)

11:05 am Discovery of DNA Polymerase theta (Pol?) Inhibitors: HTS to in vitro Probes

Dr Robert HEALD
(ARTIOS PHARMA LTD, Cambridge, United Kingdom)

11:35 am Discovery of Potent and Selective DNA-PK Inhibitors via Structure-Guided Virtual Screening Strategies

Dr Charlene FALLAN
(ASTRAZENECA, Cambridge, United Kingdom)

12:05 pm Lunch & Exhibition

12:20 pm 45-minutes Vendor Workshop by BioSymetrics
Using Machine Learning for Mechanism of Action Prediction Following Phenotypic Screening

01:20 pm Session 3: Hot Targets from NYC Academic and Biotech Scene

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01:20 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, United States)

01:25 pm Therapeutic Potential of the Gut-Brain Axis

Dr Ann WEBER
(KALLYOPE, New York, United States)

02:00 pm Rational Design of Inhibitors of Protein-Protein Interactions

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

02:35 pm Optimization of Mycobacterium Tuberculosis (Mtb) Selective Inhibitors of Lipoamide Dehydrogenase (Lpd)

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

03:10 pm Coffee Break & Exhibition

03:40 pm Next Generation Drug Discovery

Dr Steve COLLETTI
(LODO THERAPEUTICS, New York, United States)

04:15 pm Designing and Combining Cancer's Off Switches

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

04:50 pm Free Time

07:00 pm Poster Session & Networking

09:00 pm End of the Day

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Tuesday June 30, 2020

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

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

09:05 am Activating PTEN-Induced Kinase 1 (PINK1) for Parkinson's Disease

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

09:35 am The Development of Substrate Competitive and Allosteric Inhibitors of Cysteine Protease ATG4B to Prevent Autophagic Flux

Dr Jason CROSS
(MD ANDERSON CANCER CENTER, Houston, United States)

10:05 am Coffee Break & Exhibition

10:35 am Discovery of Highly Potent and Selective Vacuolar Protein Sorting 34 (Vps34) Inhibitors

Dr Jenny VIKLUND
(SPRINT BIOSCIENCE AB, Huddinge, Sweden)

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

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

11:35 am Title of talk to be confirmed

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 Opening Address

07:29 pm 2020 Division of Medicinal Chemistry Award

**07:30 pm 2020 Division of Medicinal Chemistry Award Lecture
Title of Talk to be confirmed**

Prof. Shaomeng WANG
(UNIVERSITY OF MICHIGAN, Ann Arbor, United States)

Introduction by Dr Scott Runyon, ACS Medi Division Chair 2020

08:14 pm 2020 IUPAC-Richter Prize

**08:15 pm 2020 IUPAC-Richter Prize Lecture
How I Spent my Summer Vacation: Insights from a 30-year Career in Drug Discovery (and Molecules that have Broken my Heart)**

Dr John E. MACOR
(SANOFI, Waltham, United States)

Introduction by Dr Janos Fischer, Chair of the IUPAC-Richter Prize Selection Committee

09:00 pm End of the Day

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Wednesday July 1, 2020

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

08:30 am Introduction by Session Chair

Dr Matthew VOLGRAF
(GENENTECH INC., South San Francisco, United States)

08:35 am 3 Generations of RAF Inhibitors – Learnings and Improvements Based on Clinical Data

Dr Robert AVERSA
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)

09:05 am LPA1 Receptor Antagonists for the Treatment of IPF

Dr Peter CHENG
(BRISTOL-MYERS SQUIBB R & D, Hopewell, United States)

09:35 am Evolution of Clinical PI3K Inhibitors at Genentech

Dr Steve STABEN
(GENENTECH, South San Francisco, United States)

10:05 am Coffee Break & Exhibition

10:35 am Leveraging the Human PK of PF-06882961, an Oral Small Molecule GLP-1R Agonists, in the Discovery of a 2nd Generation Candidate

Dr David GRIFFITH
(PFIZER INC., Cambridge, United States)

11:05 am Discovery of Oral CGRP Receptor Antagonists for the Treatment of Migraine: Learning from (Clinical) Experience

Dr Christopher BURGEY
(MERCK & CO., INC., West Point, United States)

11:35 am Discovery of Risdiplam, a Selective SMN2 Gene Splicing Modifier for the Treatment of Spinal Muscular Atrophy

Dr Hasane RATNI
(F. HOFFMANN-LA ROCHE LTD, Basel, Switzerland)

12:05 pm Lunch Break & Exhibition

12:20 pm 45-minutes Vendor Workshop by Schrödinger
Designing Molecules in 3D

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 Delivering Innovative Medicines: Small Changes can have a Large Effect

Dr Wendy YOUNG
(GENENTECH, South San Francisco, United States)

02:00 pm Discovery of Novel Drug Regimens for the Treatment of Tuberculosis

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

02:35 pm Discovery of Upadacitinib: a Tricyclic Janus Kinase 1 (JAK1) Inhibitor

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

03:10 pm Coffee Break & Exhibition

03:40 pm DSM265, a Dihydroorotate Dehydrogenase Inhibitor for the Treatment of Malaria

Prof. Meg PHILLIPS
(UNIVERSITY OF TEXAS SOUTHWESTERN MED CENTER, Dallas, United States)

04:15 pm Discovery of the Selective Allosteric TYK2 Inhibitor BMS-986165 for the Treatment of Autoimmune Diseases

Dr Steve WROBLESKI
(BRISTOL-MYERS SQUIBB, Princeton, 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, United States)

05:00 pm Departure