14th Winter Conference on Medicinal & Bioorganic Chemistry January 27th - 31st 2019

Steamboat Springs Resort, Colorado

Organised in collaboration with:



Provisional Program

Sunday 27th January 2019



1.00 – 5.00pm Registration

4.00 – 5.00 Welcome Coffee and Cookies

5.00 Welcome and Opening Remarks – Professor Anthony GM Barrett, Conference Chair

> Welcome to the 2019 MBCF Scholars – Professor Victor Snieckus, Member of the Board

- **5.15 8.00 pm Drug Hunting** Chair: *Dr Daniel Flynn, Deciphera Pharmaceuticals*
- **5.15 Dr Petr Vachal,** Merck The Invention of MK-8262, a CETP Inhibitor Backup to Anacetrapib (with best in class properties)
- **5.55 Dr Kevin Freeman-Cook**, Pfizer Targeting the Cell Cycle for the Treatment of Cancer
- **6.35 Dr Sandra Filla,** Eli Lilly Lasmiditan: The Long Road Home for a Novel Therapy for Acute Migraine Treatment
- 7.15 Dr Daniel Flynn, Deciphera Pharmaceuticals Drug Hunter Award Introduction and Prize
- **7.20** Dr Josh Bilenker, LOXO (Drug Hunter Award) TRK Inhibitor LOXO-101 and back up LOXO-195

8.00 – 10.00 pm Welcome Networking Reception in the Exhibition Area

Monday 28th January 2019

7.00 – 8.00 am Good Morning Buffet Breakfast

- 8.00 11.00 am Immuno-oncology Chair: Dr Wes Trotter, Merck
- 8.00 Dr Jared Cumming, Merck Novel STING Agonists for Immuno-oncology

8.45 Dr Paul Scola, BMS

Discovery of a Macrocyclic Peptide Inhibitor of Programmed Death-Ligand 1 (*PD-L1*)

9.30 Dr Cynthia Parrish, GSK Targeting the Adenosine Pathway with Non-Nucleoside Inhibitors of CD73

10.15 Dr Brendan Parr, Genentech

Design of Selective, Heme-binding Inhibitors of Tryptophan-2,3-dioxygenase (TDO)

- **11.00 End of session**
- 4.00 5.00 pm Back from the Slopes Coffee and Cookie Break
- 5.00 8.00 pm Structural and in-Silico Chemistry Chair: Dr Georgia McGaughey, Vertex
- **5.00 Dr Meihua Tu,** Pfizer The Role of Water Molecule in Ketohexokinase Inhibitor Design
- **5.45 Dr Yuan Wang,** Novartis Computational Methods Help Find Chemical Matter to Uncover Novel Biology

6.30 Dr Clara Christ, Bayer Five years of Binding Free Energy Calculations at Bayer: Impact and Future Directions

- **7.15 Dr Ed Sherer,** Merck Impact of Computational Chemistry Post Candidate Selection and Translating Lessons Learned back into Discovery
- 8.00 End of session

Tuesday 29th January 2019

- 7.00 8.00 am Good Morning Buffet Breakfast
- 8.00 11.00 am Chemical Biology for Drug Discovery Chair: Dr Paola Castaldi, AstraZeneca
- **8.00 Professor Daniel Nomura,** Berkeley *Reimagining Druggability using Chemoproteomic Platforms*
- **8.45 Professor Christina Woo,** Harvard Mapping Binding Site Hotspots in the Global Proteome by Photo-affinity Labeling Mass Spectrometry
- **9.30 Dr Paola Castaldi,** AstraZeneca Building New Bridges between Chemistry & Biology
- **10.15 Dr Andy Phillips,** C4 Therapeutics Targeted Protein Degradation
- **11.00 End of session**
- 4.00 5.00 pm Back from the Slopes Coffee and Cookie Break
- 5.00 8.00 pm Potential New Therapies for the Treatment of Chronic Pain Chair: Dr Sarah Skerratt, Vertex
- **5.00 Dr Sarah Skerratt,** Vertex Overview of Current Therapies for the treatment of Pain
- **5.30 Dr Mark Layton,** Merck Breathe Easy: Mechanistic Insights Enable a Path Forward for Highly Selective Nav1.7 Inhibitors
- **6.00 Professor Laura Bohn,** Scripps Harnessing Opioid Receptor Signaling to Improve Pain Therapeutics
- **6.30 Dr Brendan Crowley,** Merck Discovery And Optimization Of A Novel CGRP Receptor Antagonist Chemotype For The Treatment of Migraine
- **7.00 Dr Emilia Väisänen,** Orion *TRPA1: A Pain Target or a Painful Target?*
- **7.30 Dr Steven McKerrall** Genentech Structure-Based Drug Discovery in the Search for Nav1.7 Inhibitors
- 8.00 End of Session

Wednesday 30th January 2019

- 7.00 8.00 am Good Morning Buffet Breakfast
- **8.00 11.00 am** Recent Advances in Targeting Autophagy Chair: Professor Jay Debnath (UCSF)
- **8.00 Professor Jay Debnath,** UCSF Complexities of Targeting Autophagy to Treat Human Disease
- **8.45 Professor Kevan Shokat,** UCSF *Targeting the Autophagy initiating Kinase ULK1*
- **9.30 Professor Martin McMahon**, University of Utah Combined Targeting of MAP Kinase Signaling and Autophagy for the Future Therapy of Cancers Driven by the RAS Pathway
- **10.15 Professors Ravi Amaravadi & Jeffrey Winkler,** University of Pennsylvania Advances in Targeting Lysosomotrophic Agents
- **11.00 End of session**
- 4.00 5.00 pm Back from the Slopes Coffee and Cookie Break
- **5.00 8.10 pm** Advances in Synthesis and Medicinal Chemistry Chair: Professor Darren Dixon, University of Oxford
- **5.00 Professor James Barrow,** Lieber Institute for Brain Development Discovery and Evaluation of Non-Nitrocatechol COMT Inhibitors for Treatment of Psychiatric Conditions
- **5.20 Dr Scott Savage**, Bristol-Myers Squibb Intrinsic Aminomethyl Pyridine Enables Regioselective C-H Arylation in the Synthesis of IKur Inhibitor, BMS-919373
- **5.40** Dr Vishal Verma, Genentech Development of Inhibitors of MsbA: From HTS to Gram-negative Wild-type Activity
- **6.00 Professor Michael Pollastri**, Northeastern University *Hit-to-lead Medicinal Chemistry Targeting Neglected Tropical Diseases*
- **6.20 Dr Eva Prchalova**, John Hopkins University Hydrogen Bonding Leads to Improved Properties and Exposure
- **6.40 Dr Andrew Woodhead**, Astex Pharmaceuticals The Role of Solution Conformation in Structure-Guided Fragment Optimization
- 7.00 Dr John Butler, Amgen Pyridyl Urea Sulfonamide Inhibitors of NaV1.7: Intramolecular
- **7.20 Professor Darren Dixon**, University of Oxford New Broad Scope Strategies for Amine Synthesis
- 8.00 End of session

Thursday 31st January 2019

- 7.00 8.00 am Good Morning buffet breakfast
- 8.00 11.00 am Photoredox Catalysis Chair: Dr Dan DiRocco, Merck
- **8.00 Dr Dani Schultz,** Merck Recent Advances in the Remote Functionalization of Aliphatic C-H Bonds via Decatungstate Photocatalysis
- **8.35 Dr Thomas Knauber,** Pfizer Enablement of Photoredox Csp2-Csp3 Cross Coupling Reactions
- **9.10 Dr Kaid Harper,** Abbvie *Scaling Catalytic Photochemistry with Lasers*
- **9.45 Professor Corey Stephenson,** University of Michigan Photoredox Catalysis – An Enabling Platform for Discovery and Development
- **10.20 Professor Tomislav Rovis,** University of Columbia New Tools for Catalysis
- **11.00 End of session**
- 4.00 5.00 pm Back from the Slopes Coffee and Cookie Break and visit the Posters
 5.00 6.00 Chair: Professor Victor Snieckus, Queen's University
 5.00 6.00 pm Keynote Speaker: Professor Phil S. Baran, The Scripps Research Institute Translational Chemistry
- 6.00 7.30 Networking Session Pre-Dinner Drinks & Poster Session
- 7.30 9.30 Conference Dinner
- 9.30 Conference Closes

Thank you to all our Sponsors:

Gold:







Silver:







Bronze:





Gilead