

2023

Graduate Research Symposium



July 20 - 23, 2023

DOC Graduate Research Symposium

Montana State University, Bozeman, Montana, July 20-23, 2023

THURSDAY, JULY 20

- 1:45 pm - 4:30 pm Arrival and Check-in
2:30 pm - 4:30 pm Industrial Poster Session – **Ballroom A**
4:30 pm - 5:45 pm Registration and Pizza – **Ballroom A Lobby and Ballroom A**

THURSDAY EVENING Presiding: Brett Fors, Cornell University

- 5:45 pm - 6:00 pm **Welcome – P. Andrew Evans – Ballroom A**
6:00 pm - 6:50 pm **Sarah Reisman – CalTech**
Necessity is the Mother of Invention: Natural Products and the Chemistry they Inspire

- 6:50 pm - 7:10 pm **Claire Page**
Princeton University
Light Excitation of "Ene" Reductases Enables the (Hydro)alkylation of Alkenes and Heteroarenes

- 7:10 pm - 7:30 pm **Mareena Frank**
University of Wisconsin
Electrochemically-Driven, Nickel-Catalyzed Cross-Electrophile Coupling of Aryl Bromides with Alkyl Bromides

- 7:30 pm - 7:50 pm **Patrick Kelly**
University of Chicago
Strategies for Nitrogen Atom Transfer

- 7:50 pm - 8:10 pm **Zhi Xu**
Yale University
Progress Toward the Total Synthesis of (-)-lomaiviticin A

- 8:10 pm - 8:30 pm **Yu Zhu via Zoom**
Queen's University
Intramolecular Rhodium-Catalyzed [(3+2+2)] Carbocyclization Reactions with Dienylidenecyclopropanes: A Concise and Stereoselective Total Synthesis of the Sesquiterpene (+)-Zizaene

- 8:45 pm - 11:30 pm Reception and **Poster Session 1 – Ballroom A**

FRIDAY, JULY 21 Presiding: P. Andrew Evans, Queen's University

- 7:45 am - 9:00 am Breakfast
9:00 am - 9:40 am **Margaret Chu Moyer – Amgen**
Innovation in Small Molecule Drug Discovery
9:40 am - 10:00 am **Hui-Qi Ni**
The Scripps Research Institute

Anti-Selective Cyclopropanation of Non-Conjugated Alkenes with Diverse Pronucleophiles via Directed Nucleopalladation

10:00 am - 10:20 am **Nicholas Fitzpatrick**

Worcester Polytechnic Institute

Harnessing Light for Challenging Transformations: Leveraging Photoredox-Catalyzed [HAT + RPC] Formal Hydride Abstraction to Install Oxygen and Nitrogen Nucleophiles in Simple Hydrocarbons and Pharmaceutically-Active Compounds

10:20 am - 10:50 am Coffee Break – **Ballroom B/C**

10:50 am - 11:40 am **Steve Townsend – Vanderbilt University**

Synthesis of Mind and Body Altering Substances

11:40 am - 12:00 am **Brittany Haas**

University of Utah

Data Science for the Prediction of Amide Coupling Reaction Outcomes

12:00 pm – 12:15 pm **Group Photograph – Norm Asbjornsen Hall**

12:15 pm - 2:30 pm Lunch and **Poster Session 1 – Ballroom B/C and Ballroom A**

WORKSHOPS – Brett Fors

WORKSHOP 1: Academia and Entrepreneurship – Ballroom A

2:30 pm – 3:00 pm **Paul Blakemore – NSF**

Chemistry at the National Science Foundation: Our Mission, Priorities, Programs, and Modus Operandi

3:00 pm – 3:30 pm Greco Gonzalez Miera – **ACS Publications**

The Art of Scientific Publishing

3:30 pm – 4:00 pm **Chuck Frazier – Apeel Sciences**

Building from Scratch: Startups, Entrepreneurship, and Transforming Ideas into Successful Products

4:00 pm - 4:15 pm Coffee Break – **Ballroom A**

4:15 pm - 5:15 pm **WORKSHOP 2 Academic Life – Ballroom A**

Andy Evans (Queen's) and Brett Fors (Cornell)

Paul Blakemore (Oregon State University), Lou Charkoudian (Haverford College), Robert Gilliard (MIT), Sharon Neufeldt (Montana State University), Sarah Reisman (CalTech) and Steve Townsend (Vanderbilt).

5:15 pm - 6:30 pm Dinner – **Inspiration Hall**

FRIDAY EVENING Presiding: Angie Angeles, Vertex

6:30 pm – 7:10 pm **Kyle Rugg – Boehringer Ingelheim**

Process Development of BI 1808128, a 4th Generation EGFR Inhibitor

7:10 pm – 7:30 pm **Aja Nicely**

University of Texas at Austin

Pd-Catalyzed Intramolecular Aminoboration

7:45 – 9:15 pm **WORKSHOP 3: Industrial Life**

Please see the assignments in the tables at the end of the document.

9:15 pm - 11:30 pm **Reception and Poster Session 2 – Ballroom A**

SATURDAY, JULY 22 Presiding: Sharon Neufeldt, Montana State University

7:45 am – 9:00 am Breakfast

9:00 am - 9:50 am **Robert Gilliard – MIT**

Organoboron Heterocycles: From Fundamental Bonding to Functional Materials

9:50 am - 10:10 am **Alexander Oanta**

Northwestern University

Understanding the Effect of Zwitterion Incorporation on 2DP Materials Quality

10:10 am - 10:30 am **David Ryffel**

University of Illinois

Total Synthesis of Darobactin A

10:30 am - 10:50 am Coffee Break –**Ballroom A**

10:50 am - 11:30 am **Travis McMahon – FMC**

Overview of Agricultural Discovery at FMC

11:30 am - 11:50 am **Jenna Humke**

University of Minnesota

Access to "Inaccessible" 5-Membered Heteroarynes Using Transition Metal Complexes

11:50 am - 12:10 am **Matthew McVeigh**

University of California, Los Angeles

Pd-Catalyzed Annulations of Strained Cyclic Allenes

11:50 am - 12:10 pm **Aleksa Milosavljevic**

University of Rochester

Nitrogen-Interrupted Halo-Prins/Halo-Nazarov Fragment Coupling Cascade for the Synthesis of Indolines

12:30 pm - 2:30 pm Lunch and **Poster Session 2 – Ballroom B/C and Ballroom A**

SATURDAY AFTERNOON Presiding: Steven Wisniewski, BMS

2:30 pm - 3:10 pm **Joel Barrish – Jnana Therapeutics**

Drug Discovery Innovation: The Next Chapter for Medicinal Chemistry

3:10 pm - 3:30 pm **Bryan Metze**

Portland State University

Formation of Arynes by C-H Deprotonation with Weak Base: Evaluating and Expanding the Functional Group Compatibility of Aryne Generation Reactions

3:30 pm - 4:00 pm Coffee Break – **Corwin Ballroom**

4:00 pm - 4:20 pm **Patrick Gross**

Emory University
Enabling Asymmetric C–N Bond Formations using Planar Chiral Rh(III) Indenyl Catalysts

4:20 pm - 4:40 pm **Hillary Nguyen**
Colorado State University
Site-Selective Pyridine Functionalization via Nucleophilic Additions to Activated Pyridiniums

4:40 pm - 5:00 pm **Oliver Jackson**
Montana State University
C2 Site-Selective Cross-Coupling of 2,4-Dihalopyrimidines

5:00 pm - 5:20 pm **David Cabanero**
Columbia University
Deep Red (DR) to Near Infrared (NIR) Generation of Aryl(trifluoromethyl) Carbenes

5:30 pm - 8:30 pm Dinner

8:30 pm Drinks and Games: **Recreational Center**

SUNDAY, JULY 23 Presiding: Aleksandra Holownia, Abbvie

7:45 am - 9:00am Breakfast

9:00 am - 9:50 am **Lou Charkoudian – Haverford College**
Unveiling the Biological Chemistry of Polyketide Biosynthetic Pathways by Embracing the Unexplored and Unexpected

9:50 am - 10:10 am **Alina Trofimova**
University of Toronto
Cyclic Prenylated Oligomers – A New Platform for Interrupting and Diverting Terpene Biosynthesis Cascades

10:10 am - 10:40 am Coffee Break – **Ballroom A**

10:40 am - 11:00 am **Griffin Barnes**
University of California, Irvine
A Synthesis of Alstonlarsine A via Alstolucines B and F Demonstrates the Chemical Feasibility of a Proposed Biogenesis

11:00 am - 11:20 am **Meredith Pomfret**
University of Washington
Large Polymers That Behave Like Small Polymers

11:20 am - 11:40 am **Hao Tan**
Texas A&M University
N-Aminopyridinium Salts as Bifunctional Intermediates for Nitrogen Group Transfer Reactions

11:40 am – 12:00 pm **Weiyang Guan**
Cornell University
Electrochemically Driven Deoxygenative Borylation of Alcohols and Carbonyl Compounds

12:00 pm - 1:00 pm Lunch – **Ballroom B/C**

12:00 pm - 2:00 pm Check out and Depart

Friday, JULY 21: POSTER SESSION 1

- 1. Bismarck Amaniampong – Michigan State University**
Exploiting Acetylene Dicarboxylate as a Sustainable Feedstock: Mechanistic Insights into Utilization by E. coli and Bioconversion to D-Lactate
- 2. Alexandra Bodnar – Yale University**
Z-Selective Cobalt-Catalyzed Propargylic Dehydrogenation
- 3. Tyler Azbell – Cornell University**
Cobalt (III) Halide MOFs Drive Catalytic Halogen Exchange
- 4. Zhenqi Zhao – California Institute of Technology**
Accessing Strained Systems via Vinyl Carbocation Intermediates
- 5. Adilene Bernal Sánchez – University of California, Davis**
Catalyst Design and Method Optimization for the Enantioselective Synthesis of Si-Stereogenic Centers
- 6. Cassandra Youshaw – Texas A&M University**
Development of (Enantioselective) Fe-Catalyzed Multicomponent Radical Cascades/Cross Couplings
- 7. Kendelyn Bone – Colorado State University**
Development of C–H Functionalization Reactions Enabled by Base-Catalyzed Halogen Transfer
- 8. Wen Xiu – Purdue University**
[4 + 1]-Cycloaddition Logic for the Total Synthesis of Terpene Alkaloid Natural Products
- 9. Amy Chan – Princeton University**
Marcus-Inverted Excited-State Decay Kinetics as a Photocatalyst Design Principle
- 10. Hunter Warren – University of California, Davis**
Synthesis and Pharmacological Evaluation of New Psychoplastogens
- 11. Hoang Dang – University of Iowa**
Selective Functionalization of Unactivated Diamondoid C–H Bonds via Photooxidative Proton Loss
- 12. Cooper Vincent – UT Southwestern Medical Center**
Photocatalytic Sulfonyl Fluorination of Alkyl Organoboron Substrates
- 13. Louis De Lescure – Colorado State University**
Azine Functionalization and Transformation Through Zincke Imine Intermediates: A DFT Study on Reactivity and Regioselectivity
- 14. Karina Targos – University of Wisconsin**
New Strategies in Oxidative Bond Formation
- 15. Hejun Deng – UT Southwestern Medical Center**
Total Synthesis of Nimbolide and Plumisclern A
- 16. Mayank Tanwar – University of Minnesota**
Mediated ElectroOrganic Transformations for Selective C-H Activation
- 17. Simran Dhingra – Louisiana State University**

Synthesis of BODIPY-TKI Conjugates and Investigation of Their Ability for Targeting the Epidermal Growth Factor Receptor

18. **Allison Stanko – California Institute of Technology**
Enantioselective Nickel-Catalyzed α -Spirocyclization of Lactones
19. **Eric Dobias – Indiana University**
Enantioselective Construction of Acyclic Tertiary-Alkyl α -Fluoro Esters
20. **Gavin Smith – Emory University**
Radical Chain Reduction and C(sp²/sp³) Carboxylation via Carbon Dioxide Radical Anion
21. **Zaafir Dulloo – University of Florida**
Fluorinated-DDAs as Novel Anti-Cancer Agents Against EGFR+ & HER2+ Breast Cancers: Synthesis & Formulation
22. **Dipshi Singh – The Ohio State University**
Cationic Cobalt(I)-Catalyzed Functionalization of Alkynes via Chemodivergent Cycloaddition Reactions and Carboboration Reaction
23. **Cole Edwards – NC State University**
Efforts Toward the Total Synthesis of Echinospirin
- Saturday, JULY 22: POSTER SESSION 2**
24. **Roberto Silva Villatoro – University of Texas at San Antonio**
General Method for Ni-Catalyzed C-N Cross-Coupling of (Hetero)Aryl Chlorides with Anilines and Aliphatic Amines using a Dual-Base Strategy
25. **Nicholas Falcone – Princeton University**
Modern Tactics for Molecular Complexity: Exploring the Construction of Elaborate Heterocyclic Frameworks Through the Synthesis of Maeocrystal V
26. **Jagrut Shah – Stony Brook University**
Direct Synthesis of 2-Aminophenols from Triplet-State Nitro(hetero)arenes and Excited-State Cu-Catalysis
27. **Karan Goyal – University of California, Berkeley**
Exploration of Spirocyclic Topology: Reaction Discovery en route to the Total Synthesis of Urceoloids A & B
28. **Jose Ruiz – University of California, Davis**
Enantioselective Synthesis of Carbacycles by Donor/Donor Carbenes C-H Insertion
29. **Nathaniel Greenwood – Yale University**
Sulfur-Functionalization of Sulfenamides: New Approaches to High Oxidation State Sulfur Pharmacophores
30. **Jessica Paziienza – University of California, Irvine**
Efforts Towards the Synthesis of the Euphoria A Scaffold
31. **Thiago Grigolo – Florida State University**
Total Synthesis Enabled by Regioselective Asymmetric Pyridinium Dearomatization

32. **Shashwati Paul – Indiana University**
Synthesis of Bicyclic Building Blocks to Enable Medicinal Chemistry
33. **Jiachen He – Indiana University**
Metal-free, Photoinduced C(sp³)-H Borylation
34. **Anthony Palermo – University of Toronto**
Stereospecific Synthesis of Strained Rings from Photochemically Generated α -Siloxycarbenes
35. **Benjamin Hejna – Princeton University**
Catalytic Asymmetric Hydrogen Atom Transfer Enables the Hydroamination of Alkenes
36. **Claire Herbert – University of California, Irvine**
Synthesis of Vicinal Carbocycles by Intramolecular Nickel-Catalyzed Conjunctive Cross-Electrophile Coupling Reaction
37. **Casey Olen – University of Illinois**
Chemoinformatic Catalyst Selection Methods for the Optimization of Copper-Bis(oxazoline) Mediated Asymmetric Mukaiyama Aldol Reactions
38. **Fernanda Hernandez Sanchez – University of Arkansas**
Alkynylation of dihydroquinazolinones as Radical Precursors via Hypervalent Iodine compounds under Photoredox Catalysis
39. **Skylar Norman – Wake Forest University**
Solvent Dependency on the Rate-Determining Step of Gold-Catalyzed N-Propargyl Benzamide
40. **Jose Intano – University of Connecticut**
[3+2] Nitrile Oxide Cycloadditions of Strained Dipolarophiles
41. **Giulia Murbach-Oliveira – Purdue University**
Design and Synthesis of IRE1 α Inhibitors for Suppression of Necroptosis
42. **Russell Kielawa – University of Chicago**
Development of a General Synthetic Strategy Toward Akuammiline Alkaloids
43. **Bill Motsch – Temple University**
Synthesis of Pyridinium Salts via C–H Functionalization Enabled by Arene Radical Cations
44. **Matthew Lasky – University of Michigan**
Photocatalytic C-H Amination of Arenes Utilizing a Versatile Acridine-Lewis Acid Complex
45. **Adam Mitrevski – Purdue University**
Design and Synthesis of a Dual-Action Agent Capable of Simultaneously Activating HIV-1 Latency and Preventing New Infection
46. **Jonnathan Marin – University of Illinois**
Optimizing Protein Likeness Enhances Recovery of Physiology for a Molecular Prosthetic

For interactive campus map: <https://www.montana.edu/campusmap/#!/>

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Group A (Angeles)	Group B (Evans)	Group C (Fors)	Group D (Neufeldt)
Last Name: Amaniampong to Franke	Last Name: Goyal to McVeigh	Last Name: Metze to Ruiz	Last Name: Ryffel to Zhu
<i>Ballroom A</i>	<i>Ballroom B</i>	<i>Ballroom C</i>	<i>Ballroom D</i>
Anthony Mastracchio - AbbVie Margaret Chu-Moyer - Amgen Jake Song - Arcus Zachary Buchan - Corteva Adam Schrier - Gilead Cooper Taylor - Incyte Thorsten Rosner - J-Star Katie Logan - Merck Ryan Patman - Pfizer	Aleksandra Holownia - AbbVie Carolyn Wei - Amgen Kyle Rugg - Boehringer Ingelheim Erin Hancock - Corteva Gregg Barcan - GSK Nicole Behnke - Janssen Adriana Jamison - Lilly Cheng Chen - Mirati s ZhenZhen Dong - PharmaBlock	Guanlin Bao - Adesis Wenhan Zhang - Amgen Nicola Webb - BMS Travis McMahon - FMC Tyler Higgins - GSK Christopher McAtee - Janssen Tamas Benkovics - Loxo Oncology Casey Mathison - Novarti Tatsuaki Matsubara - Takeda	Yagya Subedi - Adesis Chuck Frazier - Apeel Sciences Steve Wisnewski - BMS Richard Thornbury - Gilead Marshall Law - Incyte Joel Barrish - Jnana Jamie McCabeDunn - Merck Emma McInturff - Pfizer Ving Lee - UDC

Speakers

Joel Barrish, Jnana Therapeutics
Lou Charkoudian, Haverford College
Margaret Chu Moyer, Amgen
Robert Gilliard, MIT
Travis McMahan, FMC
Sarah Reisman, CalTech
Kyle Rugg, Boehringer Ingelheim
Steve Townsend, Vanderbilt University

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