2024 Graduate Research Symposium









July 25 - 28, 2024

DOC Graduate Research Symposium University of Virginia, Charlottesville, VA, July 25-28, 2024

THURSDAY, JULY 25

1:30 pm - 4:30 pm	Registration and Check-In – Grove Pre-Function				
2:30 pm - 4:30 pm	Industrial Poster Session – Grove Pre-Function				
4:30 pm - 5:45 pm	Pizza Dinner – Grove Ballroom 3				
THURSDAY EVENIN	G Presiding: Jason Chruma – University of Virginia – Grove 1/2				
5:45 pm – 6:00 pm	Welcome – P. Andrew Evans				
6:00 pm - 6:50 pm	Javier Read De Alaniz – UC Santa Barbara Exploring Light-Responsive Materials				
6:50 pm - 7:10 pm	Jason Wang UCLA				
Identifying G	Generally Applicable Reaction Conditions via Bandit Optimization				
7:10 pm – 7:30 pm	Kaitlyn Keasler Cornell University				
Handling Fluor	inated Gases as Solid Reagents Using Metal-Organic Frameworks				
7:30 pm – 7:50 pm	Noah Bissonnette Princeton University				
Deoxygenative Phos	phonylation: Development of a General Organophosphorus Radical Trap				
7:50 pm – 8:10 pm	Camille Rubel Scripps Research				
Oxidation S	State Manipulation to Control Stability and Reactivity with Nickel				
8:10 pm – 8:30 pm	Danielle Loving University of Illinois Urbana-Champaign Directed Coevolution of Chemicals				
8:45 pm – 11:30 pm	Reception and Poster Session 1 – Grove Pre-Function				
FRIDAY, JULY 26 P	residing: P. Andrew Evans, Queen's University – Grove 1/2				
7:45 am – 9:00 am	Breakfast – Grove Ballroom 3				
9:00 am – 9:40 am Discov	Sabine Hadida – Vertex Pharmaceuticals ery of CFTR modulators for the treatment of Cystic Fibrosis				
9:40 am – 10:00 am	Hayden Bishop Purdue University Catalytic Asymmetric Synthesis of Zinc Metallacyles				
10:00 am – 10:20 am	Le Dung "July" Pham University of Minnesota				

Latent Organocatalysis from Reversible N-Heterocyclic Carbene Adducts with Carbodiimides

10:20 am – 10:50 am Coffee Break – Grove Pre-Function

10:50 am – 11:30 am Rebecca Green BMS

Data-Rich Experimentation for Safe and Sustainable Process Development

11:30 pm - 11:50 pm Amaechi Odoh

Clemson University

SuFEX-Enabled Direct Deoxy-Diversification of Alcohols via Cooperative Activation of Substrates and Nucleophiles

- 11:50 pm 12:15 pm Group Photograph TBA
- 12:15 pm 2:30 pm Lunch and Poster Session 1 Grove 3 and Pre-Function

WORKSHOPS: Presiding – P. Andrew Evans – Grove 1/2

WORKSHOP 1: Academia and Entrepreneurship

- 2:30 pm 3:00 pm **Jon Ranier NSF** *Chemistry at the NSF: Our Mission, Priorities, Programs, and Modus Operandi*
- 3:00 pm 3:30 pm **Michael Hurst RSC** Publishing with Impact with the Royal Society of Chemistry
- 3:30 pm 4:00 pm **Chuck Frazier Temporal Agriculture** Building from Scratch: Startups, Entrepreneurship, and Transforming Ideas into Successful Products
- 4:00 pm 4:15 pm Coffee Break Grove Pre-Function
- 4:15 pm 5:15 pm WORKSHOP 2 Academic Life

Erick Carreira (ETH), Javier Read De Alaniz (UCSB), Danielle Dube (Bowdoin) Jason Chruma (Virginia), Christina Cooley (Trinity) and Jon Ranier (NSF)

5:15 pm - 6:30 pm Dinner – Grove Ballroom 3

FRIDAY EVENING Presiding: Angie Angeles, Vertex Pharmaceuticals – Grove 1/2

6:30 pm – 6:50 pm So Young Lee

MIT

Selective Glycan Labeling of Mannose-Containing Glycolipids in Mycobacteria

- 6:50 pm 7:10 pm Mark Maust Emory University
 Photoredox-Enabled Reactivity of (Hetero)aryl Radicals in Switchable 5-exo and 6-endo Cyclizations and Aerobic Hydroxyarylation Reactions
 7:10 pm – 7:30 pm Alexandra Lubaev
 - **Baylor University**

Catalytic Chemo-, Regio-, Diastero-, and Enantioselective Bromochlorination of Unsaturated

Systems Enabled by Lewis Base-Controlled Chloride Release

7:45 – 9:15 pm	WORKSHOP 3: Industrial Life
Please se	ee the assignments in the tables at the end of the document.
9:15 pm - 11:30 pm	Reception and Poster Session 2 – Grove Pre-Function
SATURDAY, JULY 2	7 Presiding: Christina Cooley, Trinity University – Grove 1/2
7:45 am - 9:00 am	Breakfast – Grove Ballroom 3
	Erick Carreira – ETH s and Tactics in Natural Products as an Engine for Discovery
9:50 am - 10:10 am	Bradley Lipka University of Rhode Island Ultra-Rapid Electrophilic Cysteine Arylation
10:10 am - 10:30 am	Katelyn Kitzinger University of North Carolina at Chapel Hill hael-Aldol Annulations via Stereodivergent-Stereoconvergent Pathways
c	Coffee Break – Grove Pre-Function
	Michael Nicastri – Biogen Chemistry via High-throughput Experimentation: Applying sp2-sp3 Cross Coupling to Multistep Library Synthesis
11:30 am - 11:50 am Bulky	Cher-Tian Ser University of Toronto <i>Ligands Promote Palladium-Catalyzed Protodeborylation</i>
11:50 am - 12:10 pm	Logan Bartholomew University of California Berkeley egies for Core Atom Modification of Nitrogen Heteroaromatics
12:10 pm - 2:30 pm	Lunch and Poster Session 2 – Grove 3 and Pre-Function
SATURDAY AFTERN	IOON Presiding: Cooper Taylor, Incyte – Grove 1/2
2:30 pm - 3:20 pm Chemical Tool	Danielle Dube – Bowdoin College s to Detect, Discover, and Disrupt Sugars on Pathogenic Bacteria.
3:20 pm – 3:40 pm	Xuan Wu UCSB
Chiral Bifuncti	onal Ligand Enables Asymmetric Trapping of Vinyl Gold Carbene
3:40 pm - 4:10 pm	Coffee Break – Grove Pre-Function
4:10 pm - 4:30 pm	Danniel Arriaga Texas A&M University Constructive Ozonolysis: Capturing Primary Ozonides
4:30 pm - 4:50 pm	Melody Guo

	Yale University
Differential Cat	talyst-Substrate Pairs for Carbocyclic and Heterocyclic Systems in Atroposelective Quinazolinone Synthesis
4:50 pm - 5:10 pm	Evan Savelson
	University of Virginia
A Tetrazi	ne-Based Synthesis for Underutilized Aza-Indole Analogues
5:10 pm - 5:30 pm	Stephanie Tsang University of Delaware
Mecl	hanism of Photocatalytic Activation of Tetrazine Ligation
8:30 pm	Drinks and Games: The Graduate
SUNDAY, JULY 28 F	Presiding: Thomas Greshock, Merck – Grove 1/2
7:45 am - 9:00 am	Breakfast – Grove Ballroom 3
9:00 am - 9:40 am Design	John Curto – Pfizer and Synthesis of Small Molecule GLP-1 Receptor Agonists
9:40 am – 10:00 am	Joseph Edgecomb University of Wisconsin-Madison
Leveraging P	Potent Photoreductants for Intermolecular Ketyl Radical Coupling
10:00 am – 10:20 am	Coffee Break – Grove Pre-Function
10:30 am – 10:50 am	Riley Roberts Portland State University
Formal	Dehydrogenation of Arenes: New Paths in Aryne Synthesis
10:50 am – 11:10 am	
Phosphine Mono-C	Montana State University Dxides Formed in Situ Implicated in Chemoselectivity of Suzuki Cross- Couplings of Bromoaryl Triflates
11:10 am – 11:30 am	Yufei Zhang University of Buffalo
Direct 1,2-Diazola	tion of Alkyl Halide via Photoredox-Catalyzed Halogen Transposition
11:30 am – 12:10 pm	Veronika Kottisch – BASF Coatings Research at BASF
12:10 pm – 1:00 pm	Lunch – Grove Ballroom 3
12:10 pm – 2:00 pm	Check out and Depart

Fr	iday, JULY 26: POSTER SESSION 1 – Grove Ballrooms 1/2
1.	Souvik Adak – Indiana University Boron Enabled Photosensitized Directed Cycloadditions
2.	Sophie Bender – Princeton University Enantioselective Hydroalkylation of Alkenes using Photoenzymatic Catalysis
3.	Kevin Blanco-Herrero – University of California Davis Silanols: From Ligand Design to Blue Light Reactions
4.	Alexander Bunnell – University of Michigan Mechanism Guided Development of Directed C-H Functionalization of Bicyclo[1.1.1]Pentanes
5.	Kevin Burns – University of Virginia C-H Functionalization via Amine Organocatalysis
6.	Deepta Chattapadhyay – Texas A&M University Development of a Universal SuFEx Reagent for Deaminative C-C Cross-Couplings
7.	Andrew Cruz – University of Michigan Palladium-Catalyzed Alkene Difunctionalization Reactions for the Synthesis of Amine- Substituted Tetralin Derivatives
8.	Noah Daniecki – University of Deleware Insights into the Nature of C-H/O and N-H/N Interactions and Implications for Conformationally Biased Molecular Design
9.	Parag Das – University of Florida Designing Small-Molecule Photoswitches Inspired from Popular Organic Photovoltaics Materials
10.	Serena DiLiberti – University of Minnesota Total Synthesis of (+)-Eburnamonine via Asymmetric Alkene Cyanoamidation and C-CN Bond Activation
11.	Lauren Ehehalt – University of Wisconsin-Madison Decarbonylative Cross-Electrophile Coupling: Synthesis of C(sp2)-C(sp3) Bonds from Carboxylic Acid and Amine Substrate Pools
12.	Martina Golden – Emory University Target Guided Synthesis of Aryl-Functionalized (–)-Promysalin Analogs via Reductive Ni-Catalyzed Cross Electrophile Coupling
13.	Blaik Hopewell – Oregon State University The Total Synthesis of 1,9-diepi-Mensacarcin
14.	Jenny Hu – Cornell University Designing Plastics: Machine Learning to Predict Polymer Properties from Molar Mass Distributions
15.	Julian Kellner-Rogers – Cornell University Hydrazine-Catalyzed Ring-Opening Metathesis Polymerization of Cyclobutenes
16.	Samuel Kwain – Clemson University Selective Inhibition of Polysaccharide Metabolism in Human Gut Microbes through Small Molecules

17.	Tanya Lazarus – University of North Carolina at Chapel Hill Enantioselective Amino- and Oxycyanation of Alkenes via Organic Photoredox and Copper Catalysis
18.	Jaehoo Lee – Yale University Progress Towards the Total Synthesis of Phragmalin Natural Products
19.	Angela Lin – Princeton University Intermolecular Anti-Markovnikov Hydroamination of Alkenes with Sulfonamides, Sulfamides, and Sulfamates
20.	Huitao Ling – University of California Davis The Development of Dyes and Fuels from Sustainable Feedstocks
21.	Sabina Maurer – University of Pennsylvania Cryptic Sulfotransferases for Aziridine Formation
22.	Morgan Mayieka – Michigan State University Development of a Synthetic Strategy to Prepare Mimetics of Heparin Sulfate
	Saturday, JULY 27: POSTER SESSION 2 – Grove Ballrooms 1/2
23.	Jenna Cailin C. Molas – Yale University Cp*Rh(III)-Catalyzed N-H Functionalization for the Synthesis of Nitrogen Heterocycles
24.	Ashley Nensel – Northwestern University Proteomimetic Polymers Exhibit Anti-Angiogenic Activity for Applications in Age-Related Macular Degeneration
25.	Blake Ocampo – University of Illinois at Urbana-Champaign Regression Modeling of Substrate Effects on Enantioselectivity in the Sharpless Asymmetic Dihydrosylation
26.	Karl Ocius – University of Virginia Cell Free Screening Platform for the Identification of Inhibitors of the L,D- Transpeptidase LdtMt2 of Mycobacterium Tuberculosis
27.	Elizabeth Park – Stanford University Electrical Signaling at the Molecular Level: Chemogenetic Inhibition of Sodium Channels
28.	Harrison Reid – University of Oregon Synthesis and Materials Applications of Cycloparaphenylene-Based Polymers
29.	Christopher Reid – University of Virginia Rhodium-Catalyzed Oxidative Alkenylation of Anisole: Control of Regioselectivity
30.	Joshua Sailer – Emory University Development of Diruthenium Tetracarboxylate Catalysts for Selective Carbene Insertion Reactions
31.	Samya Samanta – Texas A&M University β-Phenethylamine Synthesis: N-Pyridinium Aziridnes as Latent Dual Electrophiles
32.	Nathan Schmitt – UT Southwestern Synthesis, Isolation, and Derivation of Unique Clerodane Diterpenes
33.	Chris Seong – University of Minnesota

	Arynes in a Bottle: Thermally Activated Additive-Free Aryne Precursors
34.	Yao Shi – University of British Columbia The Mechanistic Duality of the Suzuki-Miyaura Cross-Couplings
35.	Paolo Siano – University of Virginia Synthesis of Polycyclic Cores from Phenyl Sulfones
36.	Aniket Sole – University of Florida Asymmetric Bronsted Acid Catalyzed Hydroamination Reactions Provide Access to Elusive Pictet-Spengler Products
37.	Annika Tharp – University of Michigan Late-Stage Chlorination of Kinase Inhibitors
38.	Garrett Toth-Williams – University of California Davis Desymmetrization of Heterocyclic Sulfonimidamides via Asymmetric Allylation
39.	Brendan Wall – Iowa State University General Installation of (4H)-Imidazolone cis-Amide Bioisosteres Along the Peptide Backbone
40.	Zihao Wang – Boston University Assssment of Rocaglates as Selective Inhibitors of Glioblastoma Cancer Stem Cells: Enhancing B-ring Diversity of Rocaglates Through Diazonium Coupling
41.	Aiden Wang – MIT Synthesis of Branched-Linker PROTACs for Next-Generation Targeted Protein Degradation
42.	Dominick Witkowski – UCLA Exploring the Reactivity and Utility of Strained Cyclic Cumulenes
43.	Sicheng "Marina" Xie – Indiana University Developing Effective Fluorescent and Fluorogenic Probes for Monitoring the Biological Processes of Micro-Organisms

Industrial Workshop Panels – Organized by Student Last Name

Group A (Angeles)	Group B (Cooley)	Group C (Evans)	Group D (Chruma)
Last Name: Adak to	Last Name: Golden to	Last Name: Maurer to	Last Name: Schmitt to
Ehehalt	Lubaev	Savelson	Zhang
Grove Ballroom 1/2	Grove Ballroom 3	Academy Room	Oak Boardroom
Wenhan Zhang – Amgen	Carolyn Wei – Amgen	Robert Dyer – Adesis	Chuck Frazier – Temporal Ag
Grace Trammel – Corteva	Zachary Buchan – Corteva	Evan Hurlow – Snapdragon	Trevor Sherwood – BMS
Peter Gildner – FMC	Michael Nicastri – Biogen	Nicola Webb – BMS	Dane Holte – Gilead
Cooper Taylor – Incyte	Tarek Sammakia – Loxo	Stephen Ammann – Gilead	Marshall Law – Incyte
Ving Lee – UDC	Jing Li – PharmaBlock	Hannah Shenouda – GSK	Richard Jackson – FMC
Brian Laforteza – Janssen	Thomas Greshock – Merck	Christopher Kelly – Janssen	Danielle Schultz – Merck
Rachel Knapp – Lilly	Jiang Wang – Lilly	Austin Smith – Loxo	John Curto – Pfizer
Michael Hurst – RSC	Jon Rainer – NSF	Veronika Kottisch – BASF	Zachary Garlets – Zoetis
Jared Piper – Pfizer	Rebecca Green – BMS	Sabine Hadida – Vertex	Heather Hintz – GSK

Speakers

Erick Carreira, ETH John Curto, Pfizer Danielle Dube, Bowdoin College Rebecca Green, BMS Sabine Hadida, Vertex Veronika Kottisch, BASF Michael Nicastri, Biogen Javier Read DeAlaniz, UC Santa Barbara

Sponsors

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