Graduate Research Symposium July 26 – 29, 2018 Bloomington, IN

American Chemical Society Division of Organic Chemistry

https://www.organicdivision.org/

DOC Graduate Research Symposium Indiana University, Bloomington, IN July 26-29, 2018

Building Locations	
Neal-Marsha	II Black Culture Center (NMBCC): 275 N. Jordan Avenue, Bloomington, IN 47405
Woodburn H	all (WH): 1100 E. 7 th Street, Bloomington, IN 47405
Indiana Mem	orial Union (IMU): 900 E. 7 th Street, Bloomington, IN 47405
Willkie Quad	rangle: 7505, 150 N. Rose Avenue, Bloomington, IN 47406
THURSDAY, JULY 26	
3:00 pm - 4:30 pm	Arrival and Dormitory Check-in at Neal-Marshall Lobby
4:30 pm - 5:45 pm	Registration and Pizza – NMBCC Bridgewater Lounge
THURSDAY EVENING	Presiding: Gary A. Molander, University of Pennsylvania
5:45 pm - 6:00 pm	Welcome – NMBCC Grand Hall
6:00 pm - 6:50 pm	Jin-Quan Yu, Scripps – NMBCC Grand Hall
	Enantioselective and Remote C–H Activation Reactions
6:50 pm - 7:10 pm	Stephen Sardini
Advances in N	Indiana University Ii-Catalysis for the Stereoselective Difunctionalization of Alkenes
7:10 pm - 7:30 pm	Joseph Vasquez
Simplified Autoin	University of Wisconsin-Madison ducing Peptide Mimetics are Potent Antagonists of Staphylococcus aureus AgrC
7:30 pm - 7:50 pm	Daria Kurandina
General Vi	University of Illinois at Chicago sible Light-Induced Pd-Catalyzed Room Temperature Alkyl-Heck Reaction
7:50 pm - 8:10 pm	Andrew Zahrt
Opt	University of Illinois at Urbana-Champaign imization of Enantioselective Catalysis Through Chemoinformatics
8:10 pm - 8:30 pm	Lin Deng
	University of Chicago
Rhodium-Cat	alyzed C-C Bond Activation as a New Strategy for Natural Product Synthesis
8:45 pm - 11:30 pm	Reception and Poster Session 1 – NMBCC Bridgewater Lounge
FRIDAY, JULY 27 Pre	siding: Lisa Marcaurelle, Enko Chem
8:15 am - 9:00 am	Continental Breakfast – NMBCC Bridgewater Lounge
9:00 am - 9:40 am	Rebecca Ruck, Merck Research Laboratories – NMBCC Grand Hall
Innovation at N	1erck Process R&D via Discovery and Development of New Catalytic Reactions

9:40 am - 10:00 am	Klare Lazor	
Sj	University of Delaware Inthetic Probes to Investigate the Host-Microbiome Interaction	
10:00 am - 10:20 am	Primali Navaratne	
	University of Florida	
Engaging Knoevenag	el Adducts to Develop a Formal Dehydrocyanation via Tsuji-Saegusa-Ito Oxidation	
10:20 am - 10:40 am	Coffee Break – NMBCC Bridgewater Lounge	
10:40 am - 11:20 am	Tim Guzi, Blueprint Medicine – NMBCC Grand Hall	
Crafting Highly Selective Kinase Inhibitors: Discovery and Development of Avapritinib		
11:20 am - 11:40 am	Roy David Row	
	University of California, Irvine Cyclopropenones for Biomolecule Labeling and Assembly	
11:40 am - 12:00 am	Timothy Wright	
Enantioconvergen	Queen's University t Allylic Alkylation of β, γ-Unsaturated α-Amino Nitriles: Synthetic Homoenolate Equivalents	
12:00 - 12:15 pm	Group Photograph – Auditorium Entrance	
12:15 pm - 2:30 pm	Lunch and Poster Session 1 – NMBCC Bridgewater Lounge	
	ACADEMIC WORKSHOPS – Gary A. Molander	
2:30 pm - 3:10 pm	WORKSHOP 1: Academic Support – NMBCC Grand Hall	
	Robert G. Lees, NIGMS	
	Nicole Camasso, ACS Publications	
3:10 pm - 3:30 pm	WORKSHOP 2: Entrepreneurship – NMBCC Grand Hall	
	Jason L. Whitney, IURTC	
3:30 pm – 5:00 pm	WORKSHOP 3: Academic Life – NMBCC Grand Hall	
Sam Gellman (Wis	sconsin), Nikki Pohl (Indiana University), Gary Molander (UPenn), Kristine Nolan (University of Richmond) and Jeremiah Johnson (MIT)	
FRIDAY EVENING Pre	esiding: Nikki Pohl, Indiana University	
5:00 pm - 6:30 pm	Dinner – Indiana Memorial Union	
6:30 pm - 7:20 pm	Jeremiah Johnson, MIT – NMBCC Grand Hall	
Using Org	ganic Chemistry to Gain A Deeper Understanding of Polymer Networks	
7:20 pm - 7:40 pm	Colleen Keohane	
Synthesis and	Emory University Biological Investigation of the Narrow Spectrum Antibacterial (–)-Promysalin	
8.00 0.20 pm	WORKSHOD A. Industrial Life	

8:00 - 9:30 pm WORKSHOP 4: Industrial Life

Group B (Pohl)	Group C (Molander)	Group D (Gellman)
WH006	WH005	WH007
Tony Mastracchio, Abbvie	Ving Lee, Adesis	David Sandoval, Apeel
Chuck Frazier, Apeel	Dave St. Jean, Amgen	Fang Gao, Biogen
Tim Guzi, BluePrint Medicines	Mike Ellis, Celgene	Mike Hay, BMS
Zach Buchan, Corteva	Kimberly Steward, Corteva	Jennifer Griffin, Celgene
Matt Kraft, Gilead	Anna Wagner, Gilead	Belgin Canturk, Corteva
Neil Johnson, GSK	Eddie Yue, Incyte	Steve Staben, Genentech
Wenqing Yao, Incyte	Mark Kerr, Lilly	Mark Nilson, GSK
Kelly George, L'Oréal	John Flygare, Merck	Michael Ameriks, Janssen
Phieng Siliphaivanh, Merck	Christoph Zapf, Nurix	Rebecca Ruck, Merck
Naoko Ichiishi, Takeda	Jared Piper, Pfizer	Hiroko Tanaka, Nurix
	Group B (Pohl) WH006 Tony Mastracchio, Abbvie Chuck Frazier, Apeel Tim Guzi, BluePrint Medicines Zach Buchan, Corteva Matt Kraft, Gilead Neil Johnson, GSK Wenqing Yao, Incyte Kelly George, L'Oréal Phieng Siliphaivanh, Merck Naoko Ichiishi, Takeda	Group B (Pohl)Group C (Molander)WH006WH005Tony Mastracchio, AbbvieVing Lee, AdesisChuck Frazier, ApeelDave St. Jean, AmgenTim Guzi, BluePrint MedicinesMike Ellis, CelgeneZach Buchan, CortevaKimberly Steward, CortevaMatt Kraft, GileadAnna Wagner, GileadNeil Johnson, GSKEddie Yue, IncyteWenqing Yao, IncyteMark Kerr, LillyKelly George, L'OréalJohn Flygare, MerckPhieng Siliphaivanh, MerckJared Piper, Pfizer

9:30 pm - 11:45 pm Reception and **Poster Session 2 – NMBCC Bridgewater Lounge**

SATURDAY, JULY 28	Presiding: Kimberly Steward – Corteva Agriscience
8:15 am - 9:00 am	Continental Breakfast – NMBCC Bridgewater Lounge
9:00 am - 9:50 am	Sam Gellman, University of Wisconsin, Madison – NMBCC Grand Hall
	Functional Foldamers
9:50 am - 10:10 am	Jeff Van Raden
Ca	University of Oregon atalysis Inside of Macrocycles With Radially Oriented π -Systems
10:10 am - 10:30 am	Zhiwei Chen
Asymn	University of California, Irvine netric Intramolecular Hydroacylation via Dynamic Kinetic Resolution
10:30 am - 10:55 am	Coffee Break – NMBCC Bridgewater Lounge
10:55 am - 11:35 am	Kelly George, L'Oréal – NMBCC Grand Hall
Ca	areer Transition States – Innovating at P&G, Roche, and L'Oréal
11:35 am - 11:55 am	Hyowon Seo
	Massachusetts Institute of Technology Photoredox Activation of Carbon Dioxide in Continuous Flow
11:55 am - 12:15 am	Xiaoyang Chen
Orthanilic Acids: N	Princeton University ew Transient Directing Groups for the ortho C-H Methylation and Fluorination of Benzaldehydes via Pd Catalysis
12:15 pm - 2:30 pm	Lunch and Poster Session 2 – NMBCC Bridgewater Lounge

SATURDAY, AFTERNO	DON Presiding: David St. Jean, Amgen		
2:30 pm - 3:10 pm	Tony Mastracchio, Abbvie – NMBCC Grand Hall		
Su	ppressing Toxicity with Acids: The Case of Abbvie's CDK9 Project		
3:10 pm - 3:30 pm	Hiroki Sato		
Development of New	University of Texas at Austin Cycloaddition Reactions of Diols and their Applications: Bridge between Synthetic Chemistry and Material Science		
3:30 pm - 3:55 pm	Coffee Break - NMBCC Bridgewater Lounge		
3:55 pm - 4:15 pm	Brendon Sargent		
Enantios	University of North Carolina at Chapel Hill pecific, Cobalt-Catalyzed Carbonylations of Unactivated Alkyl Tosylates		
4:15 pm - 4:35 pm	Mina Nakhla		
	Baylor University Total Synthesis of (±)-Aspergilline A		
4:35 pm - 4:55 pm	Xin Wen		
	Boston College		
The Exploration of .	Sulfonylhydrazones as New Radical Precursors for Asymmetric C–H Alkylation via Co(II)-Based Metalloradical Catalysis		
4:55 pm - 5:15 pm	Julie Hofstra		
Deve	California Institute of Technology Iopment of Nickel-Catalyzed Asymmetric Reductive Cross-Couplings		
5:30 pm - 8:30 pm	Dinner – Downtown Bloomington		
8:30 pm	Drinks and Games: Indiana Memorial Union		
SUNDAY, JULY 29 Pr	esiding: Gary A. Molander, University of Pennsylvania		
8:15 am - 9:00 am	Continental Breakfast – NMBCC Bridgewater Lounge		
9:00 am - 9:50 am	Kristine Nolan, University of Richmond - NMBCC Grand Hall		
	Calcium-Catalyzed Addition Reactions		
9:50 am - 10:10 am	Dillion Gentekos		
Molecular	Cornell University Weight Distribution Shape as a New Handle to Tune Polymer Properties		
10:10 am - 10:30 am	Gabriel do Passos Gomes		
	Florida State University Taming Oxygen-Rich Systems with Stereoelectronic Effects		
10:30 am - 11:00 am	Coffee Break – NMBCC Bridgewater Lounge		
11:00 am - 11:20 am	Lucas Morrill		
	UCLA		
Enantio	selective Total Synthesis of Akuammiline Alkaloid (−)-Ψ-Akuammigine		

11:20 am - 11:40 am Cristian Morales-Rivera

University of Pittsburgh Predictive Model for Oxidative C–H Bond Functionalization Reactivity with 2,3-Dichloro-5,6-dicyano-1,4benzoquinone (DDQ)

11:40 am – 12:00 pm Jade Bing

Vanderbilt University A Unified Approach to Enantioenriched Carbocyclic β-Fluoroamines

- 12:00 pm 1:00 pm Lunch NMBCC Bridgewater Lounge
- 12:00 pm 2:00 pm Check out at Willkie Quadrangle
- 2:00 pm Depart

THURSDAY, JULY 26: POSTER SESSION 1

1. Paul Marcyk – Indiana University

Iron-Catalyzed Substitution of Unactivated Alcohols by Sulfonamides

2. Minsoo Ju – University of Wisconsin, Madison

Tunable, Catalyst-Controlled Syntheses of β - and γ -Amino Alcohol Motifs Enabled by Silver Complexes

3. Christopher Bemis – University of Illinois at Urbana- Champaign

Synthesis of Sesquiterpene-Tropolones

4. Nicole Godfrey – University of California, Irvine

A Concise Approach to the Nodulisporic Acids

5. Sina Rezazadeh – University of Delaware

Transition Metal-Catalyzed Alkylation of Nitroalkanes

6. William Scaggs – Indiana University

Direct Asymmetric alpha-Allylation of Esters Using BPin-Substituted Electrophiles

7. Shengyang Wang – University of Minnesota

Development and Mechanistic Studies of Pd/Lewis-Acid-Catalyzed N–CN bond Activation and Intramolecular Aminocyanation of Alkenes.

8. Michael Robo – University of Michigan

Elucidating the Activation Pathway of a Nickel Fumarate Pre-Catalyst

9. Anthony Rosales – University of Notre Dame

Predictions of Stereochemistry from Q2MM Developed Transition State Force Fields

10. Jennie Liao – University of Delaware

Transforming Alkyl Amines into Alkyl Arenes: Nickel-Catalyzed Arylation of Amine Derivatives via C-N Bond Activation

11. Adena Issaian – University of California, Irvine

Mechanistic Studies of Formal Thioboration Reactions of Alkynes

12. Blane Zavesky – University of North Carolina at Chapel Hill

Enhancing the Synthetic Utility of Enantioconvergent Reactions and Progress Toward a Convergent Synthesis of Jervine

13. Christopher Pattillo – University of Illinois at Urbana- Champaign

Synthesis of Macromolecular Architectures via Alkyne Metathesis DCC

14. Jagadeesh Manda – University of Florida

Enantioselective Synthesis of Biaryls Using StackPhos as a Chiral Ligand

15. Moustafa Gabr – University of Iowa

Platinum(II) Complexes with Sterically Expansive Tetraarylethylene Ligands as Probes for DNA Mismatches

16. Kellan Passow – University of Minnesota

Photochemically Responsive Nucleosides as Biological Tools

17. Austin Kelly – University of California, Davis

Metal-free Synthesis of 1,3-Disiloxanediols with Mechanistic Insight into the Tamao-Fleming Oxidation

18. Tyler Higgins – University of Pennsylvania

Synthesis and Chemistry of Diazabicyclo[4.4.1]undecanes

19. Nicholas P. Massaro – University of Oklahoma

Metal Carbenoid Initiated Cascades for the Synthesis of Diverse Heterocycles

20. Rene Ebule – University of Louisville

DMSO-Mediated One-Carbon Homologation of Homoallylic Amines to Access 4-Chloropiperidines: An Aza-Pummerer Cyclization Reaction

21. Alexa Barres – University of Wisconsin, Madison

Development of Highly Stable, Semifluorinated Nanoemulsions to Deliver Therapeutics and Imaging Agents

FRIDAY, JULY 27: POSTER SESSION 2

22. Logan Combee – University of Virginia

Organocatalytic C(sp³)-H Amination: Selective Intermolecular Nitrenoid Transfer Catalyzed by an Iminium Salt

23. Kondalarao Kotturi – Ohio University

Directional Self-sorting with Cucurbit[8]uril Controlled by Allosteric π – π and Metal-Metal Interactions

24. Joshua Lutz – Louisiana State University

Thioenamide Synthesis Inspired by Peptide Macrocycles

25. Grant Edwards – North Carolina State University

Synthesis and Biological Evaluation of Heterocyclic Natural Products

26. Julia Duncan – University of Nevada, Reno

Generation of Reactive Intermediates via Lewis Acid Catalysis

27. Arpan Pal – The University of Tulsa

Copper-Catalyzed Sulfide Contraction Reaction Using Diazo Compounds

28. Qile Wang – University of Arkansas

Photocatalyzed Cascade for Synthesis of the Tetracyclic Core of Akuamiline Alkaloids

29. Enrique Barragan – University of Texas at Arlington

Novel Reactivity of Alkyl and Aryl pi-Conjugated Triazenes

30. Ravi Singh – The University of Texas at Arlington

Studies Toward the Total Synthesis of Natural Products Containing 2-Aminoimidazole Moiety

31. Amir Keshavarz – University of California, Merced

Acid-Catalyzed Intramolecular Hydroarylations of beta-Homobenzylstyrenes for the Selective Synthesis of Tetralins

32. Christine Arbour – Wayne State University

Harnessing the Reactivity of the MeDbz Linker to Access C-Terminally Modified and Macrocyclic Peptides

33. Steven Loskot – California Institute of Technology

Enantioselective Total Synthesis of Nigelladine A via a Late-Stage C–H Oxidation Enabled by an Engineered P450 Enzyme

34. Kimberly Klas – Colorado State University

Synthetic Studies for the Biological Evaluation of the Paraherquamide and M albrancheamide Pathways in the Penicillium Genus

35. Nicholas Chiappini – Stanford University

Intermolecular sp3 C–H Amination: Explorations of Acope, Application and Mechanism

36. Kwaku Kyei-Baffour – Purdue University

Synthesis and Biological Evaluation of Aryl Isonitriles as Antibiotic Agents

37. Ethan Wappes – The Ohio State University

Beta C-H Functionalization of Alcohols via Radical Chaperones

38. Erika Lucas – University of California, Irvine

Stereospecific Nickel-Catalyzed Cross-Electrophile Coupling Reactions for Cyclopropane Synthesis

39. Alec Christian – University of California, Berkeley

Understanding and Developing Reactivity and Selectivity in Methionine Modification Using a Data-Intensive Approach

40. Jonathan Dannatt – Michigan State University

Achieving Exquisite Ortho Selectivity in Phenol and Aniline C–H Borylations by Optimizing Weak Interactions

41. James Burrows – University of Pittsburgh

Synthetic Studies Toward Polythiodiketopiperazines and Mechanistic Investigations of Aryl Triazine

42. Gabriel Magallanes – University of Michigan

Redox Catalysis Enables Lignin Valorization

43. James Brewster, II – University of Texas at Austin

Functionalized Heterocycles as Building Blocks for Oligoheterocyclic and Porphyrinoid Constructs

For interactive campus map: <u>https://map.iu.edu/iub/index.html</u>

Plenary Speakers

Sam Gellman, Univ. of Wisconsin-Madison Kelly George, L'Oréal Tim Guzi, BluePrint Medicines Jeremiah Johnson, MIT Tony Mastracchio, AbbVie Kristine Nolin, Univ. of Richmond Rebecca Ruck, Merck Jin-Quan Yu, Scripps Research Institute

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Professor P. Andrew Evans Professor Gary A. Molander Professor Nikki Pohl