42nd National Organic Chemistry Symposium

Princeton University Princeton, New Jersey June 5 – 9, 2011

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Welcome to Princeton University

On behalf of the Executive Committee of the *Division of Organic Chemistry* of the *American Chemical Society* and the *Department of Chemistry at Princeton University,* we welcome you to the *42nd National Organic Chemistry Symposium.* The goal of this biennial event is to present a distinguished roster of speakers that represents the current status of the field of organic chemistry, in terms of breadth and creative advances.

The first symposium was held in Rochester NY, in December 1925, under the auspices of the Rochester Section of the Division of Organic Chemistry. The early meetings were held in December but this was later changed to June. There was an interruption during WWII but the symposium was resumed in Boston in 1947 and has been held biennially ever since. In 1959, the Roger Adams Award was established and the Award Address has become a key focus of the symposium. The *National Organic Chemistry Symposium* is the premier event sponsored by the Division of Organic Chemistry of the American Chemical Society to highlight recent advances in organic chemistry. The 42nd Symposium consists of 13 invited speakers, plus the 2011 Roger Adams Awardee, Professor Robert Grubbs. The lectures will be presented during morning and evening sessions at the beautiful McCarter Theatre on the campus of Princeton University.

The poster sessions have greatly increased in popularity and impact in recent years, and will take place in the evenings (Sunday to Wednesday) from approximately 9:00 pm - midnight in the Taylor Commons Atrium of the new Frick Chemistry Laboratory. The Symposium Banquet on Wednesday evening is open to all registered attendees and guests. The Princeton area offers many recreational opportunities for everyone's taste. The organizers have arranged on-site and offsite activities that we hope you will enjoy.

We thank our Sponsors and our Exhibitors for providing financial support for the Symposium. We also thank the Princeton Conference Services, and our volunteers, including our student volunteers, for assisting with the organization of this event. Finally, thank you for attending, and being a part of the 42nd National Organic Chemistry Symposium.

William Greenlee 42nd NOS Executive Officer Merck Research Laboratories **Duane Burnett** Division Co-Organizer Merck Research Laboratories Scott Sieburth Division Co-Organizer Temple University

Paul Reider 42nd NOS Local Co-Chair Princeton University **Abigail Doyle** 42nd NOS Local Co-Chair Princeton University **Dorothea Fiedler** 42nd NOS Local Co-Chair Princeton University

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Exhibitors

The following organizations will have booths at the evening poster sessions

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Bruce Burnham Paul Chirik Michael Clift Abigail Doyle Dorothea Fiedler Jay Groves Danielle Jacobs Rob Knowles David MacMillan Tom Muir Paul Reider Erik Sorensen Jeff Van Humbeck

Symposium Program

SUNDAY, JUNE 5		
3:00 PM -Midnight	Registration	Taylor Commons, Frick Chemistry
Afternoon – free time	Minor League Baseball - Trenton Thunder Princeton University Campus Walking Tour	
8:00 PM - Midnight	Reception and Poster Session, Exhibitor Booths Sponsored by Merck	Taylor Commons, Frick Chemistry
MONDAY, JUNE 6		
7:30 AM - Noon	Registration	McCarter Theater
8:30 AM - 9:00 AM	Opening Remarks: Dr. William Greenlee, Merck Research Laboratories - Conference Chair Professor Erik Sorensen, Princeton University Department of Chemistry Mr. Eric Hamblin, Princeton University Conference Services	McCarter Theater
	Session Chair: Professor Danielle Jacobs, Rider University	
9:00 AM - 10:15 AM	Professor Amir Hoveyda , Boston College: "New Concepts, Catalysts and Methods for Efficient Z- Selective Olefin Metathesis Reactions"	McCarter Theater
10:15 AM-10:45 AM	Break - Sponsored by ACS Publications	
	Session Chair: Professor Dan Seidel, Rutgers University	

10:45 AM - Noon	Professor Michael Krische , University of Texas at Austin: "Formation of C-C Bonds via Catalytic Hydrogenation and Transfer Hydrogenation"	McCarter Theater
Afternoon – free time	Six Flags Great Adventure, Princeton University Campus Walking Tour NOS Softball Challenge	
	Session Chair: Professor David Chenoweth, University of Pennsylvania	
7:00 PM - 8:15 PM	Professor Geoffrey Coates , Cornell University: "Bimetallic Catalysis: Design, Discovery, and Applications in Organic and Materials Chemistry"	McCarter Theater
8:15 PM - 9:30 PM	Professor Colin Nuckolls , Columbia University: "From Molecules to Materials"	McCarter Theater
9:30 PM - Midnight	Mixer and Poster Session, Exhibitor Booths Sponsored by Sigma Aldrich	Taylor Commons, Frick Chemistry
	TUESDAY, JUNE 7	
6:30 AM - 7:30 AM	5K Fun Run	
8:20 AM - 8:30 AM	Session Chair: Professor Paul Reider, Princeton University	McCarter Theater
8:30 AM - 9:45 AM	Professor Benjamin Cravatt , The Scripps Research Institute: "Activity-Based Proteomics – Applications for Enzyme and Inhibitor Discovery" Sponsored by Chemical Science	McCarter Theater
9:45 AM - 10:30 AM	Break - Sponsored by Lilly	
	Session Chair: Professor Rodrigo B. Andrade, Temple University	

10:30 AM - 11:45 AM	Professor Carolyn Bertozzi, University of California at Berkeley: "Bioorthogonal Chemistries for Glycoprofiling and Beyond" Sponsored by the Journal of the American Chemical Society	McCarter Theater
11:45 AM - 1:00 PM	Professor Dieter Enders , RWTH University, Aachen: "Asymmetric Organocatalysis: Methods and Applications"	McCarter Theater
Afternoon – free time	Grounds for Sculpture, Princeton University Art Museum Tour Volleyball "Tiger" Tournament	
5:30 PM – 6:30 PM	Undergraduate Context Session: Professor Jeffrey Katz Pizza and Soda will be provided	Frick – Taylor Auditorium
	Session Chair: Professor Gary Molander, University of Pennsylvania, Chair ACS Division of Organic Chemistry	
7:00 PM - 8:30 PM	2011 Roger Adams Award Lecture: Professor Robert Grubbs, California Institute of Technology: "Development of Olefin Metathesis Catalysts for the Synthesis of Large and Small Molecules"	McCarter Theater
8:30 PM - Midnight	Mixer and Poster Session, Exhibitor Booths Sponsored by The Journal of Organic Chemistry and Organic Letters	Taylor Commons, Frick Chemistry

WEDNESDAY, JUNE 8		
	Session Chair: Professor Bruce Burnham, Rider University	McCarter Theater
8:30 AM - 9:45 AM	Professor Dennis Dougherty , California Institute of Technology: "Chemistry on the Brain: Understanding the Nicotine Receptor"	McCarter Theater
9:45 AM - 10:30 AM	Break - Sponsored by Amgen	
	Session Chair: Dr. Duane Burnett, Merck Research Laboratories	
10:30 AM -11:45 AM	Dr. Anthony Wood , Senior Vice President, Head of Worldwide Medicinal Chemistry Pfizer: "Challenges and Opportunities for Medicinal Chemistry" Sponsored by MedChemComm	McCarter Theater
11:45 AM - 1.00 PM	Dr. Joseph Armstrong , Senior Director, RNAi & Discovery Process Chemistry, Merck Research Laboratories: "Innovation as the Driver of Green Chemistry Advances in the Pharmaceutical Industry"	McCarter Theater
Afternoon – free time	Institute Woods Princeton University Art Museum Tour Ultimate Frisbee Event	
5:00 PM - 7:00 PM	Conference Banquet	Jadwin Gym
	Session Chair: Professor Abigail Doyle, Princeton University	
7:30 PM - 8:45 PM	Professor Hisashi Yamamoto , University of Chicago: "Molecular Design of Acid Catalyst for Organic Synthesis - Rapid Synthesis of Polyketides"	McCarter Theater

8:45 PM - Midnight	Mixer and Poster Session, Exhibitor Booths Sponsored by WuXi AppTec	Taylor Commons, Frick Chemistry
THURSDAY, JUNE 9		
	Session Chair: Professor Dorothea Fiedler, Princeton University	McCarter Theater
9:00 AM - 10:15 AM	Professor Vy Dong , University of Toronto: "A Few of My Favorite Rings: Catalysis Inspired by Lactones and Lactams "	McCarter Theater
10:15 AM-10:45 AM	Break - Sponsored by ACD/Labs	
	Session Chair: Professor Scott Sieburth, Temple University, Chair NOS 2013	
10:45 AM - Noon	Professor M. Christina White , University of Illinois: "The Emergence of Predictable Selectivity for Aliphatic C—H Oxidations "	McCarter Theater
	Closing Remarks	



The Roger Adams Award in Organic Chemistry

The Roger Adams Award in Organic Chemistry is sponsored jointly by the American Chemical Society, Organic Reactions, Inc., and Organic Synthesis, Inc. The award recognizes the distinguished career of Roger Adams, who played a vital role in each of these three organizations. He was Chairman of the Board of Directors as well as President of the American Chemical Society, and he co-founded Organic Syntheses and Organic Reactions.

The award is made biennially to an individual, without regard to nationality, for outstanding contributions to research in organic chemistry. The award consists of a gold medal, a sterling silver replica of the medal, and an honorarium of twenty-five thousands dollars. It is presented at the biennial National Organic Chemistry Symposium of the Division of Organic Chemistry of the American Chemical Society. The awardee is a featured lecturer in the program of the symposium.

The recipient of this year's Roger Adams Award is Professor Robert Grubbs of the California Institute of Technology in recognition of his outstanding contributions to synthetic, mechanistic, and catalytic organic chemistry. Professor Grubbs' Award Address, entitled "*Olefin Metathesis: Catalysts, Molecules and Materials*," will be delivered on Tuesday evening.

Roger Adams Awardee Professor Robert Grubbs California Institute of Technology Division of Chemistry and Chemical Engineering Pasadena, CA 91125 Presenting: Tuesday, June 7, 7:00 PM



Plenary Speakers



Professor Amir Hoveyda Boston College Presenting Monday, June 6, 9:00 AM



Professor Michael Krische University of Texas at Austin Presenting Monday, June 6, 10:45 AM



Professor Geoffrey W. Coates Cornell University Presenting Monday, June 6, 7:00 PM

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Professor Colin Nuckolls Columbia University Presenting Monday, June 6, 8:15 PM



Professor Robert Grubbs 2011 Roger Adams Awardee California Institute of Technology Presenting Tuesday, June 7, 7:00 PM



Professor Benjamin Cravatt The Scripps Research Institute Presenting Tuesday, June 7, 8:30 AM



Professor Carolyn Bertozzi University of California at Berkeley

Presenting Tuesday, June 7, 10:30 AM



Professor Dieter Enders RWTH University, Aachen Presenting Tuesday, June 7, 11:45 AM



Professor Dennis Dougherty California Institute of Technology Presenting Wednesday, June 8, 8:30 AM



Dr. Anthony Wood Senior Vice President, Head of Worldwide Medicinal Chemistry, Pfizer Presenting Wednesday, June 8, 10:30 AM



Dr. Joseph Armstrong Senior Director, RNAi & Discovery Process Chemistry, Merck Research Laboratories Presenting Wednesday, June 8, 11:45 AM

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Professor Hisashi Yamamoto University of Chicago Presenting Wednesday, June 8, 7:30 PM



Professor Professor Vy Dong University of Toronto Presenting Thursday, June 9, 9:00 AM



Professor M. Christina White University of Illinois Presenting Thursday, June 9, 10:45 AM

New Concepts, Catalysts and Methods for Efficient Z-Selective Olefin Metathesis Reactions

Amir H. Hoveyda

Joseph T. and Patricia Vanderslice Millennium Professor of Chemistry Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts 02467

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Alkenes are found in a great number of biologically active molecules and are employed in numerous transformations in organic chemistry. Many olefins exist as *E* or higher energy Z isomers. Catalytic procedures for stereoselective formation of alkenes are therefore highly valuable; nonetheless, methods enabling the synthesis of 1,2- disubstituted Z olefins are scarce. In this lecture, concepts that have resulted in the development of catalytic Z-selective cross-metathesis reactions of terminal enol ethers, which have not been reported previously, and allylic amides, employed thus far only in E-selective processes, will be presented; the corresponding disubstituted alkenes are formed in up to >98% Z selectivity and 97% yield. In addition, catalytic ring-closing metathesis reactions that deliver Z cyclic alkenes with exceptional selectivity will be unveiled. Use of reduced pressure will be introduced as a simple and effective strategy for achieving high stereoselectivity. It will be demonstrated that the above catalytic Zselective transformations, promoted by catalysts that contain the highly abundant and inexpensive molybdenum or tungsten, are amenable to gram scale operations. The utility of the concepts, catalysts and methods is demonstrated in the context of synthesis of a number of biologically active molecules, such as an anti-oxidant plasmalogen phospholipid, immunostimulant KRN7000, antibacterial nakadomarin A, and anticancer agents epothilones C and D.

Formation of C-C Bonds *via* Catalytic Hydrogenation and Transfer Hydrogenation

Michael Krische

Robert A. Welch Chair in Science Department of Chemistry, University of Texas at Austin 1 University Station, Austin TX 78712, USA email: mkrische@mail.utexas.edu

Under the conditions of homogenous hydrogenation, π -unsaturated reactants engage in byproduct-free reductive C-C coupling to carbonyl compounds and imines, offering an alternative to stoichiometric organometallic reagents in diverse C=X (X = O, NR) addition processes. This concept is extended further by "C-C bond forming transfer hydrogenations". Here, alcohol dehydrogenation triggers generation of organometallic nucleophiles from π -unsaturated reactants, enabling byproduct-free carbonyl addition *directly from the alcohol oxidation level*. These processes represent the first C-C bond forming hydrogenations beyond hydroformylation.



Selected Publications

<u>Review</u>: "Catalytic Carbonyl Addition through Transfer Hydrogenation: A Departure from Preformed Organometallic Reagents," Bower, J. F.; Kim, I. S.; Patman, R. L.; Krische, M. J. *Angew. Chem. Int. Ed.* **2009**, *48*, 34.

<u>Review</u>: "Enantiomerically Enriched Allylic Alcohols and Allylic Amines *via* C-C Bond Forming Hydrogenation: Asymmetric Carbonyl and Imine Vinylation," Skucas, E.; Ngai, M.-Y.; Komanduri, V.; Krische, M. J. *Acc. Chem. Res.* **2007**, *40*, 1394.

<u>Review</u>: "Diastereo- and Enantioselective Reductive Aldol Addition of Vinyl Ketones *via* Catalytic Hydrogenation," Han, S. B.; Hassan, A.; Krische, M. J. *Synthesis* **2008**, 2669.

Bimetallic Catalysis: Design, Discovery, and Applications in Organic and Materials Chemistry

Geoffrey W. Coates

Tisch University Professor, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York

email: gc39@cornell.edu

Society depends on polymeric materials now more than at any other time in history. Although synthetic polymers are indispensable in a diverse array of applications, ranging from commodity packaging and structural materials to technologically complex biomedical and electronic devices, their synthesis and post-use fate pose important environmental challenges. The focus of our research is the development of routes to polymers with reduced environmental impact. In this work, we aim to transition from fossil fuels to renewable resources, and are developing synthetic methods that limit energy and raw-material consumption. In addition, we are designing materials that will eventually degrade into non-toxic materials, and have properties comparable to current commodity plastics.

Over the last decade, my research group at Cornell has focused on the development of catalysts for polymer synthesis. Epoxides are ideal feedstocks in that they have significant ring strain, enabling thermodynamically favorable homopolymerization and copolymerization reactions. In my presentation, I will outline our research that involves the development of new bimetallic catalysts for the synthesis of polymers from epoxides.



From Molecules to Materials

Colin Nuckolls

Professor of Chemistry, Department of Chemistry and Nanoscale Science and Engineering Center Columbia University, New York, NY 10027

email: cn37@columbia.edu

The presentation will present methods of designing, synthesizing and assembling nanostructured forms of carbon. Methods to synthesize highly non-planar aromatic structures will be presented that allow the assembly of fullerenes in efficient solar cells, formation of aromatic bowls, and the synthesis of atomically defined graphene ribbons. Utilization of nanostructured carbon in electrical devices allows the preparation of ultrasensitive sensors and single molecule switches.

Activity-based Proteomics and Its Application for Enzyme and Inhibitor Discovery

Benjamin Cravatt

Chairman, Department of Chemical Physiology, The Skaggs Institute for Chemical Biology, and Co-director of the Center for Physiological Proteomics, The Scripps Research Institute, La Jolla, CA

email: cravatt@scripps.edu

Genome sequencing projects have revealed that eukaryotic and prokaryotic organisms universally possess a huge number of uncharacterized enzymes. The functional annotation of enzymatic pathways thus represents a grand challenge for researchers in the genome era. To address this problem, we have introduced chemical proteomic and metabolomic technologies that globally profile enzyme activities in complex biological systems. These methods include activity-based protein profiling (ABPP), which utilizes active site-directed chemical probes to determine the functional state of large numbers of enzymes in native proteomes. In this lecture, I will describe the integrated application of ABPP and complementary metabolomic methods to discover and functionally annotate enzyme activities in mammalian systems, including cancer and the nervous system. I will also present competitive ABPP platforms for developing selective inhibitors for poorly characterized enzymes and discuss ongoing challenges that face researchers interested in assigning protein function using chemoproteomic methods.

Bioorthogonal Chemistries for Glycoprofiling and Beyond

Carolyn Bertozzi

T. Z. and Irmgard Chu Distinguished Professor of Chemistry and Professor of Molecular and Cell Biology at University of California, Berkeley, an Investigator of the Howard Hughes Medical Institute and Director of the Molecular Foundry at the Lawrence Berkeley National Laboratory

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Bioorthogonal chemical reactions enable the selective labeling of biomolecules in systems as complex as live animals. This presentation will summarize progress in bioorthogonal reaction methodology as well as highlight applications toward disease biomarker discovery and in vivo imaging. In particular, we employ metabolic labeling followed by bioorthogonal chemical tagging as a means to profile changes in protein glycosylation associated with cancer and to monitor spatiotemporal changes in cell surface glycosylation during embryogenesis.

Asymmetric Organocatalysis: Methods and Applications

Dieter Enders

Professor of Chemistry, Institute of Organic Chemistry, RWTH Aachen University, Landoltweg 1, 52074 Aachen, Germany

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The research field of organocatalysis has developed rapidly since about the turn of the millennium and can now be seen as a third pillar of asymmetric catalysis beside metal and biocatalysis.¹ Numerous basic organocatalytic protocols for very efficient and highly stereoselective carbon-carbon and carbon-heteroatom bond formations are now part of the strategic arsenal of synthetic chemistry.

In this lecture some of our recent results in both methodology and target oriented asymmetric organocatalysis will be presented. Proline-catalyzed diastereo- and enantioselective aldol and Mannich reactions opened a short and efficient entry into the important natural product classes of carbohydrates and sphingolipids. The main focus, however, will be on the development of simple, triple and even quadruple domino reactions using diphenyl prolinol-TMS-ether as catalyst as well as Brønsted acid and thiourea catalysis in the asymmetric synthesis of pyrrolidines, isoindolines and tetrahydroisoquinolines. Finally, some of our recent results in the field of NHC-organocatalysis will also be presented.

For reviews from our group, see: Domino reactions: a) C. Grondal, M. Jeanty, D. Enders, *Nature Chemistry* **2010**, *2*, 167. b) D. Enders, C. Grondal, M. R. M. Hüttl, *Angew. Chem.* **2007**, *119*, 1590; *Angew. Chem. Int. Ed.* **2007**, *46*, 1570. Aza-Michael additions: c) D. Enders, C. Wang, J. X. Liebich, *Chem. Eur. J.* **2009**, *15*, 11058. NHC-organocatalysis: d) D. Enders, O. Niemeier, A. Henseler, *Chem. Rev.* **2007**, *107*, 5606. e) D. Enders, T. Balensiefer, *Acc. Chem. Res.* **2004**, *37*, 534. f) Perspective: D. Enders, A. A. Narine, *J. Org. Chem.* **2008**, *73*, 7857.

Development of Olefin Metathesis Catalysts for the Synthesis of Large and Small Molecules

Robert Grubbs 2011 Roger Adams Awardee

Victor and Elizabeth Atkins Professor of Chemistry, California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA 91125

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Ruthenium based olefin metathesis catalysts have opened a number of applications that range from the synthesis of new pharmaceuticals to the development of new composite materials. Key to the evolution of these catalysts has been a detailed mechanistic understanding. Although a number of details remain to be determined and there are still many surprises, good models for the intermediates and the isolation of intermediate structures have provided new insights into the mode of operation of the catalyst.

With highly active catalysts available that provide a starting point for many applications, the mechanistic understanding and the facile synthetic procedures for new ligand systems provide a basis for the design of catalysts for specific applications. Recent advances have been made in the development of new complexes that show greater efficiency in the ethenolysis of internal olefins, select for less substituted olefins and control the E:Z geometry of the resulting olefins from acyclic metathesis.

Ring opening metathesis polymerization (ROMP) provides a route to a variety of polymeric materials. In some cases, the catalysts can be used to efficiently produce large composite plastic parts from simple cyclic olefins. The catalytic complexes also serve as initiators for living polymerization of strained olefins. The functional group tolerance of the initiators allow for the synthesis of polymers with low polydispersities for use in biomaterials and photonic applications.

Chemistry on the Brain: Understanding the Nicotine Receptor

Dennis Dougherty

George Grant Hoag Professor of Chemistry, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125

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The human brain is the most complex object known to man. It presents daunting challenges at all levels, from the anatomical, to the cellular, to the molecular. Our work seeks to provide a chemical-scale understanding of the molecules of memory, thought, and sensory perception; of Alzheimer's, Parkinson's, and schizophrenia. An area of particular interest has been the chemistry of nicotine addiction. The initial chemical event of nicotine addiction involves nicotine binding to and activating acetylcholine (ACh) receptors in the brain. Using the mindset and methodologies of physical organic chemistry, we have probed these complex membrane proteins with a precision and subtlety normally associated with small molecule studies. We have established that the cation- π interaction plays a pivotal role in promoting the high potency of nicotine in the brain, leading to its addictive properties. We have also discovered key hydrogen bonding interactions that uniquely contribute to the binding of nicotine to ACh receptors. These chemical studies provide a high-precision structural model for the interaction of potent drugs at brain receptors.
Challenges and Opportunities for Medicinal Chemistry

Anthony Wood

Senior Vice President, Head of Worldwide Medicinal Chemistry, Pfizer

email: anthony.wood@pfizer.com

The lecture will cover opportunities for medicinal chemistry to continue to make an impact on modern drug discovery. These will range from the challenge of designing better molecules to reduce discovery costs through fewer design cycle iterations and improved survival to new chemical biology techniques that promise to provide a more detailed understanding of molecular interactions and selectivity to the synthetic challenges posed by the need for more efficient synthesis of complex scaffolds and the opportunities presented by protein conjugation.

- 1. more effective design through improved computational chemistry, knowledge management and decision making tools
- 2. reducing compound toxicity based project failure
- 3. innovative synthesis to improve efficiency and access new chemical space
- 4. the application chemical biology to better understand target interactions

NOTES

Innovation as the Driver of Green Chemistry Advances in the Pharmaceutical Industry

Joseph Armstrong

Senior Director, RNAi & Discovery Process Chemistry, Merck Research Laboratories

email: joe.armstrong@merck.com

- Highlighting Merck's approach of incorporating Green Chemistry principles into discovering and developing manufacturing routes for its products
- Developing an environmentally benign 'Asymmetric Hydrogenation' manufacturing route to sitagliptin, the active pharmaceutical ingredient in JANUVIA® (a new treatment for Type II Diabetes)
- Collaborating to produce a novel transaminase that is capable of catalyzing the production of the chiral amine for sitagliptin on a manufacturing scale

NOTES

Molecular Design of Acid Catalyst for Organic Synthesis Rapid Synthesis of Polyketides

Hisashi Yamamoto

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New reagents and catalysts have unlimited potential for the future of organic synthesis. We have been interested in Lewis and Brønsted acid catalysis for a number of years. In this lecture, I am going to focus on several of these acid and related catalysts from the aspect of their molecular design and engineering.

Acid is the classical reagent in organic synthesis. Lewis and Brønsted acids can be utilized as more effective tools for chemical reactions by sophisticated engineering such as "designer acids". Needless to say, the ultimate goal of such "designer acids" is to achieve high reactivity, selectivity, and versatility as a useful tool of organic synthesis. Even now, the full potential of acid catalysts has not yet been realized. The lecture will be focused on the combination of super Brønsted acid and super silyl group to establish a cascade reaction to generate complex molecules in a single pot. This successive aldol process is a completely new version of the Mukaiyama aldol reaction and provides numerous opportunities to flexible and straightforward control the stereochemistry of the product molecule.

NOTES

A Few of My Favorite Rings: Catalysis Inspired by Lactones and Lactams

Vy Dong

Professor of Chemistry, Department of Chemistry, University of Toronto, Toronto, Canada

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Lactones and lactams make up a range of structurally complex and useful compounds, from antibiotics to nanomaterials. Inspired by these cyclic architectures, we have developed catalytic methods that feature the enantioselective functionalization of carbon-hydrogen bonds. This lecture will focus specifically on the reaction design, scope, and mechanism of ketone- and olefin-hydroacylation. Our goal is to develop green and efficient strategies for constructing cyclic structures and other common motifs.

References:

Shen, Z.; Dornan, P. K.; Khan, H. A.; Woo, T. K.; Dong, V. M. "Mechanistic Insights into the Rhodium-Catalyzed Intramolecular Ketone Hydroacylation." *J. Am. Chem. Soc.* **2009**, 131, 1077.

NOTES

The Emergence of Predictable Selectivity for Aliphatic C—H Oxidations

M. Christina White

Professor of Chemistry, Department of Chemistry, University of Illinois, 270 Roger Adams Laboratory, 600 South Mathews Ave., Urbana, IL 61801

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Aliphatic C—H oxidations have appeared in the literature sporadically over the past century. However, synthetic chemists considered these transformations to be too poorly selective and/or reactive for routine utilization in synthesis. As recently as 2007, chemists considered bio-inspired catalysts with elaborate binding pockets to be the most promising candidates for achieving site-selectivity for intermolecular reactions with unactivated, aliphatic C-H bonds. Reactivity differences between these very inert bonds were thought to be too minor for a small molecule catalyst to discriminate effectively. Remarkably, only four years after this sentiment pervaded, it is now widely accepted that predictable selectivity and good reactivity for aliphatic C-H oxidations is possible with electrophilic small molecule catalysts and simple organic reagents. Three factors have that have been crucial to this paradigm shift in how the reactivity of C-H bonds is viewed will be discussed: first, the discovery of a selective Fe(PDP) catalyst that operates under synthetically useful conditions (limiting substrate) and reliably furnishes \geq 50% isolated yields of mono-oxidized products; second, the systematic delineation of predictable "rules" for the selectivities observed that are generalizable to other electrophilic oxidants; and, third, the demonstration that these rules persist in complex molecule settings.

NOTES

Listed below are the advanced graduate students who were awarded a Division of Organic Chemistry Graduate Fellowships in the past two years. All of these students are presenting a poster at the symposium. Also listed are the names of their institution, faculty research advisor, and the company that sponsored the specific award. The Division of Organic Chemistry is pleased to honor these extraordinary students and to gratefully acknowledge the substantial financial support provided by their generous sponsors.

2010 – 2011 Fellowship Recipients





Adam Brown Sponsor: Eli Lilly Harvard University Advisor: Eric Jacobsen

Ming Chen Sponsor: Pfizer The Scripps Research Institute Advisor: William Roush





Hee Yeon Cho Sponsor: Roche Boston College Advisor: Larry Scott, James Morken

Juana Du Sponsor: GlaxoSmithKline University of Wisconsin Advisor: Tehshik Yoon -----42nd National Organic Chemistry Symposium 2011 • Princeton University





Claire Filloux Sponsor: Genentech Colorado State University Advisor: Tomislav Rovis

Dawn Makley Sponsor: Organic Reactions/Organic Syntheses Vanderbilt University Advisor: Jeffrey Johnston



R





Kyle Quasdorf Sponsor: Organic Syntheses UCLA Advisor: Neil Garg

Daniel Robbins Sponsor: Boehringer Ingelheim University of Illinois Advisor: John Hartwig

Danielle Schultz Sponsor: Organic Syntheses (Nelson Leonard Fellowship) University of Michigan Advisor: John Wolfe

Gretchen Stanton Sponsor: Amgen University of Pennsylvania Advisor: Patrick Walsh

2009 – 2010 Fellowship Recepients







Judy Chen Sponsor: Organic Syntheses/Organic Reactions Columbia University Advisor: Nicholas Turro

Alison Donnelly Sponsor: Roche University of Kansas Advisor: Brian Blagg

Brett Fors Sponsor: Boehringer Ingelheim Massachusetts Institute of Technology Advisor: Stephen Buchwald





Stephen Lathrop Sponsor: Sanofi Aventis Colorado State University Advisor: Tom Rovis

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Joann Um Sponsor: Novartis University of California, Los Angeles Advisor: Kenneth Houk

Kathy Woody Sponsor: Organic Syntheses, Nelson J. Leonard Fellowship Georgia Institute of Technology Advisor: David Collard

SCHEDULE OF PRESENTERS

Sunday – 5 June 2011 Poster Session A

- A–01 **On the Origin of Conformational Kinetic Isotope Effects** <u>Daniel J. O'Leary</u>,*¹ Matthew P. Meyer² and Paul R. Rablen³ ¹Department of Chemistry, Pomona College, Claremont, CA 91711; ²Department of Chemistry, University of California, Merced, Atwater, CA 95301 ³Department of Chemistry, Swarthmore College, Swarthmore, PA 19081
- A–02 A Comparative Study of the Photophysical Properties of Carbazolo- and Diphenylamino-based Heterocyclophanes
 E.A. Hernberg, A.J. Wagenhals, D. Gagnon, M.J. Novak, <u>A.B. Brown</u>,* J.C. Baum Department of Chemistry, Florida Institute of Technology, 150 W. University Blvd., Melbourne, FL 32901
- A–03 A Hands-On Method for Learning Chemical Shift Correlation in Nuclear Magnetic Resonance Spectroscopy Kyle T. Smith and Christian S. Hamann, Ph.D.* Albright College, Reading, PA 19604
- A–04 Is This Carbocation Rearrangement One Step or Two? Using Computational Chemistry to Answer the Question Danielle M. Russo and Christian S. Hamann, Ph.D.* Albright College, Reading, PA 19604
- A-05 Catalytic, Atom-Efficient Aromatic Substitution Through Radical Intermediates Dhandapani Sadasivam,¹ Todd Maisano,¹ Robert A. Flowers II^{1,*} and Andreas Gansäuer²
 1. Lehigh University; 2. University of Bonn
- A–06 Effect of surfactant on electrical conductivity in carbon nanotube thin films Juliet Hahn Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400
- A–07 **A Heterocyclic Radical Cation Acts as a Hydrogen Atom Acceptor** Brittney L. Tiley, Crina M. Sasaran, Samantha R. Cordisco, Jeffrey P. Wolbach, <u>Ian J. Rhile</u>* Albright College

- A–08 Investigation and Application of Newly Synthesized Oxypyridinium Salts Christian T. N. H. Hubley, Lauren D. Bannister and <u>Philip A. Albiniak</u>* Ball State University, Muncie, IN 47306
- A–09 Development of functionalized chiral allylboranes via allene hydroboration and applications in natural product synthesis <u>Ming Chen</u>, William R. Roush* Scripps Florida, 130 Scripps Way, 3#A2, Jupiter, FL 33458
- A–10 Development of a 2-Aza-Cope-[3+2] Dipolar Cycloaddition Strategy for the Synthesis of Quaternary Proline Scaffolds <u>Michael P. McCormack</u>, Xiaoxi Liu, Stephen P. Waters* Department of Chemistry, University of Vermont, 82 University PI. Burlington, VT 05405
- A–11 Multicatalytic, Asymmetric Michael/Stetter Reaction of Salicylaldehydes and Activated Alkynes <u>Claire M. Filloux</u>, Stephen P. Lathrop, and Tomislav Rovis* Chemistry Department, Colorado State University, Fort Collins, CO 80523
- A–12 Quantum Mechanical Investigation of the Effect of Catalyst Fluorination in the Intermolecular Asymmetric Stetter Reaction
 Joann M. Um [1], D. A. DiRocco [2], Elizabeth Noey [1], Tomislav Rovis [2],* K. N. Houk [1]*
 [1]UCLA, Los Angeles; [2]Colorado State University
- A–13 **Current Explorations of the Aza-Piancatelli Rearrangement** <u>Gesine K. Veits</u>, Donald R. Wenz, Leoni Palmer, Javier Read de Alaniz* University of California, Santa Barbara
- A–14 **Mild Generation and Reactivity of Acylnitroso Compounds** <u>Charles P. Frazier</u>, Jarred R. Engelking, Javier Read de Alaniz* Department of Chemistry & Biochemistry, University of California, Santa Barbara
- A–15 Low temperature [3,3]-sigmatropic rearrangements of benzyl alkynyl ethers: synthesis of substituted 2-indanones and indenes Armen A. Tudjarian and <u>Thomas Minehan</u>* Department of Chemistry and Biochemistry, California State University, Northridge
- A–16 **T3P®: The Green Reagent for Amide Bond Formation and Other Condensation Reactions** <u>James Schwindeman</u>*, Richard Wisdom, Juergen Brockmann Archimica, Inc., 479 Jenny Drive, Yardley, PA 19067

- A–17 Organocatalyzed Reactions for the Asymmetric Synthesis of Unnatural, Fmoc-protected Amino Acids <u>Timothy J. Peelen</u>*, Nicholas C. Boaz, Samantha J. Bowen Department of Chemistry, Lebanon Valley College, 101 N. College Ave., Annville, PA 17003
- A–18 Atropisomeric *N*-Heterocyclic Carbenes: A New Scaffold in Asymmetric Catalysis

<u>Milena Czyz</u>, Marcus L. Cole,* Jonathan C. Morris* School of Chemistry, University of New South Wales, Sydney, Australia

- A–19 Supramolecular catalysts exhibiting remarkable substrate discrimination in catalytic asymmetric hydroboration <u>Kazuya Toyama</u> and James M. Takacs* Department of Chemistry, University of Nebraska, Lincoln, Nebraska 68588-0304
- A–20 Synthesis of Carbo- and Heterocycles by 5-endo and 5-exo cyclisations <u>Wilfried Hess</u>, Jonathan W. Burton* Chemistry Research Laboratory, 12 Mansfield Road, Oxford, OX13TA, United Kingdom
- A–21 Chelation-controlled Addition of Organozinc Reagents to Silyloxy Aldehydes and Ketones
 <u>Gretchen R. Stanton</u>, Corinne N. Johnson, Meara C. Kauffman, Gamze Koz, and Patrick J. Walsh*
 Department of Chemistry, University of Pennsylvania, P. Roy and Diana T. Vagelos Laboratories, 231 S. 34th Street, Philadelphia, PA 19104-6323
- A–22 Borylative multicomponent coupling reactions and novel chemistry of polycyclic hydrocarbons <u>Hee Yeon Cho</u>, James P. Morken* and Lawrence T. Scott* Boston College, Merkert Chemistry Center, 2609 Beacon St. Rm# 013, Chestnut Hill, 02467
- A-23 Enones as Radical Precursors: Brønsted Acid Activators in Visible Light Photocatalysis Juana Du, Laura Ruiz Espelt, and Tehshik P. Yoon*
 - University of Wisconsin–Madiso
- A-24 Enantioselective Catalytic alpha-Alkylation of Aldehydes via an SN1 Mechanism

<u>Adam R. Brown</u>, Wen-Hsin Kuo, and Eric N. Jacobsen* Harvard University

A-25 Highly enantioselective synthesis of *anti* aryl β -hydroxy α -amino esters via DKR transfer hydrogenation

Zhuqing Liu,*[†] C. Scott Shultz,*[†] Candice A. Sherwood,[†] Shane Krska,[†] Peter G. Dormer,[†] Richard Desmond,[†] Claire Lee,[‡] Edward C. Sherer,^{\$} Joseph Shpungin,[%] James Cuff[‡] and Feng Xu[†]

[†]Department of Process Chemistry, Merck Research Laboratories, Rahway, New Jersey 07065, USA; [‡]Department of Analytical Chemistry, Merck Research Laboratories, Rahway, New Jersey 07065, USA; ^{\$}Chemistry Modeling and Informatics, Merck Research Laboratories, Rahway, New Jersey 07065, USA; [%]Scientific Computing, Merck Research Laboratories, Rahway, New Jersey 07065, USA

A-26 Epoxide-based synthesis of the C14–C25 bafilomycin A1 polypropionate fragment

<u>Elizabeth M. Valentín</u> and José A. Prieto, PhD Department of Chemistry, University of Puerto Rico, Río Piedras Campus, PO Box 23346, San Juan, PR 00931-3346

A-27 Computationally-Guided Stereocontrol of the Combined C—H activation/Cope Rearrangement

<u>Yajing Lian</u> and Huw M. L. Davies* Department of Chemistry, Emory University, 1515 Dickey Drive, Atlanta, Georgia, 30322

A-28 Setting Two Stereocenters in the Synthesis of a Design of a Gamma Secretase Modulator- BIIB042

Hexi Chang, John Guzowski, Corrie Hulten, <u>Michael Humora</u>,* Erwin Irdam, William Kiesman, Adam Littke, Hairuo Peng, Xianglin Shi, Tina Talreja, and Zhili Xin

Biogen Idec, 14 Cambridge Center, Cambridge, MA 02142

A–29 Studies on the mechanism, selectivity and synthetic utility of lactone reduction

<u>Dixit Parmara</u>, Kieran Pricea, Malcolm Spaina, Hiroshi Matsubarab, Paul A. Bradleyc, David J. Proctera*

(a) School of Chemistry, University of Manchester, Oxford Road, Manchester, M13 9PL, UK; (b) Department of Chemistry, Graduate School of Science, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan; (c) Pfizer Global R & D, Ramsgate Road, Sandwich, Kent, CT13 9NJ, UK.

A–30 **Directing a Sml2 radical cyclization using a C-Si bond: A Second generation approach to pestalotiopsin A and 6-epitaedolidol** Harb, H. Y.; Procter, D. J.*

School of Chemistry, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

- A–31 **A One-Pot, Asymmetric Synthesis of Highly Functionalized Cyclopentanes** <u>Brendan T. Parr</u>,¹ Zhanjie Li² and Huw M. L. Davies¹* ¹Emory University & ²Harvard University
- A–32 Exploiting reagent evolution in samarium-mediated reaction cascades: Application in a tag removal-cyclisation approach to spirooxindole scaffolds <u>S. Quenum</u>, S. C. Coote, D. J. Procter* School of Chemistry, Oxford road, University of Manchester, Manchester, M13 9PL, UK
- A–33 Catalytic asymmetric cyclopropanation An enabling technology for CNS drug development Spandan Chennamadhavuni, Josh Alford, Huw M.L. Davies* Emory University, Atlanta, GA.
- A–34 Chemistry of Complexes between N-Heterocyclic Carbenes and Boranes Andrey Solovyev, Shau-Hua Ueng, Julien Monot, Dennis P. Curran* Department of Chemistry, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
- A–35 A Novel, Mild, and Regioselective Cobalt Catalyzed Addition of Sulfides to Unactivated Alkenes V. Girijavallabhan*, Carmen Alvarez, and F. George Njoroge Merck Research Laboratories, Kenilworth, NJ
- A–36 An Iterative Approach towards Fluorous Mixture Synthesis (FMS) of 4 Isomers of 4, 8, 12-Trimethylheptadecanol with Traceless Ultra-Light Fluorous Phenylthionocarbonate Tags Edmund A.-H. Yeh, Dennis P. Curran* University of Pittsburgh, PA
- A–37 **Biomimetic C-H Activation of Nitrogen-Containing Compounds** <u>Zachary D. Aron</u>,¹ Albert Felton,¹ Mani R. Chaulagain,² Ping Fang,¹ Abraham Verdoes¹ and Alyssa Pirinelli¹ ¹Indiana University, Bloomington; ²Sabic Americas
- A–38 **The Preparation and Reactions of an Indole Containing Iminium Salt Building Block** <u>John Gupton</u>*, Nakul Telang, Peter Barelli, Kara Finzel, John Stafford and Spencer Bates Dept. of Chemistry, University of Richmond, Richmond, VA, 23173.
- A–39 Efficient synthesis of substituted furans and polyfunctional cyclopentanones via oxidation of α-diazo-β-ketoacetates <u>Phong Truong</u>, Michael Doyle* University of Maryland College Park

A–40 Enantioselective Synthesis of Siloxyallenes from Alkynoylsilanes Via Tandem Enantioselective Reduction/Brook Rearrangement and Their Subsequent Trapping by [4 + 2] Cycloaddition

<u>Yasuhiro Kondo</u>, Michiko Sasaki, Kei Takeda* Department of Synthetic Organic Chemistry, Graduate School of Medical Sciences, Hiroshima University

A-41 Direct Catalytic Asymmetric Aminoallylation of Aldehydes ? Scope, Mechanism and Application

Hong Ren, William D. Wulff* Chemistry Department, Michigan State University

A-42 [4+4] Ortho-Quinone Methide: A New Reaction Pathway

Moon Young Hur, John P. Flynn, Thiwanka B. Samarakoon, Alan Rolfe and Paul R. Hanson*

Department of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045. The University of Kansas Center for Chemical Methodologies and Library Development (KU-CMLD), 2034 Becker Drive, Shankel Structural Biology Center, West Campus, Lawrence, KS 66047.

A-43 **ROMP-Derived Oligomeric Phosphates for the Application in Facile Benzylation and Triazolation**

<u>Saqib Faisal</u>,^{a,b} Toby R. Long,^a Pradip K. Maity,^a Alan Rolfe,^a Fatima Z. Basha^b and Paul R. Hanson^{*a}

^aDepartment of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045. The University of Kansas Center for Chemical Methodologies and Library Development (KU-CMLD), 2034 Becker Drive, Shankel Structural Biology Center, West Campus, Lawrence, KS 66047. ^bH.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan.

A-44 Reaction Pairing Strategies for DOS

Joanna K. Loh, Thiwanka B. Samarakoon, Sun Young Yoon and Paul R. Hanson*

Department of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045. The University of Kansas Center for Chemical Methodologies and Library Development (KU-CMLD), 2034 Becker Drive, Shankel Structural Biology Center, West Campus, Lawrence, KS 66047.

A-45 Synthesis of Isothiazolidine 1,1-dioxide Libraries via One-Pot Transformations

<u>Naeem Asad</u>, Alan Rolfe, Thomas Painter, Conrad Santini and Paul R. Hanson* Department of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045. The University of Kansas Center for Chemical Methodologies and Library Development (KU-CMLD), 2034 Becker Drive, Shankel Structural Biology Center, West Campus, Lawrence, KS 66047.

- A–46 An Intramolecular [3+2] Cycloaddition Reaction of Azomethine Ylide Stabilized by Pyrimidine Ring Hongxiang Xie, Jinbao Xiang, Qun Dang and <u>Xu Bai</u>* The Center for Combinatorial Chemistry and Drug Discovery, The School of Pharmaceutical Sciences and The College of Chemistry, Jilin University, 1266 Fujin Road, Changchun, Jilin 130012, P. R. China
- A–47 Strategies for the Synthesis and Use of β-Stereogenic α-Keto Esters <u>Kimberly M. Steward</u> and Jeffrey S. Johnson* The University of North Carolina at Chapel Hill
- A–48 **On the Nature of the Oxidative Heterocoupling of Lithium Enolates** <u>Brian M. Casey</u> and Robert A. Flowers, II* Department of Chemistry, Lehigh University, Bethlehem, PA 18015, USA
- A–49 New chiral DMAP type catalysts based on chiral relay strategy and their application in asymmetric kinetic resolution of alcohols Jun Deng and Mukund P. Sibi* Department of Chemistry and Biochemistry, North Dakota State University, Fargo, North Dakota 58105
- A-50 Single step, regioselective synthesis of diazadioxacalix[4]arene macrocycles

<u>Alex Hymanson</u>, Nick Bizier, Jack Vernamonti and Jeffrey Katz* Department of Chemistry, Colby College, 7934 Mayflower Hill, Waterville, ME 04901

- A–51 Diastereoselective 6π-electron electrocyclic ring closures of 2-haloamidotrienes via a remote 1,6-asymmetric induction Mary C. Walton, Ryuji Hayashi†, John H. Schwab and Richard P. Hsung* Department of Chemistry and Division of Pharmaceutical Sciences, University of Wisconsin—Madison, Rennebohm Hall, 777 Highland Ave, Madison, WI, 53705
- A–52 Ring Contraction Strategy for the Practical, Scalable, Catalytic Asymmetric Synthesis of Versatile gamma-Quaternary Acylcyclopentenes <u>Allen Y. Hong</u>, Michael R. Krout, Thomas Jensen, Nathan B. Bennett, Andrew M. Harned, Brian M. Stoltz* California Institute of Technology
- A–53 Zincke Aldehydes: Complex Intermediates for the Synthesis of Strychnos Alkaloids - A Six-Step Synthesis of Strychnine David Martin, Lucas Nguyen and Chris Vanderwal* UC Irvine

A-54 Divergent Synthesis of Allenoates and Alkynoates from Stereodefined Enol Triflates

<u>Bobbi Neff</u>, Ian Crouch and Doug E. Frantz* The University of Texas at San Antonio, Department of Chemistry, San Antonio, TX 78249

A-55 Asymmetric, organocatalytic interrupted Feist-Benary reaction of tosyloxyketones

<u>Alexander Korotkov</u> and Michael Calter* Department of Chemistry, Wesleyan University, Middletown, CT, United States

- A–56 **Photoredox Catalysis: Using Visible Light to Enable Reaction Discovery** <u>Joseph W. Tucker</u>, Jagan M. R. Narayanam and Corey R. J. Stephenson* Department of Chemistry, Boston University, Boston, MA
- A–57 **Stork–Danheiser Transposition of a Seven-Membered Ring Vinylogous Ester toward Enantioenriched gamma-Quaternary Cycloheptenones** <u>Nathan Bennett</u>, Allen Y. Hong, Andrew M. Harned and Brian M. Stoltz* California Institute of Technology
- A–58 **Factors Controlling Selectivities in Wittig Rearrangements of α- and γ-Silyl Allylic Benzyl Ethers** <u>Luis M. Mori-Quiroz</u>, Edith Onyeozili and Robert E. Maleczka, Jr.* Department of Chemistry, Michigan State University
- A–59 **Dynamic Kinetic Resolution of Allylic Sulfoxides via Hydrogenation** <u>Kevin G. M. Kou</u>, Peter K. Dornan, and Vy M. Dong* Department of Chemistry, University of Toronto
- A–60 A Process for Preparing 2-(quinolin-5-yl)-4,5-disubstituted-oxazole Derivatives: Application to Initial Kilogram Scale-up of PDE4 Inhibitors <u>Timothy D. Cutarelli</u>*, Xiaoyong Fu, Mathew Maust, Timothy L. McAllister, Michael R. Reeder, Jianguo Yin, Kelvin H. Yong, Shuyi Zhang, and Man Zhu Department of Process Research, Merck & Co., Inc., Rahway, NJ
- A–61 Development of a Tandem Diels-Alder/Pauson-Khand Strategy for the Synthesis of Tetracycles Sarah J. Perlmutter, Catriona E. W. Blunt, Kevin M. Shea* Smith College, Department of Chemistry, Northampton, MA 01063
- A–62 **Development of Oppolzer-Type Intramolecular Diels-Alder Cycloadditions via Isomerizations of Allenamides** <u>John B. Feltenberger</u> and Richard P. Hsung* University of Wisconsin, Madison

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- A–63 Metathesis Reactions of β-Acyloxysulfones in Synthesis
 Kyle C. Carter, Jennifer M. Storvick, Erasmus O. Volz, Daniel J. Moser, and
 <u>Gregory W. O'Neil</u>*
 Department of Chemistry, Western Washington University, Bellingham, WA, 98225
- A–64 Visible Light-Mediated Conversion of Alcohols to Halides <u>Chunhui Dai</u>, Jagan M. R. Narayanam & Corey R. J. Stephenson* Boston University
- A–65 Visible Light Photoredox Catalysis: Mannich Reactions via C-H Functionalization David B. Freeman, Laura Furst and Corey R. J. Stephenson* Department of Chemistry, Boston University
- A–66 **The generation and reactivity of aza-oxyally cationic intermediates: aza-**[4+3] cycloaddition reactions for heterocycle synthesis Christopher S. Jeffrey,* <u>Korry L. Barnes</u>, John A. Eickhoff and <u>Christopher R.</u> <u>Carson</u> Department of Chemistry: University of Nevada, Reno 89557
- A–67 Formal Oxidative Arylation Strategy for the Synthesis of Propolisbenzofuran B Brian T. Jones and Regan J. Thomson* Department of Chemistry, Northwestern University
- A–68 **Organic Solvent-Free Preparation of Sulfones** <u>Igor R. Likhotvorik</u>*, Marlon R. Lutz Jr., and Kevin D. Boyer Regis Technologies., 8210 Austin Avenue, Morton Grove, IL 60053, USA
- A–69 Enantioselective Generation of Mesomerically-Stabilized Lithiocarbanions and Evaluation of Their Configurational Stability <u>Michiko Sasaki</u>, Tomo Takegawa, Misato Fujiwara, Hidaka Ikemoto, Kei Takeda* Department of Synthetic Organic Chemistry, Graduate School of Medical Sciences, Hiroshima University
- A-70 Can ?Free? Proton Be The Counter Cation Of Chiral Borate Anions In Absence Of Base

<u>Anil Kumar Gupta</u>, Gang Hu and William D. Wulff* Department of Chemistry, Michigan State University, East Lansing, MI 48824

A–71 Modular Synthesis of P-chirogenic PN-, PNN- and PNNP-Amino and Amidophosphines Ligands Kristian H. O. Andersson, Karin B. Lundberg and Nina Kann

Division of Organic Chemistry, Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-41296 Gothenburg, Sweden

- A–72 **Rapid Assembly Of Complex Nitrogen Heterocycles Utilizing Allenamides** <u>Andrew G. Lohse</u>, Richard P. Hsung Pharmaceutical Sciences, Division and Department of Chemistry, University of Wisconsin – Madison, Madison WI, 53705
- A-73 Cooperative Catalysis in the Enantioselective Ring Opening of Epoxides and Aziridines by Fluoride Anion

<u>Julia A. Kalow</u> and Abigail G. Doyle* Princeton University

- A–74 **Stereoselective Halocyclization** <u>Weiping Tang</u>,* Jenny B. Werness, Wei Zhang, and Wen Zhang School of Pharmacy and Department of Chemistry, University of Wisconsin, Madison, WI 53705
- A–75 New Methodology Towards α,β–unsaturation of Carboxylic Acid Gregory P. Tochtrop* and <u>Qingjiang Li</u> Department of Chemistry, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106, USA
- A–76 Urea Functionalized Bis-Salen Catalysts for Asymmetric Epoxide Opening <u>Michael J. Rodig</u>, Jongwoo Park and Sukwon Hong* Department of Chemistry, University of Florida, P.O. Box 117200, Gainesville, FL 32611-7200
- A–77 In situ phosphine oxide reduction: a catalytic Appel reaction <u>Henri A. van Kalkeren</u>, Stefan H. A. M. Leenders, Rianne A. Hommersom, Floris P. J. T. Rutjes and Floris L. van Delft* Institute for Molecules and Materials, Radboud University Nijmegen Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands

Monday – 6 June 2011 Poster Session B

- B–01 **Recent advances in intramolecular alkene carboamination reactions** <u>Dani M. Schultz</u> and John P. Wolfe* Department of Chemistry, University of Michigan, 930 N. University Ave, Ann Arbor, MI, 48109
- B–02 **Palladium-catalyzed carbenylative aminations with** *N***-tosylhydrazones** <u>Avinash Khanna</u>, Kyle Johnson, David L. Van Vranken* Department of Chemistry, University of California, Irvine, Irvine, CA 92697-2025
- B-03 Palladium-Catalyzed Carboetherification For The Synthesis Of Benzopyrans

<u>Amanda F. Ward</u> and John P. Wolfe* Department of Chemistry, University of Michigan, 930 N. University Ave, Ann Arbor, MI, 48109

B-04 Synergistic approaches to the synthesis of diverse cyclophane derivatives by Suzuki coupling, Claisen rearrangement and ring-closing metathesis as key steps

<u>Arjun S. Chavan</u> and S. Kotha* Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai-400 076 INDIA

B-05 Synthesis of Complex Molecules via Pd-catalzyed Functionalization of C(sp³)-H Bonds

<u>Gang He</u>, Yingshen Zhao and Gong Chen* Department of Chemistry, The Pennsylvania State University, University Park, PA 16802

- B-06 New Approaches to the Development of Transition Metal Catalysis Daniel W. Robbins and John F. Hartwig* Department of Chemistry, University of Illinois, Urbana-Champaign, Urbana, IL 61801
- B–07 **Towards a bioorthogonal organometallic reaction** <u>Ellen M. Sletten</u>, Carolyn R. Bertozzi* University of California, Berkeley, B84 Hildebrand Hall, Berkeley, CA 94720
- B-08 **Two Palladium-Catalyzed Syntheses of Diarylmethanes** Jason R. Schmink,*¹ Nicholas E. Leadbeater,¹ Matthew Tudge,² Gary A. Molander³

¹Department of Chemistry, University of Connecticut, Storrs, CT; ²Department of Process Research, Merck & Co., Rahway, NJ; ³Roy and Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA.

- B-09 **Ru(bpy)₃Cl₂ Photocatalyzed Reductive Cyclization of Enones** <u>Kristopher W. Randall</u>, Brandon W. Parks, Timothy J. Peelen* Department of Chemistry, Lebanon Valley College, 101 N. College Ave., Annville, PA 17003
- B-10 Construction of All-carbon Quaternary Stereogenic Center Containing Organic Building Blocks through NHC-Cu-Catalyzed Enantioselective Allylic Substitution Reactions: Use of Alkenyl-, Aryl- and Heteroarylaluminum Reagents as Effective Nucleophilic Partners Fang Gao, Yunmi Lee, Kevin P. McGrath, Kyoko Mandai and Amir Hoveyda* Department of Chemistry, Boston College, Merkert Chemistry Center, 2609 Beacon St., Chestnut Hill, MA 02467
- B-11 Pd-Catalyzed C-H Activation Reactions using Air or Oxygen as the Terminal Oxidant

<u>Kara J. Stowers</u>, Kevin C. Fortner, Melanie S. Sanford* University of Michigan, 930 N. University Ave. Ann Arbor MI, 48109

- B–12 **Ruthenium Catalyzed Eschenmoser Coupling Reaction** Syed Raziullah Hussaini,* Justin Cox, Michael L. Coffin, Halee Scott, and Lindsay C. Glicksberg Department of Chemistry and Biochemistry, The University of Tulsa, Keplinger Hall, 800 S. Tucker Dr., Tulsa, OK 74104
- B–13 Stereoselective Palladium-Catalyzed [2,3]-Stevens Rearrangement Arash Soheili and Uttam K. Tambar* UT Southwester Medical Center
- B-14 Development of a Multiligand Based System for Pd-Catalyzed C-N Cross-Coupling Reactions

<u>Brett P. Fors</u> and Stephen L. Buchwald* Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139

- B-15 Base Metal Catalysis: Mechanistic Insights and Catalyst Development with Iron and Cobalt" Jonathan M. Darmon,^{1,2} Emil Lobkovsky² and Paul Chirik^{1*} ¹Princeton University, ²Cornell University
- B-16 Optimization of a novel palladium-catalyzed cross coupling of protected thiols and aryl halides

Wager, Krista M.¹ and <u>Daniels, Matthew H.²</u>* ¹Northeastern University, Boston, MA; ²Merck Research Laboratories, Boston, MA

- B–17 Direct Synthesis of Enones via Pd-Catalyzed Aerobic α,β-Dehydrogenation of Carbonyl Compounds
 <u>Tianning Diao</u>, Shannon S. Stahl*
 Chemistry Department, UW-Madison
- B–18 **Copper-Catalyzed Oxidative Trifluoromethylation Reactions** <u>Andrew T. Parsons</u>, Todd D. Senecal, Stephen L. Buchwald* Massachusetts Institute of Technology
- B–19 Chiral Triarylcyclopropane Carboxylate Ligand for High Symmetry Dirhodium Catalyst: Design, Synthesis and Application Changming Qin, Vyacheslav Boyarskikh, Jørn H. Hansen, Djamaladdin Musaev and Huw M. L. Davies* Department of Chemistry, Emory University, 1515 Dickey Drive, Atlanta, Georgia 30322, United States
- B-20 Synthesis of imidomethyltrifluoroborates and their use in Suzuki-Miyaura cross-coupling reactions with aryl chlorides

Gary A. Molander,^{*,b} <u>Rammohan Devulapally</u>,^a Nicolas Fleury-Brégeot,^b and Dave G. Seapy^{a,*}

^aDepartment of Chemistry, Texas A&M University at Qatar, Doha, Qatar. ^bRoy and Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, United States.

B-21 Early Transition Metal Binaphtholate Complexes for Stereoselective Intermolecular Hydroamination and Hydroaminoalkylation

<u>A. L. Reznichenko</u>, T. J. Emge, H. N. Nguyen, E. G. Klauber, K. C. Hultzsch^{*} Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, New Jersey 08854-8087, USA

B-22 A Catalytic Synthesis of Conjugated Diene Esters from Stereodefined Enol Triflates

<u>Ian Crouch</u>,¹ Timothy Dreier¹ and Doug E. Frantz^{*1,2}
1. Department of Chemistry, The University of Texas at San Antonio, San Antonio, TX;
2. UTSAHSCSA, Department of Biochemistry, San Antonio, TX 78229

- B–23 **Copper Catalyzed Reductive Claisen Rearrangement** <u>Kong-Ching Wong</u>, Dr. Pauline Chiu* The Department of Chemistry, The University of Hong Kong
- B-24 **Diastereoselective Intramolecular Rhodium-Catalysed [2+2+2] and [4+2+2] Cycloisomerisation Reactions and their Application in Total Synthesis** <u>Helen J. Laidlaw</u> and P. Andrew Evans* Department of Chemistry, University of Liverpool, Liverpool, L69 7ZD, U.K.

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- B-25 Stereoselective Synthesis of Cyclopropenes Using Donor/Acceptor Carbenoid Chemistry John F. Briones and Huw M. L. Davies Emory Univ
- B-26 A Structure-Activity Study of VANOL-Boroxinate Catalyzed Asymmetric Aziridination Reactions

Yong Guan and William D. Wulff* Department of Chemistry, Michigan State University, East Lansing, MI 48824

B-27 Development of Nickel-Catalyzed Intermolecular Enoate-Alkyne [3+2] Cycloadditions

<u>Aireal Jenkins</u> and John Montgomery* University of Michigan

- B–28 Palladium-Catalyzed Asymmetric Synthesis of Allylic Fluorides <u>Matthew H. Katcher</u> and Abigail G. Doyle* Department of Chemistry, Princeton University
- B–29 Ruthenium-catalyzed asymmetric transfer hydrogenation of ketones in ethanol <u>Helena Lundberg</u>*, Hans Adolfsson Stockholm University, Sweden
- B–30 Hammett NMR Studies of Phosphinooxazoline (PHOX) Chiral Ligands in π-Allyl Palladium Catalysis

<u>Elizabeth A. Dembicer, Nathaniel C. Nelson</u>, and Richard C. Bunt* Middlebury College, Middlebury, VT 05753, USA

B-31 Nickel-Mediated Decarbonylative Cross-Coupling of Imides with Organozinc Reagents

<u>Thomas B. D. Endean</u>, Jessica M. Simmons, Valerie J. Winton, Jeffrey B. Johnson* Hope College Department of Chemistry, Holland, MI 49423

- B-32 Rhodium-Catalyzed Carbon-Carbon Bond Activation: Mechanistic Investigation and Reaction Developmen
 J. Patrick Lutz, Colin M. Rathbun, Susan M. Stevenson, <u>Jeffrey B. Johnson</u>* Hope College Department of Chemistry, Holland, MI 49423
- B-33 A General Catalytic System for the Intermolecular Hydroacylation of Terminal Alkenes with Salicyl Aldehydes <u>Max von Delius</u> and Vy M. Dong* Lash Miller Chemical Laboratories, University of Toronto, 80 St. George Street, Toronto, Canada M5S 3H6

B-34 Enantioselective synthesis of chiral lactones and lactams via rhodiumcatalysis

<u>Hasan A. Khan</u>, Vy M. Dong* Lash Miller Chemical Laboratories, University of Toronto, 80 St. George Street, Toronto, Canada M5S 3H6

- B-35 Sequential Rhodium-, Silver- and Gold-Catalyzed Reactions for the Rapid Construction of Polycyclic Compounds Hengbin Wang,¹ Justin R. Denton,² Huw M.L. Davies,^{1,*}
 1. Emory University, 2. SUNY at Buffalo
- B-36 **Chemistry in Water: Radical Coupling Reactions Using Fenton's Reagent** Jennifer L. Meyer,¹ Mark D. Naber,¹ Christopher Sears-Dundes,¹ <u>Richard P.</u> <u>Hotz</u>,^{1,*} Allan R. Pinhas² ¹Department of Chemistry, College of Mount St. Joseph, Cincinnati, OH 45233-1670 ²Department of Chemistry, University of Cincinnati, Cincinnati, OH 45221-0172
- B–37 **Silver-Catalyzed Ring-Opening Hydroamination of Cyclopropenes** <u>Diem T. H. Phan</u>, Vy M. Dong* Department of Chemistry, University of Toronto, Canada.
- B–38 **Further Developments of an Enantioselective Pd-Catalyzed Polyene Cyclization: Surprising Solvent and Ligand Effects** Daniela Lucciola and <u>Brian A. Keay</u>* Department of Chemistry, University of Calgary, Calgary, AB, Canada, T2N 1N4
- B-39 Transition Metal Catalysis: Activating CO₂, C-H, and C-O Bonds En Route to Carboxylic Acids, Biaryls, and N-Containing Heterocycles Charles S. Yeung, Vy M. Dong* Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, ON, M5S 3H6, Canada
- B–40 Rh(II)-catalyzed cascade reactions of styryl azides produce 2,3disubstituted indoles
 <u>Ke Sun</u>, Sheng Liu, Patryk M. Bec and Tom G. Driver*
 Department of Chemistry, University of Illinois at Chicago, 845 W Taylor st, Chicago, IL USA
- B–41 Rh₂(II)-Catalyzed Nitro-Group Migration Reactions: Selective Synthesis of 3-Nitroindoles from β-Nitro Styryl Azides
 Benjamin J. Stokes, <u>Sheng Liu</u>, and Tom G. Driver*
 Department of Chemistry, University of Illinois at Chicago, 845 W Taylor st, Chicago, IL USA

- B–42 Novel Strategies in Heteroatom-Directed Olefin Hydroacylation <u>Matthew M. Coulter</u> and Vy M. Dong* Department of Chemistry, University of Toronto 80 St. George Street, Toronto, Ontario, Canada M5S 3H6
- B-43 **Chiral Phosphinine and Phosphabarrelene Ligands** <u>Dana Horgen</u>, Jason Bell, Dr. Charles Garner* Baylor Department of Chemistry and Biochemistry
- B-44 Palladium-catalyzed cascade reaction for the synthesis of substituted isoindolines

<u>Florence J. Williams</u>, Elizabeth R. Jarvo* University of California, Irvine

B-45 Nickel-Catalyzed Reductive Coupling of Unactivated Alkyl Halides with Other Electrophiles

Yijing Dai, Xiaolong Yu, Fan Wu, <u>Hegui Gong</u>* Department of Chemistry, Shanghai University, 99 Shang-Da Road, Shanghai 200444, China

B-46 Transition Metal Catalysis: Preparation of Nitrogen Heterocycles and Chiral Esters

<u>Tom H. H. Hsieh</u>, Vy M. Dong* Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, ON M5S 3H6 Canada

- B–47 Synthesis and Suzuki Coupling of B/Sn Bismetallic Arenes <u>Hao Li</u>, Milton R. Smith, III, and Robert E. Maleczka, Jr.* Department of Chemistry, Michigan State University
- B-48 Accessing enatiopure and highly reactive iron and cobalt olefin hydrogenation catalysts Sebastien Monfette, Jonathan M. Darmon, Bastian M. Theis and Paul J. Chirik* Department of Chemistry, Princeton University
- B-49 **Palladium-Catalyzed Hydrogenolysis Of Secondary Amines** <u>Maria del Rosario I. Amado-Sierra</u> and Robert E. Maleczka, Jr.* Department of Chemistry, Michigan State University, East Lansing, MI 48824
- B–50 **Pyridyl and Benzoquinolyl Amine Ligands for Chromium Catalyzed Ethylene Trimerization** <u>Catherine A. Faler</u>* and Steven D. Brown ExxonMobil Chemical Company, 5200 Bayway Drive, Baytown, TX 77520

- B–51 Synthesis of Highly Functionalized Cyclohexenone Rings: Rhodium-Catalyzed 1,3-Acyloxy Migration and Subsequent [5+1] Cycloaddition
 <u>Dongxu Shu</u>,² Xiaoxun Li,¹ Min Zhang,¹ Patrick J. Robichaux,² Weiping Tang^{1,*}
 (1) The School of Pharmacy, (2) Department of Chemistry, University of Wisconsin, Madison, WI 53706-1322 (USA)
- B-52 Development of New Ir-Catalyzed Transfer Hydrogenative C-C bond forming Reactions and their Application toward Total Synthesis of (+)-Roxaticin

<u>Abbas Hassan</u>, Soo Bong Han, In Su Kim, Jason R. Zbeig, Michael J. Krische* University of Texas at Austin

- B–53 Palladium-Catalyzed β-Hydride Elimination Reactions of HX from Alkyl Halides and Pseudo Halides <u>Alex C. Bissember</u> and Gregory C. Fu* Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139 USA
- B–54 Syntheses of Diaryl[d,f][1,3]diazepines via One-pot Suzuki Coupling Followed by Direct Ring Closure With Carboxylic Acids
 Longjia Yan, Xin Che, Xu Bai and Yazhong Pei*
 The Center for Combinatorial Chemistry and Drug Discovery, The School of Pharmaceutical Sciences and The College of Chemistry, Jilin University, 1266 Fujin Road, Changchun, Jilin 130012, P. R. China
- B-55 Organoaluminum and zwitterionic effect on stereoselection in heterocyclic amines

Juliet Hahn

Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400

B-56 Exploration of Novel Rearrangements of N-Allyl Ynamides

<u>Kyle A. DeKorver</u>, Yu Zhang, Whitney L. Johnson, Yan-Shi Zhang, Andrew G. Lohse, Jun Deng, Huifang Dai, and Richard P. Hsung* Department of Chemistry and Division of Pharmaceutical Sciences, University of Wisconsin – Madison, Rennebohm Hall, 777 Highland Ave, Madison, WI 53705

B-57 Combining transition metal catalysis with enzyme catalysis for polyketide synthesis

Nadine Borduas, Peter K. Dornan, Vy M. Dong* Chemistry Department, University of Toronto

B–58 Nickel-Catalyzed Cross Coupling of Styrenyl Epoxides with Boronic Acids Daniel K. Nielsen and Abigail G. Doyle* Princeton University B-59 Development of Novel Cationic Diels-Alder Dienophiles Stabilized by Cobalt-Complexed Alkynes

Sarah A. Rothstein and Kevin M. Shea* Smith College, Department of Chemistry, Northampton, MA 01063

- B–60 High Valent Palladium Catalysis: Application in Carbon-Carbon Bond Forming Wacker Cyclization Cascades
 Bryan S. Matsuura, Allison G. Condie, Ryan C. Buff, Greg S. Karahalis and Corey R. J. Stephenson*
 Boston University Department of Chemistry, Boston, MA
- B–61 The Preparation of Chiral Amines via Asymmetric Hydrogenation Joseph A. Pignatelli and Vy M. Dong* Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6, Canada
- B-62 Nickel-catalyzed asymmetric Suzuki-Miyaura cross-couplings of γ-chloro amides

Susan Zultanski and Gregory C. Fu*

B-63 Palladium Hydroxyl-Bridged Dimers as Air and Water-Tolerant Masked Cations: Applications Toward Oxidative Transformations and Olefin Oligomerization

<u>Matthew S. Winston</u>, Paul F. Oblad, Jay A. Labinger, John E. Bercaw* California Institute of Technology

B-64 The Role of Women in the Discovery and Development of Named Organic Reactions

<u>Julie A. Olson</u> and Kevin M. Shea* Smith College, Department of Chemistry, Northampton, MA 01063

B-65 New Synthetic Methods for the Preparation of Donor-Acceptor Block Copolymers

<u>Kathy Beckner Woody</u>, David M. Collard* 901 Atlantic Drive, Atlanta GA 30332; 502-727-7553 B-66 Theory and Spectroscopy of an Incarcerated Quantum Rotor. The Infrared Spectroscopy, Inelastic Neutron Scattering and Nuclear Magnetic Resonance of H2@C60 at Cryogenic Temperatures Judy Y.-C. Chen,¹ Rangeet Bhattacharyya,² Malcolm H. Levitt,² Ronald G.

Judy Y.-C. Chen, ' Rangeet Bhattacharyya,² Malcolm H. Levitt,² Ronald G. Lawler,³ Anthony J. Horsewill,⁴ Toomas Rõõm,⁵ Zlatko Bac`ic⁶ and Nicholas J. Turro^{*1}

¹Department of Chemistry, Columbia University, New York, NY 10027, USA; ²School of Chemistry, University of Southampton, University Road, Southampton SO17 1BJ, UK; ³Department of Chemistry, Brown University, Providence, RI 02912, USA; ⁴School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK; ⁵National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, Tallinn 12618, Estonia; ⁶Department of Chemistry, New York University, New York, NY 10003, USA

B-67 Positive Heterotropic Cooperativity and Fluorescence Chemosensing for Metal Ions in Aqueous Solution Scott A. Van Arman*, Yana Hristova and Matthew Taylor

Franklin and Marshall College, Lancaster, PA

- B–68 **Computationally Inspired Diastereo- and Enantioselective Rhodium-Catalyzed Pauson-Khand Reaction at Room Temperature** <u>Paolo Ricci</u>, Mu-Hyun Baik and P. Andrew Evans Department of Chemistry, University of Liverpool, L69 7ZD, Liverpool, United Kingdom
- B–69 Synthesis of 5a,13-methano-1,3-benzoxazepino[3,2-a]indole derivatives as a new type of ultrafast photochromic switches
 Greta Ragaite, ^a Vytas Martynaitis, ^a Lukas Kontenis, ^b Mikas Vengris, ^b <u>Algirdas Sackus</u>^{*,a}
 (a) Department of Organic Chemistry, Kaunas University of Technology, Radvilenu pl. 19, LT-50254, Kaunas, Lithuania
 (b)Department of Quantum Electronics, Vilnius University, Sauletekio 10, LT-10223, Vilnius, Lithuania
- B–70 A fluorescent photoinduced electron transfer (PET) sensor for cations with a separate PET channel to suppress proton signals
 Supun Pathirana, Christopher Chu, Agnieszka Chojnowski, Brent Westcott, Maryam Alapa, Sketa Patel, Umme Habiba, Arpita Patel, Agnieszka Zieba, Matthew Rossi and Saliya de Silva*
 Department of Chemistry & Biochemistry, Montclair State University, Montclair, NJ 07043
- B-71 Molecules for Improving Charge Separation at the Organic-Inorganic Interface in Hybrid Photovoltaics

<u>Timothy A. Su</u>, Jill E. Millstone, Olivia P. Lee, Claire H. Woo, Mark S. Chen, Alan T. Yiu, Andrew C. Olson, A. Paul Alivisatos, Jean M.J. Fréchet* UC Berkeley, Lawrence Berkeley National Laboratory B-72 Novel *n*-type C₃-symmetric Discotic Materials: Synthesis, Self Assembly and Physical Properties

David Hanifi,^{1,*} Dennis Cao,^{1,2} Yue Zhang,¹ Liana M. Klivansky¹ and Yi Liu¹ (1) Lawrence Berkeley National Laboratory, Berkeley, CA; (2) Northwestern University, Evanston, IL

B-73 Mixed oxygenase-desaturase activity in carboxylic acid-directed non-heme iron catalyzed C-H oxidations

Marinus A. Bigi, Sean A. Reed, M. Christina White* University of Illinois at Urbana-Champaign

B-74 A New Approach to the Synthesis of Asymmetric Push-Pull [14]-Dehydrobenzo-annulenes

> <u>K.C. Russell</u>,* Wil Talbert, Brittany Cramer, Robert Wherle, Virginia Perleberg, Taylor Mason, Kaitlin Cahill, Elizabeth Kramer and Teddy Mcentire Department of Chemistry, Northern Kentucky University, Highland Heights, KY 41099

B-75 Synthesis of α,α-Disubstituted Allylic Aryl Amines by Rhodium Catalyzed Substitution of Tertiary Allylic Trichloroacetimidates

<u>Jeffrey S. Arnold</u> and Hien M. Nguyen* Department of Chemistry, University of Iowa

B-76 Copper and Palladium Catalyzed Amination of Arenes via C-H Functionalization

<u>Alex John</u> and Kenneth M Nicholas* Department of Chemistry & Biochemistry, Stephenson Life Sciences Research Center, 101 Stephenson Parkway, University of Oklahoma, Norman, OK – 73019

B-77 Synthesis of Organometallic Chromium Complexes as Model Systems for Conjugated Polyalkenes

<u>Jack A. Terrett</u> and Jeffrey H. Byers* Middlebury College, Middlebury VT 05753

Tuesday – 7 June 2011 Poster Session C

C-01 Optimization of *N*-benzyl-benzoxazol-2-ones as receptor antagonists of macrophage migration inhibitory factor (MIF) <u>Alissa A. Hare</u>,¹ Lin Leng,² Sunilkumar Gandavadi,¹ Xin Du2, Zoe Cournia,¹ Richard Bucala,^{2,*} William L. Jorgensen,^{1*} ¹Department of Chemistry, Yale University, New Haven, CT 06520, USA ²Department of Medicine, Yale University School of Medicine, New Haven, CT 06520-8066, USA

C-02 Discovery of MK-7655: A Beta-Lactamase Inhibitor For Combination With Primaxin.®

Timothy A. Blizzard,*¹ Helen Chen,¹ Seongkon Kim,¹ Jane Wu,¹ Candido Gude,¹ Jason Imbriglio,¹ Rena Bodner,¹ Katherine Young,² Young-Whan Park,² Aimie Ogawa,² Susan Raghoobar,² Ron Painter,² Nichelle Hairston,² Doug Wisniewski,² Sang Ho Lee,² Drew Misura,² Andrew Galgoci,² Mary Ann Powles,² Sookhee Ha,¹ Paula Fitzgerald,³ Nandini Sharma,³ Jun Lu,³ Jeff Hermes,² and Milton L. Hammond^{1,2}

Departments of ¹Medicinal Chemistry, ²Infectious Diseases, and ³Structural Biology. Merck Research Laboratories P.O. Box 2000 Rahway, NJ 07065

C-03 Novel Neurokinin 1 (NK1) Receptor Antagonists for Urge Urinary Incontinence

<u>Andrew J. Kassick</u>,^a Jinlong Jiang,^a Jianming Bao,^a Huagang Lu,^a Jonathan Young,^a Jaime Bunda,^a Peter Lin,^a David Wilson,^a Xinchun Tong,^c Song Zheng,^c Kwei-Lan C. Tsao,^b Hong Wang,^b Gary Chicchi,^b Bindhu Karanam,^c Richard Tschirret-Guth,^c Koppara Samuel,^c Donald F. Hora,^d Sanjeev Kumar,^c Maria Madeira,^c Sander G. Mills^a and Robert J. DeVita.^a

Departments of Medicinal Chemistry,^a In Vitro Pharmacology,^b Drug Metabolism,^c and Laboratory Animal Resources,^d; Merck Research Laboratories, Rahway, New Jersey 07065

C-04 Hexahydroazepinoindoles as MCH1 Antagonists

<u>Emily E. Freeman</u>^{*,1}, James Grabowski,¹ Alexander Usyatinsky,¹ Mark Hadden,¹ Dustin M. Deering,¹ Matthew D. Surman,¹ Peter R. Guzzo, Michele Luche,¹ Yuri Khmelnitsky,¹ Jean Viggers,² Sharon Cheetham²

1) AMRI, 26 Corporate Circle, PO Box 15098, Albany, NY 12212-5098 USA

2) RenaSci Consultancy Ltd, Biocity, Nottingham, NG1 1GF, UK

C-05 Phenylpyrrolidine Phenylglycineamides as Potent, Selective and Orally Bioavailable FVIIa Inhibitors

Wen Jiang, Xiaojun Zhang*, Swanee Jacutin-Porte, Yan Zou, Alexandra H. Nirschl, Jeffrey M. Bozarth, Joseph Luettgen, Alan R. Rendina, Pancras C. Wong, Ruth R. Wexler, E. Scott Priestley Bristol-Myers Squibb R&D, P.O. Box 5400, Princeton, NJ 08543

C-06 **Design and Synthesis of Discodermolide-Paclitaxel Hybrids** Amos B. Smith, III,[†]* <u>Adam T. Hoye</u>,[†] Keizo Sugawara,^{†‡} Onur Atasoylu,[†] Chia-Ping Huang Yang,[§] Susan Band Horwitz[§]

† Department of Chemistry, Monell Chemical Senses Center and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, Pennsylvania.

§ Department of Molecular Pharmacology, Albert Einstein College of Medicine, Bronx, NY

‡ Current affiliation: Astellas Pharma Inc., Tsukuba-shi, Ibaraki 305-8585, Japan

C–07 **New Applications for High Performance Dyes** <u>Kyle Brubaker</u>, Elizabeth M. Sanford*, Marco Tori and Robert Muterspaugh Hope College

- C–08 Alteration of Redox Potentials of L-Dopa in Short-Chain Peptides <u>Gillian E. Morris</u>, Laura Kavlie, and Chad D. Tatko* Calvin College
- C-09 Synthesis of Isoxazole Small Molecules That Induce Stem Cell Diferentiation Towards Cardiogenesis and Cardiac Repair

<u>Hector R. Aguilar¹</u>, Doug E. Frantz^{*1,2}, Jay Schneider³, Jamie L. Russell³, Sean C. Goetsch³

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2. The University of Texas Health Science Center at San Antonio, Department of Biochemistry, San Antonio, TX 78229

3. University of Texas Southwestern Medical Center, Department of Internal Medicine, Dallas, TX 75390

C-10 **Development of** *P. aeruginosa* **Quorum-Sensing Antagonists**

Laura C. Miller, Colleen T. O'Loughlin, Devin L. Stauff, Bonnie L. Bassler, Martin F. Semmelhack*

Princeton University
- C-11 Small-Molecule Signaling Pathways in Vibrio cholerae and Vibrio harveyi Lark J. Perez,¹ Wai-Leung Ng,² Yunzhou Wei,² Christina Kraml,³ Bonnie L. Bassler,^{2,4,*} Martin F. Semmelhack¹
 1 Department of Chemistry, Princeton University
 2 Department of Molecular Biology, Princeton University
 3 Lotus Separations LLC, Princeton
 4 Howard Hughes Medical Institute
- C-12 **Proline Editing: A General Approach To Synthesize Chemically Diverse Peptides and To Control Peptide Structure** <u>Anil K. Pandey</u>, Devan Naduthambi, Krista M. Thomas, and Neal J. Zondlo* Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716
- C–13 Identifying the Role of Aromatic Networks in Amyloid Fibril Formation and Anti-Alzheimer's Therapeutic Action Ian Robertson*, Chad Tatko Calvin College, Grand Rapids, Michigan
- C-14 **A Convergent Synthesis of a Novel Imidazolospiroketone Core** <u>Chris Limberakis</u>*, Shawn Cabral, David A. Griffith, Daniel W. Kung, Suvi T. M. Orr, and Aaron C. Smith CVMED Chemistry, Pfizer Worldwide Research and Development, Eastern Point Road, Groton, CT 06340
- C-15 **Synthesis of 4-thiophenylalanine in peptides** <u>Christina R. Ford</u> & Neal J. Zondlo* Department of Chemistry & Biochemistry, University of Delaware, Newark DE 19716
- C–16 Long-range S to N acyl migration of S-acylated cysteine containing peptides to form native peptides <u>Khanh Ha</u>*, Charles Ocampo and Aaron Lillicotch University Of Florida
- C–17 **Design of Minimal Protein Kinase-Inducible Domains for Detection of Kinase Activity** <u>Caitlin M Tressler</u>, Feng Gao, Devin Naduthambi, Blair S. Thornley and Neal Zondlo* Department of Chemistry and Biochemistry, University of Delaware, Newark DE 19702

C–18 **Discovery and Synthesis of IspF Inhibitors** <u>Timothy J. Hagen</u>,¹ Zheng Zhang,¹ Michael Clare,² Darren W. Begley,^{3,4} Robert Hartley,³ Courtney Burris,³ Bart L Staker³ and Lance J. Stewart³ ¹Northern Illinois University. ²Clare Associates LLC. ³Emerald Biostructures. ⁴Seattle Structural Genomics Center C-19 Radiosynthesis and In Vivo Evaluation of [18F]C8-Ceramide Analogues as Potential Tumor Imaging Agents

<u>Kristin Graf</u>,¹ Matthew Hellman,¹ Spiro Kavathas,¹ Stephen Dewey,¹ Wynne Schiffer,¹ Gopal Subramaniam² and Thomas Chaly^{*,1}

(1) Department of Radiochemistry, Feinstein Institute for Medical Research, Manhasset, NY

(2) Department of Chemistry, Queens College, Flushing, NY

C-20 **Design and synthesis of new pleuromutilin scaffolds for antibiotic** development

Junjia Liu, Stephen D Lotesta, Maurice A Marsini, Bedell A Thomas, Emma V Yates, Erik J Sorensen* Department of Chemistry, Princeton University

 C-21 Tandem Cross-Coupling/Electrocyclization Method to the Development of a Medicinal Chemistry Library of 3,4,5-Trisubstituted 1H-Pyrazoles David J. Babinski,¹ Hector R. Aguilar,¹ Margie DeYoung,¹ Dr. Doug Frantz^{*,1,2}
 (1) Universit of Texas at San Antonio, Department of Chemistry, San Antonio, TX, 78249
 (2) UTHSCSA, Department of Biochemistry, San Antonio, TX 78229

C–22 Synthesis and evaluation of new ChK2 kinase inhibitors. Potential adjuvants for cancers therapy Rahman Saleem, Teri Lansdell, Jetze Tepe* Department of Chemistry, Michigan State University, East Lansing, MI, 48823

C-23 **Photodimerization of a thymine derivative as a bioorganic model for the photodimerization implicated in skin cancer** <u>Juliet Hahn</u>

Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400

C-24 Discovery of a Nortropanol Derivative as a Potent and Orally Active GPR119 Agonist for Type 2 Diabetes

<u>Charles Jayne</u>*, Yan Xia, Samuel Chackalamannil, William J. Greenlee, Bernard Neustadt, Andrew Stamford, Henry Vaccaro, Xiaoying (Lucy) Xu, Hana Baker, Morgan Woods, Brian Hawes, and Tim Kowalski Merck Research Laboratories, 2015 Galloping Hill Road, Kenilworth, New Jersey 07033

C-25 Development and Application of Redox Sensors for Cellular Oxidative Stress

<u>Michael J. Scheuermann</u> and Neal J. Zondlo* Department of Chemistry and Biochemistry, University of Delaware, Newark DE 19716

C-26 Towards responsive lanthanide probes for multiplex detection in the near infrared

Johanna Laakso and <u>K. Eszter Borbas</u>* Department of Organic Chemistry, Stockholm University

- C–27 Characterization of TRIF Selectivity in the AGP Class of Lipid A Mimetics: Role of Secondary Acyl Chains <u>Khalaf, J.K.</u>; Bazin-Lee, H.; Bowen, W.S.; Ward, J.R.; Evans, J.S.; Dutta, N.; Burkhart, D.J.; Johnson, D.A.* GlaxoSmithKline Biologicals, 553 Old Corvallis Road, Hamilton, MT 59840, USA
- C–28 Cross-Couplings of Unconventional Electrophiles and Progress Toward the Total Synthesis of Welwitindolinones Kyle W. Quasdorf, Neil K. Garg* UCLA, Los Angeles, CA
- C-29 Synthesis of Leustroducsin B and Efforts Toward the Total Synthesis of Pactamycin

<u>Justin T. Malinowski</u>, Stephen N. Greszler, Jeffrey S. Johnson* University of North Carolina at Chapel Hill

C-30 Natural Products with a Twist: Towards the Synthesis of the A-B Fragment of RP-66453

<u>David J. Skinner</u>*, David C. Harrowven, Scott Twiddy, David J. Klauber[†] School of Chemistry, University of Southampton, Southampton, SO17 1BJ; [†]Chemical Science, Pharmaceutical Development, AstraZeneca Avlon Works, Bristol, BS10 7ZE

- C–31 **Synthesis and Evaluation of a Cembranoid-like Library** <u>Amanda Welford</u>, Florence Raynaud, John Caldwell, Ian Collins* Cancer Research UK Centre for Cancer Therapeutics, Institute of Cancer Research, Sutton, London UK
- C-32 **Rapid Construction of [5-6-7] Tricyclic Ring Skeleton of Calyciphylline Alkaloid Daphnilogeranin B** <u>Chen Xu</u>[†], Zheng Liu[†], Huifei Wang[†], Bo Zhang[†], Zheng Xiang[‡], Xiaojiang Hao[§]*,

<u>Chen Xu</u>⁺, Zheng Llu⁺, Hulfel Wang⁺, Bo Zhang⁺, Zheng Xiang⁺, Xiaojiang Hao^{3*}, David Zhigang Wang[†]* Shenzhen Graduate School of Peking University, [‡]Peking University, [§]Kunming Institute of Botany

C-33 Development of Tandem Processes for the Synthesis of Marine Ladder Polyether Natural Products Matthew G. Beaver and Timothy F. Jamison*

Massachusetts Institute of Technology

C–34 **Progress Towards the Total Synthesis of Citrinadins A & B** Ke Kong, <u>Genessa M. Smith</u>, John L. Wood* Department of Chemistry, Colorado State University, Fort Collins, CO 80523 C-35 **Total Synthesis of Dibromophakellin and Related Analogs** <u>Nicole Hewlett</u>, Theresa A. Lansdell, Jetze J. Tepe* Michigan State University, Department of Chemistry, East Lansing MI, 48824

C-36 The Total Syntheses of Heimiol A and Hopeahainol D, Two Resveratrol-Derived Natural Products

Jason J. Pflueger,¹ Nathan E. Wright,¹ Steven P. Breazzano^{1,2} and Scott A Snyder^{1*}

¹Columbia University, ²Scripps Research Institute

C-37 Concise, biomimetic syntheses of artemone, davanone, and related terpenoids <u>David A. Vosburg</u>,* Veerasak Srisuknimit, Eric D. Nacsa, Mary J. Van Vleet, Kanny K. Wan

Department of Chemistry, Harvey Mudd College, Claremont, CA 91711

C–38 **Formal Synthesis of Diazonamide A** <u>Cheng-Kang Mai</u>, Matthew F. Sammons, Tarek Sammakia* Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309

C–39 Studies Towards the Total Synthesis of Lancifodilactone G Sanil Sreekumar and P. Andrew Evans* Department of Chemistry, University of Liverpool

C–40 **A rapid entry to branched sugars and aminosugars** <u>Ruomeng (Cynthia) Wang</u> and Michael S. Sherburn* Research School of Chemistry, Australian National University, Canberra, ACT, Australia

C–41 **Progress toward concise, modular syntheses of endiandric acids** <u>Zara M. Seibel</u>, Laura J. Poindexter, Katerina P. Hilleke, David A. Vosburg* Department of Chemistry, Harvey Mudd College, Claremont, CA 91711

C-42 **Convergent Synthesis of the Kibdelones** John Butler, Chao Wang, and Joseph Ready* Department of Biochemistry, University of Texas Southwestern Medical Center

C–43 **Synthesis of cyclic peptide natural products** <u>Hanae Benelkebir</u>,¹ 2Marcel Jaspars,² Mostafa E. M. Rateb,² Wael E. Houssen,² Annette Hayden,³ Graham Packham,³ A. Ganesan^{1*} ¹School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK; ²Department of Chemistry, University of Aberdeen, Aberdeen, AB24 3UE, UK; ³School of Medicine, Southampton General Hospital, Southampton, SO16 6YD, UK

- C-44 **Total Syntheses of Saliniketal A, Salinisporamycin and Rifsaliniketal employing Pt(II)-catalyzed cycloisomerrization** <u>Yu Feng</u>, Jun Liu, Yazmin Carrasco, John MacMillan & Jef K. De Brabander* Department of Biochemistry, UT Southwestern Medical Center
- C-45 N-Heterocyclic Carbene Catalysis: Application to the Total Synthesis of Cephalimysin A, and the Development of Multicatalytic Cascade Reactions Stephen P. Lathrop and Tomislav Rovis Colorado State University
- C-46 **Phosphate Tether-Mediated Natural Product Synthesis** <u>Rambabu Chegondi</u>, Susanthi Jayasinghe, Phanindra Venukadasula, Soma Maitra, Christopher D. Thomas, Joshua D. Waetzig, Alan Whitehead and Paul R. Hanson* Department of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS, 66045.
- C–47 **Towards the total synthesis of muamvatin** <u>Mohammad M. Zahedi</u>, and Dale E. Ward* Department of Chemistry, University of Saskatchewan, 110 Science Place, Saskatoon, SK S7N 5C9, Canada
- C–48 **Determining the Structure of Elatenyne by Total Synthesis** <u>Bryony S. Dyson</u> and Jonathan W. Burton* Department of Chemistry, University of Oxford
- C–49 **Progress Towards the Total Synthesis of Tetrapetalone A** <u>Jennifer M. Howell</u>, Matthew W. Haley, and John L. Wood* Colorado State University, Fort Collins, CO 80523
- C–50 Scope and Limitations of a β-lodoallenolate Cyclization; Efforts Towards the Total Synthesis of Phomactin A Jennifer Ciesielski, Kevin Cariou, Dan Canterbury, Alison J. Frontier* University of Rochester, Rochester, New York, 14627

C-51 Identification of Two Unexpected Rearrangement By-Products of the Epothilone-A Derivatives Yande Huang

Analytical & Bioanalytical Development, Bristol-Myers Squibb Company, New Brunswick,

New Jersey, USA

C–52 Synthetic Studies Towards C1-C30 Fragment of Amphidinol 3 Aleksandr Grisin and P. Andrew Evans* Department of Chemistry, University of Liverpool C-53 **Progress toward the synthesis of a sesquiterpene natural product as a potential antifouling agent**

Nicholas S. Duca, Benjamin R. Eyer, <u>Jeremy D. Mason</u>, S. Shaun Murphree* Allegheny College, Meadville, PA

C–54 **Studies Towards the Total Synthesis of (–)-Irciniastatin B** <u>Chihui An</u>, Adam T. Hoye, Amos B. Smith III* Department of Chemistry, Laboratory for the Research on the Structure of Matter, and Monell Chemical Senses Center, University of Pennsylvania, Philadelphia, Pennsylvania 19104

C-55 **Studies Toward the Synthesis of (+)-Nodulisporic Acid A** Jason Melvin, Junha Jeon, Stephen Gonzales, Matthew Spafford, Amos B. Smith

|||*

Department of Chemistry, Laboratory for Research on the Structure of Matter and Monell Chemical Senses Center, University of Pennsylvania, Philadelphia, PA 19104

C-56 A short total synthesis of (±)-epimeloscine and (±)-meloscine enabled by a cascade radical annulation of a divinylcyclopropane Hanmo Zhang and Dennis P. Curran*

Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260

C–57 **Progress toward the Total Synthesis of Nakadomarin A** <u>Troy E. Reynolds</u>* and David Y. Gin Department of Molecular Pharmacology and Chemistry, Memorial Sloan–Kettering Cancer Center, New York, NY 10021

C-58 New Challenges in Indole Chemistry: The Synthesis of Indole Alkaloids by IMDAF Reaction

<u>Filip Petronijevic</u> and Peter Wipf* Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260

C–59 Efforts Toward the Total Synthesis of Pleurotin <u>Marija D. Manojlovic</u> and Peter Wipf* Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260

C-60 Scaleable formal total synthesis of dehydrogliotoxin <u>Travis C McMahon(1)*</u>, Sarah Stanley(2), Edward Kazyanskaya(2), Deborah Hung(2), John L Wood(1) (1) Colorado State University, Department of Chemistry, Fort Collins, CO 80523 USA (2) The Broad Institute, Infectious Disease Initiative, Cambridge, MA 02142 USA

C–61 **Synthesis of Sphinganines and Phytosphingosines from Chiral Aziridines** <u>Munmun Mukherjee</u> and William D. Wulff* Department of Chemistry, Michigan State University, East Lansing, MI 48824 C-62 Synthetic studies of colletoic acid as a promising therapeutic agent for metabolic syndrome

<u>Katsuhiko Mitachi</u>*, Taotao Ling and Fatima Rivas Chemical Biology and Therapeutics, St. Jude Children's Research Hospital, Memphis, Tennessee, USA 38105

C-63 **Preparation of A 4***H***-Pyrimido**[1,6-*a*]**pyrimidine Libray via A One-Pot Threecomponent Reaction**

Jinbao Xiang,^a Hanghang Li,^b Kai Yang,^a Lang Yi,^a Yongnan Xu,^b Qun Dang,^a <u>Xu</u> <u>Bai^{a,}*</u>

(a) The Center for Combinatorial Chemistry and Drug Discovery, The School of Pharmaceutical Sciences and The College of Chemistry, Jilin University, 1266 Fujin Road, Changchun, Jilin 130012, P. R. China

(b) Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang

- C–64 **[4 + 2]-Heteroannulation Strategy toward the Guanidinium Neurotoxins** <u>Michael R. Krout</u>*, Sudeep Prajapati and David Y. Gin Department of Molecular Pharmacology & Chemistry, Memorial Sloan–Kettering Cancer Center, New York, NY 10065
- C-65 [4 + 2] Heteroannulation Strategy toward the Synthesis of Polycyclic Guanidine Natural Products

<u>Sudeep Prajapati</u>*, Nicholas R. Perl, Michael R. Krout and David Y. Gin Department of Molecular Pharmacology & Chemistry, Memorial Sloan-Kettering Cancer Center, 1275 York Avenue, New York, New York 10065

C-66 Total Synthesis of Gliocladin C Enabled by Visible Light Photoredox Catalysis

Laura Furst, Jagan M. R. Narayanam and Corey R. J. Stephenson* Department of Chemistry, Boston University, Boston, MA

- C–67 **Complexity Generating Reactions Mediated by Manganese(III) Acetate** <u>Angus W.J. Logan</u>,¹ Jeremy S. Parker,² Jonathan W. Burton^{1,*} (1) University of Oxford, (2) AstraZeneca, Macclesfield
- C–68 **Total synthesis of trapoxin B and its analogues** <u>Byoungmoo Kim</u> and Vy M. Dong* Lash Miller Chemical Laboratories, University of Toronto, Toronto, Canada
- C–69 A boron-based approach to the Antimycin A family Total synthesis of (+)-Antimycin A_{1b} and related congeners Janetzko, J. and Batey R. A.* Department of Chemistry, University of Toronto, Toronto, Ontario, Canada, M5S 3H6

- C–70 **Novel Synthesis of Bis-Indole Heterocycles Including Staurosporinone** <u>Jessica Greger</u>, Nathan Bechtold, Scott Flewelling, Catherine Downey, Sarah Yoon-Miller and Erin Pelkey* Hobart and William Smith Colleges Chemistry Department
- C–71 **Progress towards the total synthesis of 6-deoxyerythronolide B** Dornan, P.K.; Borduas, N.; Hsieh, T.H.H.; Kou, K.G.M. and Dong, V.M.* Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, M5S 3H6, Canada
- C-72 Progress Toward the Total Synthesis of Virosecurinine Samantha R. Levine (1), Matthew R Medeiros (2) and John L. Wood* (1) (1) Colorado State University, Department of Chemistry, Fort Collins, Colorado, 80523-1872, United States (2) Yale University, Department of Chemistry, New Haven, Connecticut, 06520, United States
- C-73 Cascade Rearrangements of Cyclobutenones: Mechanistic insights and Applications to Total Synthesis

<u>J. P. Petrou</u>, M. Kenworthy, D. C. Harrowven* Department of Chemistry, University of Southampton, Highfield, Southampton, UK, SO17 1BJ

C-74 **Progress Towards the Total Synthesis of Maoecrystal V** <u>Kiel E. Lazarski</u>, Dennis X. Hu and Regan J. Thomson* Department of Chemistry, Northwestern University

C-75 Macrocyclic Pro-Drugs of HIV Protease Inhibitors

<u>Rachel A. Storr</u>*,^[a] Keith P. Moore,^[a] Philippe G. Nantermet,^[a] Abbas M. Walji,^[a] Theresa Williams,^[a] Michael J. Bogusky,^[b] Steve S. Carroll,^[c] Christine Burlein,^[c] Ming-Tain Lai,^[c] Jay A. Grobler,^[c] Kate Holloway,^[d] Sinoeun Touch,^[e] Daniel J. DiStefano,^[e] and Rosa I. Sanchez ^[f]

Merck Research Laboratories, West Point, PA. ^[a] Department of Medicinal Chemistry, ^[b] NMR Group, ^[c] Department of Antiviral Research, ^[d] Department of Molecular Modeling, ^[e] Department of Vaccine Basic Research, ^[f] Department of Drug Metabolism and Pharmacokinetics.

- C–76 **Nickel (II) Catalyzed Stereoselective Synthesis of α-Glycosyl Ureas** <u>Matthew J. McKay</u> and Hien M. Nguyen* Department of Chemistry, University of Iowa
- C–77 Nickel-catalyzed cross-couplings of secondary and tertiary alkyl nucleophiles with aryl halides <u>Amruta Joshi-Pangu</u>*, Mark Biscoe, Chao-Yuan Wang and Madhu Ganesh City University of New York

- C–78 Alteration of Bryonolic Acid Carbocyclic Skeleton for the Study of Novel Triterpenoid Chemopreventives Gregory P. Tochtrop* and <u>Vasily Ignatenko</u> Department of Chemistry, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106, USA
- C–79 Atom Transfer Radical Addition Mediated by Photoredox Catalysts John D. Nguyen, Joseph W. Tucker, Marlena D. Konieczynska and Corey R. J. Stephenson* Boston University Department of Chemistry, Boston, MA
- C–80 **Progress Toward Przewalskin B** <u>Kristy Tran</u> and Brian M. Stoltz* California Institute of Techonlogy, Pasadena, CA, 91125

Wednesday – 8 June 2011 Poster Session D

- D–01 **Chemical Synthesis of Thyroid Stimulating Hormone** <u>Jennifer L. Stockdill</u>,[§] Baptiste Aussedat,[§] and Samuel J. Danishefsky^{*,§,†} [§]Memorial Sloan-Kettering Cancer Center, [†]Columbia University
- D-02 Umpolung Amide Synthesis: Application to the Enantioselective Preparation of Peptides <u>Dawn M. Makley</u>, Bo Shen, Jeffrey N. Johnston* Department of Chemistry,Vanderbilt University, 7330 Stevenson Center, Station B 351822,Nashville, TN 37235
- D–03 **All-organic macrocycles for sensing and catalysis** <u>Mindy Levine</u>*, Kayla Flynn, Michael Lazar Department of Chemistry, University of Rhode Island, Kingston, RI
- D–04 Novel fluorescent derivatives of flax peptides <u>Pramodkumar D. Jadhav</u>¹, Denis P. O. Owiti², Jianheng Shen², Peta-Gaye Burnett² and Martin J.T. Reaney^{2*}
 ¹Department of Food and Bioproduct Sciences, University of Saskatchewan, 51 Campus Drive, Saskatoon, Saskatchewan, Canada S7N5A8, ²Department of Plant Sciences, University of Saskatchewan, 51 Campus Drive, Saskatoon, Saskatchewan, Canada S7N5A8
- D-05 Development of a Project-based Laboratory that Introduces Students to Drug Discovery

<u>Justin M. Kontra</u>, Brandon W. Parks, Timothy J. Peelen* Department of Chemistry, Lebanon Valley College, 101 N. College Ave., Annville, PA 17003

D-06 **Reactivity of Biarylazacyclooctynones in Copper-Free Click Chemistry** <u>Chelsea G. Gordon</u>, Joel Mackey, John C. Jewett, Ellen M. Sletten, K. N. Houk, Carolyn R. Bertozzi*

University of California, Berkeley, B84 Hildebrand Hall, Berkeley, CA 94720

D-07 Amino acid amides and hydroxamic acids as ligands for the aqueous ATHreaction

<u>Katrin Ahlford</u> and Hans Adolfsson* Department of Organic Chemistry, Stockholm University, The Arrhenius Laboratory, SE-106 91 Stockholm, Sweden

D-08 **The development of pyrrolopyrimidines as kinase inhibitors** <u>Belinda Huff</u>*, Jonathan Morris School of Chemistry, University of New South Wales, Sydney, Australia

D-09 **Design and Evaluation of Paldoxins for Treatment of Fungal Diseases of Crops**

<u>M. S. C. Pedras</u>*, Z. Minic, V. K. Sarma-Mamillapalle Department of Chemistry, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Canada

D–10 Efficient Methods for Regioselective Functionalization of 6-Substituted Furo[3,2-b]pyridines for Indole Isosteres Charles D. Beard, Ving J. Lee, Susan Swansburg, Stephen A. Waller, Kenneth J. Leavitt, L. Radu Denes, James V. Hay, John Chiarello, <u>Andrew Cottone, III</u>

Department of Chemistry, Adesis, Inc. 27 McCullough Drive, New Castle DE 19720-2080.

D–11 **Studies on the Novobiocin Coumarin Core** <u>Alison C. Donnelly</u> and Brian S. J. Blagg* The University of Kansas, Department of Medicinal Chemistry, 1251 Wescoe Hall Drive, Malott Hall 4070, Lawrence, KS 66045-7583

D–12 **Synthesis of emetine-like inhibitors of the HIF-1 pathway** <u>Jennie Hickin</u> and Keith Jones* Cancer Research UK Cancer Therapeutics Unit, Institute of Cancer Research, Sutton, UK

D-13 **Design and Synthesis of Non-benzamidine FVIIa Inhibitors**

Yan Zou, Peter W. Glunz*, Xiaojun Zhang, Wen Jiang, Indawati DeLucca, Alexandra H. Nirschl, Xuhong Cheng, Carolyn A. Weigelt, Daniel L. Cheney, Anzhi Wei, Xiao Wen, Jeffrey M. Bozarth, Diane E. Normandin, Karen S. Hartl, Alan R. Rendina, Frank A. Barbera, Joseph M. Luettgen, Randi L. Brown, Tara Peterson, Ge Zhang, Pancras C. Wong, Mark Harpel, Li Shen, Robert Knabb, Ruth R. Wexler, E. Scott Priestley Bristol-Myers Squibb R&D, P.O. Box 5400, Princeton, NJ 08543

D-14 **Rapid HATU-Mediated Solution Phase siRNA Conjugation**

<u>Jeffrey G. Aaronson</u>^{*†}, Lee J. Klein[‡], Aaron A. Momose[†], Ann M. O'Brien[‡], Anthony W. Shaw[†], Thomas J. Tucker[†], Yu Yuan[†], and David M. Tellers[†] [†]Department of Medicinal Chemistry, and [‡]Department of Pharmaceutical Analytical Chemistry, Merck Research Laboratories, Merck & Co., Inc., West Point, Pennsylvania 19486

D–15 Inhibition of Acinetobacter baumannii biofilm formation on a methacrylate polymer containing a 2-aminoimidazole subunit Lingling Peng,¹ Joseph DeSousa,¹ Zhaoming Su,¹ Bruce M. Novak,¹ Alexander A. Nevzorov,¹ Eva R. Garland² and Christian Melander^{1,2*} ¹North Carolina State University, Dept. of Chemistry, Raleigh, NC 27695; ²Agile Sciences, Inc., 840 Main Campus Dr., Lab 3550, Raleigh, NC 27606

D–16 **Synthesis of Unnatural Substrates for PikC Oxidation Studies: Exploring Macrolide Biosynthetic P450's as Biocatalysts for sp3 C-H Oxidation** <u>Solymar Negretti-Emmanuelli</u>,^a* Karoline Chiou,^b David H. Sherman^{a,b,c} and John Montgomery^{a,b}

^aDepartment of Medicinal Chemistry, ^bDepartment of Chemistry, ^cLife Sciences Institute, University of Michigan

D-17 Synthesis of Small Molecule HIV-1 Entry Inhibitors: Region III Analogs of NBD-556

Alexander W. Sun,¹ David M. Jones,¹ Akihiro Sugawara,¹ Mark A. Elban,¹ Joel R. Courter,¹ Takahiro Soeta,¹ Judith M. LaLonde,² Navid Madani,³ Amy M. Princiotto,³ Young Do Kwon,⁴ Peter D. Kwong,⁴ Arne Schön,⁵ Ernesto Freire,⁵ Joseph Sodroski³ and Amos B. Smith III¹*

¹Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA; ²Department of Chemistry, Bryn Mawr College, Bryn Mawr, PA 19010, USA;

³Department of Cancer Immunology and AIDS, Dana-Farber Cancer Institute, 44 Binney Street, Boston, MA 02115, USA; ⁴Vaccine Research Center, National Institute of Allergy and Infectious Diseases, Bethesda, MD 20892, USA; ⁵Department of Biology, The Johns Hopkins University, Baltimore, MD 21218, USA

D–18 **Design and synthesis of inhibitors of FabF, a novel antibacterial target, using a combined in silico and diversity-oriented synthesis approach.** <u>Martin Fisher</u>*, Adam Nelson*, Bruce Turnbull*, Colin Fishwick* School of chemistry, Astbury centre for structural molecular biology, University of Leeds*

D-19 Novel Methods to Functionalize Thiazolo[4,5-c]pyridines

<u>V. Girijavallabhan</u>*, Carmen Alvarez, Ashok Arasappan, Frank Bennett, Yuhua Huang, and F. George Njoroge Merck Research Laboratories, Kenilworth, NJ

D-20 Synthesis and Applications of Isotopomers of Azide, Cyanate, and Nitrile Probes for Nucleic Acids Edward E. Fenlon,* Scott H. Brewer,* Xin Sonia Gai, Anne T. Gillies, Basil A. Coutifaris, Rui Song, Jacob S. Lipkin

Department of Chemistry; Franklin & Marshall College, Lancaster, PA 17604 USA

D-21 Stereoselective Synthesis of PSI-7977: A Chiral Phosphoramidate Nucleotide Prodrug for the Treatment of HCV P. Ganapati Reddy,* Hai-Ren Zhang, Bruce S. Ross, Michael J. Sofia

Pharmasset, Inc., 303A College Rd East, Princeton, NJ 08536

D-22 Application of 3+2 dipolar cycloaddition for the synthesis of γ-secretase modulators

<u>Dmitri Pissarnitski</u>*, Zhiqiang Zhao, Zhaoning Zhu, Zhong-Yue Sun, Xianhai Huang, Theodros Asberom, David Cole, Gioconda Gallo, Hubert Josien, Hongmei Li, Murali Rajagopalan, Thomas Bara, Monica Vicarel, Ruo Xu, Xiaohong Zhu, John Clader, Lili Zhang, Lixin Song Merck Research Laboratories, 2015 Galloping Hill Road, Kenilworth, NJ, USA

- D-23 An Efficient Process for the Synthesis of a Novel LFA-1/ICAM Antagonist Douglas D. McLeod,* Albert J. DelMonte, Robert E. Waltermire, Yu Fan, Kirsten D. Gesenberg, Alan D. Braem Chemical Development, Bristol-Myers Squibb, New Brunswick, NJ, USA 08903.
- D–24 Acridinium Label Photosensitivity <u>Jonathan Grote</u>*, Joan Peart, and Thomas Spring Diagnostics R&D Organic Chemistry, Abbott Diagnostic Division, Abbott Laboratories, 100 Abbott Park Rd. Abbott Park, IL 60064-6016 USA
- D-25 Phosphate Tether-Mediated Cross Metathesis Studies in Application of Bioactive Natural Products and Analog Synthesis Susanthi Jayasinghe, James P. McParland and Paul R. Hanson* Department of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045.
- D-26 Hetero Michael Pathways to Sultam Library Synthesis

<u>Salim Javed</u>,^{a,b} Qin Zang,^a Danse Bi,^a Fatima Z. Basha^b and Paul R. Hanson^{*a} ^aDepartment of Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045. The University of Kansas Center for Chemical Methodologies and Library Development (KU-CMLD), 2034 Becker Drive, Shankel Structural Biology Center, West Campus, Lawrence, KS 66047. ^bH.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan.

- D–27 **Vinyl Sulfonamides as Versatile Synthons in Diversity-Oriented Synthesis** <u>Kyu Ok Jeon</u> and Paul R. Hanson* Department of Chemistry, 1251 Wescoe Hall Dr. University of Kansas, Lawrence, KS 66045. The Center for Chemical Methodologies and Library Development at the University of Kansas (KU-CMLD), 2034 Becker Dr. Shankel Structural Biology Center, West Campus, Lawrence, KS 66047.
- D-28 Natural Products With a Twist: Synthesis of the BOC macrocycle of RP-66453
 <u>Scott T. Twiddy</u>,*¹ David J. Skinner1 Mathew L. Jones,² Lana Nanson,¹ David Klauber,³ David C. Harrowven¹
 (1) University of Southampton, (2) Eli Lilly and (3) AstraZeneca

D-29 Cyclopropanation Reactions for Simultaneous Arming/SAR Studies of Natural Products

<u>Omar Robles</u> and Daniel Romo* Department of Chemistry, Texas A&M University, P.O. Box 30012, College Station, Texas 77842-3012

- D–30 **The Design and Construction of Novel Discretely Folded Peptoids** <u>J. Aaron Crapster</u>, Joseph R. Stringer, Ilia A. Guzei, and Helen E. Blackwell* Department of Chemistry, University of Wisconsin-Madison
- D–31 An Improved Synthesis of Phenylethynyl[1,2,4]methyltriazines and Evaluation of Novel mGluR5 Antagonists Jeremy P. Olson, Moses Gichinga, Elizabeth Butala, Hernan A. Navarro, Brian P. Gilmour and F. Ivy Carroll* Research Triangle Institute International; 3040 Cornwallis Rd, Research Triangle Park NC 27709
- D-32 Toward Eradicating HIV Reservoirs: Dimeric Prodrug Inhibitors of Pglycoprotein with Antiviral Activity

<u>Hilda A. Namanja</u>,¹ Dana Emmert,¹ David A. Davis,² Christine Hrycyna¹ and Jean Chmielewski^{*1}

(1) Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907-2084, USA. (2) HIV and AIDS Malignancy Branch, Retrovirology Disease Section, Center for Cancer Research, National Cancer Institute, Building 10, Room 6N106, NIH (National Institutes of Health), Bethesda, MD 20892, U.S.A.

D-33 A Mild Synthesis of Furans Bearing a Chiral Quaternary Carbon Substituent at the 2-Position

Satoshi Kojima,* Akihasa Iwamoto, Yoshiaki Sashihara, Aki Katori. and Yohsuke Yamamoto

Department of Chemistry, Graduate School of Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan

- D-34 Studies towards the synthesis of 3,4-epoxy alcohols as precursor for the syn-anti-syn stereotetrad using the Ireland-Claisen rearrangement <u>Alejandra Cruz Montañez</u> and José A. Prieto Department of Chemistry, University of Puerto Rico, Río Piedras Campus PO Box 23346, San Juan, PR 00931-3346
- D-35 Lithium Iodide-Catalyzed Synthesis of *N*-Propargyl Pyridones <u>Keun Ah Ryu</u> and Carolyn E. Anderson* Department of Chemistry and Biochemistry, Calvin College, Grand Rapids, MI 49546
- D–36 **Gold-Catalyzed Synthesis of Ketone-Containing N-Alkyl Pyridones** <u>Nathan A. Romero</u>, Benjamin M. Klepser, and Carolyn E. Anderson* Department of Chemistry and Biochemistry, Calvin College, Grand Rapids, MI 49546

- D-37 **Isolation, Characterization, and Application for an Unusual N-Alkenyl Pyridone** <u>Carolyn E. Anderson</u>* Department of Chemistry and Biochemistry, Calvin College, Grand Rapids, MI 49546
- D-38 **Ring opening of aziridine-2-carboxylic acid with oxalyl chloride** <u>Li Huang</u> and William D, Wulff* Michigan State University, East lansing, MI, 48824
- D–39 **Novel N-based rearrangements.** Silvana Dormi, Juliette Rivero-Castro, <u>Kolawole Ayinuola</u>, Matt Mcintosh* University of Arkansas Fayetteville, AR.
- D–40 **Formation of Boronate Ester Linked Covalent Organic Frameworks** <u>Marissa Giovino</u>, Eric Spitler, Sarah White, William Dichtel Department of Chemistry and Chemical Biology, Cornell University, Baker Laboratory, Ithaca, New York, 14853-1301
- D-41 Studies Towards the Use of Diaminocyclopropenylidenes in Umpolung and Nucleophilic Catalysis <u>M. M. D. Wilde</u>* and M. Gravel Department of Chemistry, University of Saskatchewan, Saskatoon, SK
- D-42 Are Acetylenes Electron Withdrawing Groups? Hammett Measurements and Application To Complex Macrocycle Synthesis Jeffrey L. Katz*, (a) Jay W. Wackerly, (b) Eric D. Braunstein, (a) Mengfei Zhang, (a) and Stephen M. Carlin, (a)
 (a) Department of Chemistry, Colby College, 5754 Mayflower Hill, Waterville, ME 04901; (b) Department of Chemistry, Central College, 812 University, Pella, IA 50219
- D-43 **Carbon-carbon bond formation and heterocycle syntheses using malononitrile** <u>Robert E. Sammelson</u>*, Lee Moores and Dheeptha Murali Department of Chemistry, Ball State University, Muncie, IN 47306
- D-44 Abnormal Nazarov Cyclization with Wagner Meerwein Rearrangement <u>David Leboeuf</u>, Jie Huang, Alison J. Frontier* Department of Chemistry, University of Rochester, Rochester, NY 14627
- D-45 Lithiation of Aromatic Substrates: New Methodologies <u>D. W. Slocum</u>*, Damir Kusmic, Thomas K. Reinscheld, Brian Jones, Kristen M. Clark, Erica G. Holland, and Paul E. Whitley Dept. of Chemistry, Western Kentucky University, Bowling Green, KY 42101

- D–46 **Flow Chemistry vs. Batch Chemistry: Halogen/Metal Exchange Studies** D. W. Slocum*, Damir Kusmic, Thomas K. Reinscheld, Maria A. DiLoreto, Jeffrey C. Raber[§], and Paul E. Whitley Dept. of Chemistry, Western Kentucky University, Bowling Green, KY 42101 [§]KinetiChem Inc., 19100 Von Karman Ave, Suite 400, Irvine, CA 92612
- D-47 Stereoselective Synthesis of Pyrrolidine Derivatives via Heterogeneous Hydrogenation of Substituted Pyrroles Steven Jacob, Chao Jiang, Alison J. Frontier* University of Rochester, Rochester, New York, 14627
- D-48 Sonogashira-type reactions with 5-chloro-1-phenyl-1H-pyrazole-4-carbaldehydes: a straightforward approach to pyrazolo[4,3-c]pyridines
 Gytė Vilkauskaitė, ^[a,b] Algirdas Šačkus, *^[b] and Wolfgang Holzer*^[a]
 [a] Department of Drug and Natural Product Synthesis, Faculty of Life Sciences, University of Vienna, Althanstrasse 14, A-1090 Vienna, Austria; [b] Institute of Synthetic Chemistry, Kaunas University of Technology, Radvilenu pl. 19, LT-50254 Kaunas, Lithuania
- D-49 **Conjugate Addition Initiated Nazarov Cyclization** Joshua L. Brooks, C. Rose Kennedy, Alison J. Frontier* University of Rochester, Rochester, NY 14627
- D–50 Application of Continuous Flow Operations and PAT Tools for the Synthesis of Dihydro-1H-imidazoles Ana C. Barrios Sosa,^{1*} Ryan Conway,¹ R. Thomas Williamson,¹ James P. Suchy,¹ William Edwards,¹ Jean-Michel Adam² and Thomas Cleary¹ ¹Roche, Florence, South Carolina 29506, U.S.A. ²Roche, CH-4070 Basel, Switzerland.
- D–51 **Oxidation-Initiated Nazarov Cyclization of Vinyl Alkoxyallenes** <u>Spencer, W. T</u>.; Levin, M. L.; Frontier, A. J.* University of Rochester
- D–52 Unexpected N-nitrosation-dealkylation of *N*,*N*-dialkylanilines by iodane/quartenary ammonium halide in nitromethane <u>Hima K Potturi</u>, Ras K. Gurung, and Yuqing Hou* Meyers Institute for Interdisciplinary Research in Organic and Medicinal Chemistry, Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, Illinois 62901
- D-53 Solvent-Dependent Enantiodivergent Chlorocyclization of Unsaturated Carbamates

<u>Atefeh Garzan</u>, Arvind Jaganathan, Daniel C. Whitehead, Babak Borhan* Department of Chemistry, Michigan State University, East Lansing, MI 48824, Michigan, USA, email: garzanat@msu.edu

D-54 Synthesis of 1,5-Substituted Sulfonyl Triazoles from Alkynes and Sulfonyl Azides

<u>Mitchell P. Croatt</u>,* Maria Elena Meza-Avina, Mudita Kishor Patel, Cylivia B. Lee, Thomas J. Dietz

Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC 27402

D-55 Development of a Scalable Synthesis of a Cav2.2 Blocker for Treatment of Chronic Pain

Xin Linghu^{*}, Qinghao Chen, Kevin M. Maloney, Kathleen Linn, Mark McLaughlin, Gang Qian, Lushi Tan and Paul Devine Process Research, Merck & Co., Inc. Rahway, NJ

D–56 **Progress Towards the Total Synthesis of Emetine** <u>Grant S. Buchanan</u>, Richard P. Hsung* Division of Pharmaceutical Sciences and Department of Chemistry, University of Wisconsin, Madison, WI 53705

- D–57 Synthesis of Pyrido[1,2-b]indazoles and Indazolo[3,2-a]isoquinolines via Aryne Cycloaddition
 <u>Feng Shi</u>,^{1,*} Chunrui Wu,^{1,*} Pan Li,¹ Jingjing Zhao,¹ Richard C. Larock²
 1. Henan University, Kaifeng, 475004, Henan, China; 2. Iowa State University, Ames, IA 50010, USA
- D–58 **Development and Application of a Novel "Desilylative Click" Methodology** <u>Ronald G. Brisbois</u>*, Hannah Haley and Lucas Erickson Macalester College, 1600 Grand Avenue, St. Paul, MN 55105-1899
- D-59 **Optimization of "Desilylative Click" Methodology and Application to Synthesis of 4,5'-bis-1,2,3-Triazoles** <u>Aubrey Ellison</u> and Ronald G. Brisbois* Macalester College, 1600 Grand Avenue, St. Paul, MN 55105-1899
- D–60 Direct Synthesis of Chiral pyrrolo[1,2-a]pyrazines via an Catalytic Asymmetic Intramolecular Aza-Friedel-Crafts Reaction
 Yuwei He (1), Maohui Lin(1), Zhongming Li(1), Xinting Liang(1), Guilong Li *(1), and Jon Antilla(2).
 (1)School of Chemistry and Chemical Engineering, Sun Yat-sen University, China
 (2)Department of Chemistry, University of South Florida, US
- D–61 **Cycloaddition reactions of oxazolium salts: A facile approach to nitrogencontaining heterocycles** <u>Stephen A. Habay</u>*, Corey Basch, Jameson Brinck, William Reid, John Schnoor Department of Chemistry, Henson School of Science and Technology, Salisbury University, 1101 Camden Ave., Salisbury, MD 21801

- D–62 **Phosphine-catalyzed asymmetric synthesis of trans-β-lactams** <u>Shi Chen</u> and Nessan J. Kerrigan* Department of Chemistry, Oakland University, 2200 N. Squirrel Road, Rochester, MI 48309
- D-63 **Development of Methods for the Synthesis of Natural Product-Like** Macrocycles

<u>Mark Dow</u>,¹ Adam Nelson^{1,*}, Francesco Marchetti^{1,*} and Luis-Manuel Vaz^{2,*} (1) University of Leeds and (2) AstraZeneca

D-64 Thiol Catalyzed Radical Dehalogenation with *N*-Heterocyclic Carbene Boranes

<u>Xiangcheng Pan</u> and Dennis P. Curran* Department of Chemistry, University of Pittsburgh, Pittsburgh, Pennsylvania 15260

D-65 Use of conformational bias and memory of chirality to control stereochemistry in the Lewis acid-mediated aza-Cope Mannich reaction of conformationally mobile iminium cations

<u>Micyus, T. M</u>.; Pendleton, I. M.; <u>Lindsay, H. A</u>.* Chemistry Department, Eastern Michigan University, Ypsilanti, MI, 48197

D-66 Stereoselectivity in a catalytic aza-Cope rearrangement—Mannich cyclization

<u>Pendleton, I. M</u>.; Micyus, T. M.; Lindsay, H. A.* Chemistry Department, Eastern Michigan University, Ypsilanti, MI, 48197

- D–67 Carbon-halide bond activation with HMPA <u>Kimberly A. Choquette</u>, Amanda N. Guzman, Dhandapani V. Sadasivam, Robert A. Flowers II* Department of Chemistry, Lehigh University, Bethlehem, PA
- D-68 **Preparation of 2-Substituted Indoles by Alkylation with Epoxides and Oxidation**

Brendan M. Riley, Jessica A. Hurtak, <u>C. Eric Ballard</u>* University of Tampa, Department of Chemistry, Biochemistry, and Physics, 401 West Kennedy Boulevard, Campus Box U, SA 103, Tampa, FL 33606-1490

D–69 **Catalytic Asymmetric Heterodimerization of Ketenes** <u>Ahmad A. Ibrahim</u>, Divya Nalla, Nessan J. Kerrigan* Department of Chemistry, Oakland University, 2200 N. Squirrel Road, Rochester, MI 48309

- D-70 Structure Enantioselectivity Relationship (SER) Studies of Cinchona Alkaloid Dimers in Stereoselective, Organocatalytic Chlorocyclizations Sarah E. Marshall, Daniel C. Whitehead, Roozbeh Yousefi, Arvind Jaganathan, and Babak Borhan* Department of Chemistry, Michigan State University, East Lansing, MI 48824
- D-71 Mechanistic Studies on the Asymmetric Organocatalytic Chlorolactonization <u>Roozbeh Yousefi</u>, Daniel C Whitehead, Sarah Marshal and Babak Borhan* Department of Chemistry, Michigan State University, East Lansing, MI 48824
- D-72 **Development of a Catalytic Asymmetric [4+2] Addition of Ethyl-2,3-Butadienoate with Acyclic Enones** <u>Kumar Dilip Ashtekar</u> and Babak Borhan* Department of Chemistry, Michigan State University, East Lansing, MI 48824
- D–73 Stereoselective Intermolecular Aza-[3 + 3] Annulation of Exo-cyclic Vinylogous Amides and an Unanticipated Regioselective Outcome Grant S. Buchanan, <u>Huifang Dai</u>, Richard P. Hsung* Division of Pharmaceutical Sciences and Department of Chemistry, University of Wisconsin, Madison, WI 53705
- D-74 Beta and Gamma Hydroxy Ketones via Olefin Hydroacylation <u>Murphy, S.K.;</u> Coulter, M.M.; Dong, V.M.* Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6, Canada
- D-75 Synthesis of Stereodefined Homoallylic Amines via Asymmetric Cross-Coupling of Allylic Alcohols with Imines Ming Z. Chen and Glenn C. Micalizio* The Scripps Research Institute, Scripps Florida
- D–76 **Synthetic applications of C-H insertion on sulfonyl substrates** <u>Christain S. Jungong</u>, Joseph P. Bequette, Alexei V. Novikov* Department of Chemistry, University of North Dakota, Grand Forks, ND 58202
- D-77 Development of a Scalable, One-Pot Synthesis of Fmoc-Bn-Phosphoserine, A Key Raw Material in Forigerimod Daniel E. Petrillo^{*}, Dale R. Mowrey, Shawn P. Allwein and Roger P. Bakale Chemical Process Research and Development, Cephalon, Inc., 383 Phoenixville Pike, Malvern, PA

D-78 An Improved Protocol for the Preparation of Protected (R)-2-Methylcysteine and its Use in Solution Phase Synthesis of a Glutathione Analogue Douglas S. Masterson(a)*, <u>Brant L. Kedrowski</u>(b), and Amanda Blaira(a)
 a) Department of Chemistry and Biochemistry, The University of Southern Mississippi, 118 College Drive #5043, Hattiesburg, MS 39406
 b) Department of Chemistry, University of Wisconsin Oshkosh, 800 Algoma Blvd

b) Department of Chemistry, University of Wisconsin Oshkosh, 800 Algoma Blvd., Oshkosh, WI 54901

D-79 A Tool for the Evolution of Modified DNA Aptamers: Application to HIV Glycocluster Antigen Design

Iain S. MacPherson,^{†,‡} J. Sebastian Temme,[‡] Sevan Habeshian,[‡] Krzysztof Felczak,[§] Krzysztof Pankiewicz,[§] Lizbeth Hedstrom^{†,‡*} and <u>Isaac J. Krauss</u>^{‡*} [†]Department of Biology, MS 009, Brandeis University, Waltham, MA 02454-9110 [‡]Department of Chemistry, MS 015, Brandeis University, Waltham, MA 02454-9110 [§]Center for Drug Design, University of Minnesota, Minneapolis, MN 55455

D-80 Metabolism of Lipid Peroxidation Products Using a Selective Isotope Labeling Strategy

<u>Sushabhan Sadhukhan</u>,† Yong Han,† Guo-Fang Zhang,‡ Henri Brunengraber,‡ Gregory P Tochtrop†*

Department of Chemistry⁺ and Department of Nutrition,[‡] Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106, USA

D-81 Trapping Transition States with Mechanical Force

Jeremy M. Lenhardt,¹ Mitchell T. Ong,² Robert Choe,¹ Christian Evenhuis,² James W. Ogle,¹ Todd J. Martinez,² Stephen L. Craig¹* Department of Chemistry, Duke University, Durham NC; ²Department of Chemistry, Stanford University, Stanford CA

GENERAL INFORMATION

Shuttle Buses:

The final Shuttle Bus schedule will be provided during on-site registration.

Shuttle Buses will be available between the Hyatt Regency and McCarter Theatre for the Morning and evening Oral Sessions, and between the Hyatt and Frick Hall for the evening Poster Sessions.

Shuttle Buses will be available between the Nassau Inn and Frick Hall for the evening Poster Sessions.

The Nassau Inn is a short walk from McCarter Theatre, so no Shuttle Bus service is planned. Likewise McCarter Theatre is a short (<10 minute) walk from Frick Hall. If you will need help with transportation during the NOS, please contact Tara Zarillo at (609-258-6117 or 609-258-6115).

Shuttle buses will also be provided for the planned off-site activities and for the Wednesday evening Banquet at Jadwin Gym. Please check the Shuttle Bus schedule.

A shuttle operated by the Hyatt Regency will be available for trips to downtown Princeton and the campus during the day. Please check with the Concierge about this service.

NOS Information Desk:

NOS Registration and Information Desk will be available on Sunday, June 5, 2011, from 3:00 PM – 12:00 AM in the Frick Hall Atrium located on Washington Road. On Monday – Wednesday from 7:30 AM – 1:30 PM and on Thursday from 7:30 AM – 1:00 PM there will be an NOS Information Desk in the McCarter Theater Lobby.

The NOS Information Desk will move to Frick Hall for the evening poster sessions. Representatives will be available each evening to answer questions.

If you have a question outside of the Information Desk hours, please call Conference and Event Services at 609-258-6115.

Campus Guest Cards:

Attendees (and guests) residing on campus will receive a prox card and meal card for their stay. The prox card is used to gain access to your dormitory and the meal card is for use in the dining hall. Participants who have purchased a commuter meal plan will also receive a meal card to be used in the dining hall. Lost cards can be replaced at the office of Conference and Event Services which is located at 71 University Place (next to McCarter Theater.

Restrooms:

Restrooms are located in McCarter Auditorium on the main and lower levels.

ATM's:

ATMs can be found in the WaWa convenience store (located just down the street from McCarter Theater) or in the 100 Level of the Frist Campus Center on campus.

Parking:

On campus parking is available in Lot #32. On-campus parking is free and permits will be available at the registration desk. Metered parking is also available near McCarter Theater. Lot #21 is also available for daytime parking and for parking for the poster sessions. If you are commuting each day, Lot #32 is closer to McCarter than Lot #21.

Computer Access:

Free wireless internet access is available throughout campus. The campus network can be accessed through the puvisitor wireless network.

Printing and Copying:

Triangle Printing, located at 150 Nassau Street, offers a full line of copying and printing services. Hours are Monday – Friday: 8:30 AM - 5:30 PM. Their telephone number is 609-924-4630.

Emergency Services/ Campus Safety:

In case of an emergency, call Public Safety at 609-258-1000. Public Safety will contact the fire and police departments for ambulance or rescue services. Emergency (panic) telephones are located strategically throughout the campus and in parking structures; these are recognizable by their blue lights. These phones will automatically place an emergency help call at the reported located when the button is pushed. They are visible at night by the bright blue light on the top of the poles above the phones.

Princeton Medical Center is the closest hospital and is located at 253 Witherspoon Street, Princeton, NJ. Their telephone number is 609-497-4000.

The Princeton Primary and Urgent Care facility is available for non emergiences. PPUC is located at 707 Alexander Road, Suite 201 and their telephone number is 609-919-0009.

Alcohol/Tobacco:

All conference attendees, their family or guests must adhere to all applicable state and local laws and university regulations related to the sale and use of alcoholic beverages.

- Persons under 21 years of age cannot legally possess or consume malt beverages, fermented malt liquor, or vinous or spirituous liquor. The furnishing of alcoholic beverages to under aged persons is prohibited.
- Neither person under legal drinking age nor any obviously intoxicated person shall be furnished, served, or given an alcoholic beverage.
- Alcohol cannot be consumed or carried in open containers on any street, sidewalk, alley, automobile, or public area.

Princeton University prohibits smoking in any of its buildings. This includes Residence Hall sleeping rooms and lounges, hallways, classrooms, offices, restrooms, meeting rooms, lobbies, elevators, shops, cafeterias, snack bars, waiting rooms, indoor or open-air athletic facilities and performance halls.

On-Campus Shopping:

The Princeton University Store has two locations for your shopping pleasure. The Insignia Store is located at 114-116 Nassau Street and sells official Princeton apparel and gifts. The Insignia Store is open 9:00am – 9:00pm Monday-Friday and 11:00am – 6:00pm Sundays. The PU Store,

located at 36 University Place, has a convenience store, school supplies and dorm living supplies.

Gym Access/Recreation:

Dillon Gym is available for participants of the NOS meeting. Daily passes may be purchased at registration for \$5/visit. Dillon Gym offers a fitness center, basketball courts and a swimming pool.

Gym Hours:

Summer hours TBD, will be available at NOS Information Desk Pool Hours:

Summer hours TBD, will be available at NOS Information Desk

Dining:

Conference meals included in room and board packages or commuter meal packages will be served in Wilson Dining Hall. The meal card must be presented at the dining hall; cash is not accepted. Breakfast is served from 7:00am – 10:00am; Lunch is served from 11:00am – 2:00pm and Dinner is served from 4:30pm – 7:30pm.

Guests wishing to use cash can go to the Frist Campus Center for Breakfast or Lunch. Frist is open from 8:00am – 5:00pm Monday – Friday..

Dormitory Services:

Campus guests will be provided with sheets, towels, pillow and blanket. Telephones are not provided in rooms. TV lounges are located in each building. All rooms are nonsmoking. Bunking beds is prohibited. Furniture in the common rooms and study rooms must remain in those locations; they may not be placed in individual residence rooms. To avoid climate control problems with your air conditioned room, please do not open your window, as this places strain on your unit and increases the temperature of all surrounding rooms.

Keys:

Brass keys, prox cards and meal cards will be issued to each resident. The prox card opens the exterior doors to your dormitory and the key works on your dorm room. If you lose any of these items during your stay, please contact Conference and Event Services at 609-258-6115 to get a replacement. There is a \$50 charge for lost dorm keys.

Maintenance:

If a maintenance problem or repairs are needed in your room, call 8-6115 (609-258-6115).

Fire:

Please locate the fire extinguishers and exits on your floor and be aware of the evacuation procedures posted on the inside of your room door. Always leave the building when a fire alarm sounds.

Personal Property:

Our buildings are locked 24 hours a day for your security. Please carry your prox card and room key with you at all times and lock your door when you leave the room. Keep all outside doors shut.

Princeton University assumes no responsibility and has no liability for the theft, destruction of, or loss of money, valuables, or other personal property, belonging to, or in the custody

of, the residents, whether such losses occur in the resident's room, public area, elsewhere in the hall, or in baggage handling related to shipment or storage.

Laundry Facilities/Vending:

Laundry rooms are located in each building. The washers and dryers operate free of charge.

Princeton University Attractions

Art Museum (609) 258-3788):

McCormick Hall, Princeton University

The Princeton University Art Museum houses permanent collections of African, Asian, Pre-Columbian, medieval, classical and American art, as well as European Renaissance and the baroque and impressionists styles.

The Chapel (609) 258-3047

Located behind the library, it is the largest university chapel in the world where the academic year begins and ends. It is used for services of all faiths, and contains a collection of stained glass by American artists.

FitzRandolph Gateway

Located in front of Nassau Hall, these wrought iron main gates, erected in 1905, were opened for commencement exercises. At the request of the class of 1969, they have remained open since.

Nassau Hall

Completed in 1756, Nassau Hall was the largest academic structure in the thirteen colonies. The Battle of Princeton ended when Washington captured Nassau Hall, then serving as barracks. The Hall served as Capital of the United States for six months in 1783. Its Memorial Hall commemorates the University's war dead. The faculty room, a replica of the British House of Commons, serves as a portrait gallery.

Princeton Area Attractions

Bainbridge House (609) 921-6748 - http://www.princetonhistory.org/

158 Nassau Street, Princeton

This 1766 Georgian brick house contains a museum with changing exhibits, a library and photo archives – the headquarters of the Historical Society of Princeton. Tuesday – Sunday – 12:00pm – 4:00pm

Drumthwacket (609) 921-6748 - http://www.drumthwacket.org/

Rt. 206, Princeton

This Greek Revival mansion was built circa 1834 for Charles S. Olden, Governor of New Jersey during the Civil War. Moses Taylor Pyne, the second owner, enlarged the house in the late 1890's. Now owned by the State of New Jersey, it is the official residence of the Governor. Open Wednesday, 12:00pm – 2:00pm

Morven (609) 683-4495 – historicmorven.org

55 Stockton Street, Princeton A national historic landmark, Morven was built in the 1750's by Richard Stockton, a signer of the Declaration of Independence. It served as Lord Cornwallis' headquarters, and until recently was the residence of New Jersey's governors. Wednesday, Thursday, Friday – 11:00am – 3:00pm

Tours at 11:15am, 12:15pm 1:15pm and 2:15pm

Princeton Battle Monument

Monument Drive, Princeton

Designed by Thomas Hastings, sculpted by Frederick MacMonnies, and unveiled in 1922 by President Warren Harding, it depicts General Washington on horseback, refusing defeat at the Battle of Princeton and inspiring his troops to victory.

Princeton Cemetery (609) 924-1369

Witherspoon and Wiggins Streets, Princeton Legible gravestones date back to the year 1760 includes those of Aaron Burr, Grover Cleveland, John Witherspoon, Paul Tulane, and others.

Princeton Theological Seminary (609) 921-8300 - http://www.ptsem.edu/

Mercer Street, Princeton

Established in 1812, this is the oldest and largest Presbyterian Seminary in the United States. Tours are available by appointment.

Shopping

Palmer Square

Located across from Princeton University, Palmer Square boasts a unique collection of shopping and dining right in the heart of downtown. Experience charming classical architecture mixed with contemporary elements, while you stroll along the tree lined streets. You'll find the best in apparel, shoes, jewelry, beauty, gifts, home furnishings and specialty food and drink. There are a selection of great restaurants, cafes, and artisian ice cream shops, plus The Green plays host to many seasonal events throughout the year.

Princeton Shopping Center

Located a few blocks from Princeton's Central Business District, the Princeton Shopping Center provides a unique selection of shopping, dining and services. Designed as a "California-style" mall when it opened in 1956, the Princeton Shopping Center differs from other shopping experiences in its layout and general ambiance, accounting for its popularity. Some 50 shops and restaurants, the majority of which are locally owned and operated, outline a rectangular courtyard, home to beautifully manicured floral displays and the central lawn.

PLANNED ACTIVITIES (TENTATIVE)

Sunday, June 5th

Baseball Game (1:05 PM), Trenton Thunder, Mercer County Waterfront Park, Trenton, NJ (www.trentonthunder.com/)

This AA affiliate of the NY Yankees and two-time defending league champion of the Eastern League will play their archrival, the New Hampshire "Fisher Cats." Cost - \$12 (pay in advance during online registration) Activity includes – Game Ticket and transporation Activity duration – Approximately 3 hours Departure Time - 12:00 Noon at McCarter Theatre Tour limit – 50

Princeton University Campus Walking Tour

(www.princetontourcompany.com/)

Learn about the famous students and residents that help to make Princeton the most treasured lvy League town in America. On this scenic stroll, you'll see architectural wonders on campus as well as outside the gates.

Cost - \$10 (pay in advance during online registration)

Activity duration – Approximately 2 hours

Departure Time 2:30 at McCarter Theatre

Monday, June 6th

Great Adventure & Wild Safari, Jackson Township, NJ

(http://www.sixflags.com/greatAdventure/index.aspx)

Join us for an afternoon at the Great Adventure theme park, featuring the world's tallest roller coaster "Kingda Ka" and other amazing rides.

Cost - \$28 (pay in advance during online registration)

Activity includes: Admission to park, transportation and box lunch

Departure Time – 12:00 noon at McCarter Theatre (returning at 5:30 PM) Tour Limit – 50

Princeton University Campus Walking Tour

(www.princetontourcompany.com/)

Learn about the famous students and residents that help to make Princeton the most treasured lvy League town in America. On this scenic stroll, you'll see architectural wonders on campus as well as outside the gates.

Cost - \$10 (pay in advance during online registration)

Activity Duration – Approximately 2 hours

Departure Time 2:30 at McCarter Theatre

NOS Softball Challenge – Location and time to be announced. (Please remember to bring your softball glove to the NOS!)

Kayak, Canoe Rentals (Princeton Canoe and Kayak Rental)

(<u>www.Canoenj.com/</u>) Canoe or Kayak on the Stoney Brook and Carnegie Lake. Canoe - \$14/hour Kayak – \$11-17/hour Please pay on-campus during the Symposium

Tuesday, June 7th

5K run (6:30 AM) - Location to be Announced

An enjoyable early morning run along the Delaware & Raritan Canal State Park trail, a dirt path with views along Carnegie lake and Princeton. See: <u>http://www.dandrcanal.com/natural.html</u> for a history of the D&R Canal.

Total Duration: 1.5 hours

Grounds For Sculpture – Hamilton Township, NJ

(www.groundsforsculpture.org/index.html)

The Grounds For Sculpture will take us on a guided tour of this 35-acre landscaped sculpture park, composed of works by well-known and emerging American and international artists. Cost - \$10 (pay in advance during online registration) Tour includes: Admission for guided tour, transportation and box lunch Departure Time – 1:00 at McCarter Theatre (returning at 4:00) Tour Limit – 100

Princeton University Art Museum Tour

(<u>http://artmuseum.princeton.edu/</u>) The Museum offers an impressive range of art from ancient to modern times. Cost - Free Departure Time – 3:30 at the McCarter Theatre Activity Duration – Approximately 1.5 hours Tour limit – 45

Princeton University Campus Walking Tour

(www.princetontourcompany.com/)

Learn about the famous students and residents that help to make Princeton the most treasured lvy League town in America. On this scenic stroll, you'll see architectural wonders on campus as well as outside the gates.

Cost - \$10 (pay in advance during online registration) Activity duration – Approximately 2 hours Departure Time 2:30 at McCarter Theatre

Volleyball "Tiger" Tournament – Location and time to be announced

Wednesday, June 8th

Institute Woods (Institute for Advanced Study Grounds)

(http://www.ias.edu/about/institute-grounds)

A 589-acre permanently conserved nature reserve that forms a key link in a network of green spaces in central New Jersey. Cost - Free Tour includes: Transportation Departure Time – 2:30 at McCarter Theatre Activity Duration – approximately 2 hours Activity Limit – 100

Princeton University Art Museum Tour

(<u>http://artmuseum.princeton.edu/</u>) The Museum offers an impressive range of art from ancient to modern times. Cost - Free Departure Time – 3:30 at McCarter Theatre Activity Duration – Approximately 1.5 hours Tour limit – 45

NOS Ultimate Frisbee Event - Location and time to be announced

Kayak, Canoe Rentals (Princeton Canoe and Kayak Rental)

(<u>www.Canoenj.com/</u>) Canoe or Kayak on the Stoney Brook and Carnegie Lake. Canoe - \$14/hour Kayak – \$11-17/hour Please pay on-campus during the Symposium





C. Dale Poulter EDITOR-IN-CHIEF of The Journal of Organic Chemistry

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John A. Widtsoe Distinguished Professor of Chemistry at the University of Utah

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Preeminent Researcher, Preeminent Journal.

Carolyn R. Bertozzi, the T.Z. and Irmgard Chu Distinguished Professor of Chemistry and Professor of Molecular and Cell Biology at UC Berkeley, an investigator of the Howard Hughes Medical Institute, and a member of the National Academy of Sciences, has published several articles in *JACS* including **"Rapid Cu-Free Click Chemistry with Readily Synthesized Biarylazacyclooctynones"** as featured in the March 24, 2010 issue of the journal.

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The *Journal of the American Chemical Society* is proud to sponsor Professor Bertozzi's presentation at this 42nd National Organic Symposium: "Bioorthogonal Chemistries for Glycoprofiling and Beyond."

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