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## VISIONS IN CHEMISTRY

### SYMPOSIUM

on Thursday, May 15, 2008  
at the Raritan Valley Community College  
North Branch, NJ

The **Visions in Chemistry Symposium** features speakers who are pioneers in their respective areas of expertise and whose work is considered visionary in the field of Chemistry.

#### Schedule at-a-Glance

<b>8:00 am</b>	<b>Registration and Continental Breakfast Reception</b> Raritan Valley Community College, North Branch, NJ
<b>8:45</b>	Introductory Remarks: <b>Dr. Philip Weintraub</b> , <i>Chair, Visions in Chemistry-2008</i> <b>Dr. Paul Scheuler</b> , <i>Prof. of Chemistry; Chair of Science &amp; Eng., Raritan Valley Comm. College</i> <b>Dr. James Hendrix</b> , <i>Director, CNS Medicinal Chemistry</i>
<b>9:00</b>	Speaker 1 -- <b>Professor Glenn C. Micalizio</b> , <i>Yale University</i>
<b>10:00</b>	Speaker 2 -- <b>Professor John A. Porco, Jr.</b> , <i>Boston University</i>
<b>11:00</b>	<b>Coffee Break</b>
<b>11:15</b>	Speaker 3 -- <b>Professor Dalibor Sames</b> , <i>Columbia University</i>
<b>12:15 pm</b>	<b>Lunch Break</b>
<b>2:00</b>	Speaker 4 -- <b>Professor Karl A. Scheidt</b> , <i>Northwestern University</i>
<b>3:00</b>	Speaker 5 -- <b>Professor M. Christina White</b> , <i>University of Illinois</i>
<b>4:00</b>	Closing Remarks: <b>Dr. Philip Weintraub</b>

For directions to RVCC campus: <http://www.raritanval.edu/info/directions.html>

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P R O G R A M

**8:00 – Registration and Continental Breakfast**

**8:45 – Introductory Remarks**

**9:00 – Professor Glenn C. Micalizio - *Yale University***

**“Cross-Coupling Reactions via Directed Carbmetalation:  
Development and Application”**

[ [Speaker's Bio](#) ]

**Abstract:** Professor Micalizio's laboratory is focused on the development of new reaction methodology to facilitate the synthesis of complex bioactive molecules. Over the past four years, research in his group at Yale University has targeted the development of new strategies for convergent C–C bond formation and application of these processes to complex molecule synthesis.

The Micalizio group has been deeply interested in the development of new metal-mediated coupling processes for the assembly of stereochemically dense structural motifs. Specifically, the Micalizio laboratory has discovered a number of novel titanium-mediated cross-coupling processes that enable the the following regio- and stereoselective cross-coupling reactions:

1. internal alkyne + internal alkyne and internal alkyne + terminal alkyne (for the synthesis of 1,3-dienes)
2. internal alkyne + substituted olefin (for the synthesis of allylic systems)
3. allylic alcohol + internal alkyne (for the synthesis of 1,4 dienes)
4. allenic alcohol + internal alkyne (for the synthesis of 1,4-dienes or cross-conjugated trienes)
5. aromatic imine + internal alkyne (for the synthesis of unsaturated 1,5-aminoalcohols, pyrroles and lactams)
6. aromatic imine + allenic alcohol (for the synthesis of polyunsaturated allylic amines)
7. aromatic imine + substituted olefin (for the synthesis of saturated 1,5-aminoalcohols and piperidines)
8. internal alkyne + aldehyde (for the synthesis of allylic alcohols)

In addition to the contribution of new synthetic methods, the Micalizio lab is actively involved in the efforts to demonstrate the significance of these methods in the context of target-oriented synthesis. Projects aimed at such contributions include the synthesis of polyketide-derived natural products (i.e. benzoquinone ansamycins, leptomycins, dictyostatin, jerangolid D) as well as alkaloids (sarain A and the nuphar alkaloid dimers) and terpenes (i.e. phorbacin A).

The development of these synthetic methods and application to a selection of natural product targets will be discussed in the lecture.



**10:00 – Professor John A. Porco, Jr. - *Boston University***

**“New Approaches to the Discovery of Novel Chemical  
Reactions and Chemotypes”**

[ [Speaker's Bio](#) ]

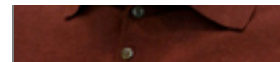
**Abstract:** Professor Porco's research is focused in two major areas: the development of new synthetic methodologies for efficient chemical synthesis of complex molecules and synthesis of complex chemical libraries. Synthetic methodologies developed in his laboratory include: copper (I)-mediated formation of enamides, oxa-electrocyclization/dimerization of dienals enroute to complex epoxyquinoid frameworks; enantioselective oxidative dearomatization using chiral copper complexes and molecular oxygen; photocycloaddition using oxidopyryliums enroute to the rocaglamides and related



natural products, and catalytic ester-amide exchange using group (IV) metal alkoxide-activator complexes. In the past six years, his research group has synthesized twenty-three complex natural product targets, including nine epoxyquinoid natural products, four salicylate enamide macrolides, the rocaglamides, and kinamycin C.

At the NIH-funded Center for Chemical Methodology and Library Development at Boston University, Professor Porco and coworkers have recently focused on approaches to identify transformations leading to complex chemotypes. Reaction development has historically been guided by problems in total synthesis or interest in developing chemical transformations of broad scope and utility. Chemical methodology development has increasingly relied on systematic evaluation of catalysts and other variables including solvent, temperature, and supporting ligands. Screening approaches have increased the efficiency of reaction development with regard to discovery of active catalysts or conditions but have generally been focused on specific transformations of interest.

An emerging but underdeveloped method for chemical reaction discovery involves high-throughput screening. A few examples have been reported in which new reactions were discovered through screening of either multicomponent systems or reaction partners and catalysts. As a part of our overall interest in the synthesis of new chemotypes and structural frameworks, we have initiated a program to identify novel chemical transformations using both “multidimensional screening” and “reaction discovery” approaches. In this approach, substrates may be reacted with various catalysts and reaction partners in an array format and analyzed for unique reaction processes. In this lecture, we will report our recent studies on this mode of reaction screening and the identification and exploration of several new transformations discovered during initial screening efforts.



#### 11:00 – Coffee Break

#### 11:15 – Professor Dalibor Sames - *Columbia University*

##### “C-H Bond Functionalization in Complex Organic Synthesis”

[ [Speaker's Bio](#) ]

**Abstract:** The possibility of direct and selective introduction of a new functionality or a new C-C bond via C-H bond functionalization has long intrigued organic chemists as it provides new strategic opportunities for the synthesis of complex organic compounds. In this lecture, I will describe the efforts in the Sames laboratory aimed at development of new catalytic transformations of both  $sp^2$  and  $sp^3$  C-H bonds. The main focus will center on C-C bond forming reactions in the context of diverse organic substrates (e.g., C-arylation of heteroarenes and saturated heterocycles, cross-coupling of alkenes and cyclic amines, electrophilic C-H/alkene coupling triggered by intramolecular hydride transfer). Both new mechanistic insights and the synthetic scope of these processes will be discussed. I will also present recent applications of the alkyne hydroarylation method (developed earlier in our group) to the synthesis of novel neuro-imaging probes, which were designed to illuminate the dopamine neurotransmission in the brain.



#### 12:15 – Lunch Break

#### 2:00 – Professor Karl A. Scheidt, - *Northwestern University*

##### “New Discoveries with Carbene Catalysis”

[ [Speaker's Bio](#) ]

**Abstract:** Professor Scheidt's research has focused on the development of new catalytic reactions and the total synthesis of molecules with important biological and structural attributes. Current methodology research in the Scheidt group involves the development of catalytic multi-component coupling processes, organosilicon chemistry, and the discovery of new catalytic reactions with N-heterocyclic carbenes (NHCs). In exploring this new field of carbene catalysis, he and his research group have discovered numerous innovative approaches to carbonyl/acyl anion equivalents, homoenolate reactivity, hydroacylations of ketones, formal [3+3] cycloadditions, Michael reactions, aldol reactions, and acylvinyl anion equivalents. The overarching theme in these investigations is the discovery of new or



unconventional reactivity modes that facilitate the synthesis of target molecules, utilize simple precursors, and produce minimal waste.

The total synthesis program in the Scheidt laboratory focuses on the construction of complex natural products containing oxygen heterocycles. Using new Lewis acid-catalyzed cyclization reactions with dioxinones, we are pursuing the synthesis of tetrahydropyran-containing natural products with anti-tumor activity. With our recent discovery of the first catalytic enantioselective synthesis of flavanones, our laboratory is engaged in the synthesis of this broad and important family of medically relevant compounds. This presentation will present our recent exciting discoveries of new chemical reactions using carbene catalysis and highlight our recent successful total synthesis endeavors.



### 3:00 – Professor M. Christina White - *University of Illinois*

#### “Streamlining Synthesis via C—H Oxidation”

[ [Speaker's Bio](#) ]

**Speaker's Bio:** M. Christina White was born in Athens, Greece where she lived until the age of five. She received her undergraduate degree in biochemistry at Smith College, where she worked with Professor Stuart Rosenfeld in the area of host-guest chemistry. After a brief stint in the biology graduate program at Johns Hopkins University working with Professor Christian Anfinsen, she began her doctoral studies in chemistry under the direction of Professor Gary Posner. During that time, she initiated the hybrid Vitamin D3 analog program in his group.

In 1999, she joined Professor Eric Jacobsen's labs at Harvard University as an NIH postdoctoral fellow. During this time, she developed the first synthetically useful methane monooxygenase (MMO) mimic system for catalytic epoxidations with hydrogen peroxide. Christina began her independent career as a member of the chemistry faculty at Harvard University in July of 2002. She joined the department of chemistry at the University of Illinois in the summer of 2005, where she is currently an Assistant Professor of Chemistry. Her group's research interests center around the development of highly selective C—H functionalization methods for streamlining the process of complex molecule synthesis.

She has received numerous awards including the Camille and Henry Dreyfus New Faculty Award (2002), the NSF CAREER Award (2006), the Eli Lilly Grantee Award (2007), the Alfred P. Sloan Research Fellowship (2008), the BMS Unrestricted “Freedom to Discover” Grant (2008), the Pfizer Award for Creativity in Organic Chemistry (2008), Amgen Young Investigator Award (2008), Boehringer Ingelheim Pharmaceuticals New Investigator Award (2008).



**Abstract:** Although it has been well demonstrated that given ample time and resources, highly complex molecules can be synthesized in the laboratory, too often current methods do not allow chemists to match the efficiency achieved in Nature. The discovery and development of highly selective C—H oxidation methods, similar to those found in Nature, for the direct installation of oxygen and nitrogen functionalities into allylic and aliphatic C—H bonds of complex molecules and their intermediates will be presented. Unlike Nature which uses elaborate enzyme active sites, we rely on the subtle electronic and steric interactions between C—H bonds and small molecule transition metal complexes to achieve high selectivities. Our current understanding of these interactions gained through preliminary mechanistic studies will be discussed. Novel strategies for streamlining the process of complex molecule synthesis enabled by these methods will be presented.

### 4:00 – Closing Remarks



## Registration

**Please Note:** There is no fee for this event, thanks to the generosity of our sponsor, sanofi-aventis. The Symposium will

include a continental breakfast, luncheon, and refreshment break. If you have any questions related to the 2008 Visions in Chemistry Symposium, please contact Bao-Guo Huang at 908-231-3828 or [Bao-Guo.Huang@sanofi-aventis.com](mailto:Bao-Guo.Huang@sanofi-aventis.com)

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