CINTACS



Newsletter of the Cincinnati Section of the American Chemical Society

December, 2007 Vol. 45, No. 3

Meeting Calendar

Dec. 11	M. Platz, Ohio State U. @ Xavier University
Jan. 16	Chemist of the Year @ Sharonville Conv. Ctr.

Feb. 20	H. Bungay, R.P.I.
	@ Museum Center

Mar. 19	Zymurgy (Beer Brewing)
	@ Great Wolf Lodge
	(Joint w. Dayton section)

Apr. 16	Awards Night	
	@ Northern Kentucky U.	

May (?) Party Night: Reds Game

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December Meeting: Xavier University December 11, 2007

Sponsored by the Department of Chemistry, Xavier University



Speaker: Prof. Matt Platz, Ohio State University

"Making the Blood Supply Safer by Applications of Physical Organic Chemistry – Sterilizing Blood Products with Riboflavin and Light"

Abstract: In the developed world, blood products used in transfusion medicine undergo a battery of tests to probe for the presence of pathogens. These tests can eliminate blood from donors with characterized disease markers. These tests can only determine the presence of known pathogens. The emergence of a new pathogen is a potential challenge to the safety of the blood supply. This lecture will trace the development of technology to eradicate pathogens in blood products using riboflavin and light. The advantages of this technology relative to competing pathogen reduction technologies will also be discussed.

THE CINTACS NEWSLETTER

Vol. 45, No. 3 December, 2007

Editor.....Kevin Ashley Advertising....Ed Hunter

CINTACS is published eight times a year (September through May) by the Cincinnati Section of the American Chemical Society. The submission deadline will be approximately December 10 for the January 2008 issue. Electronic submission is strongly preferred. All materials should be sent to:

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From the Chair

We welcome members of the National Society for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) to our joint meeting on December 11 at Xavier University. Our meeting has a busy agenda with two discussion group talks in addition to our after dinner speaker, Professor Matt Platz. Matt is Distinguished University Professor and Vice Provost at Ohio State University. Matt graciously agreed to an Organic Discussion Section talk ("Ultrafast Studies of Reactive Intermediates") in addition to the after dinner talk about making the blood supply safer by applications of physical organic chemistry principles ("Sterilizing Blood Products with Riboflavin and Light"). Matt is an excellent speaker (winner of the OSU outstanding teacher award) and makes even complex problems comprehensible. Stefan Paula from NKU is the Biochemistry Discussion Group speaker and he will discuss the application of computational modeling in his talk on "Virtual Screening for Novel Calcium ATPase Inhibitors by Computational Modeling". Thanks to XU and Dan McLouglin for sponsoring this meeting and for assisting with the venue arrangements.

September and October were busy for the section. Our September picnic at Germania Park was fun as usual. Thanks again to our picnic meeting sponsor and 55-year ACS member, Frank Diehl. October's activities began with the Chemical Educator discussion group led by Linda Ford. A Science Café, organized by the Center for Chemical Education, was held at Miami University Middletown on October 6. Bill Carroll, former National ACS president, was the headline speaker along with several chemists from the area who presented a broad range of chemistry. About 80 chemists, teachers and other interested people discussed the current contributions and the exciting challenges of professional chemistry.

On October 19-20, the Oesper Symposium was held at UC in honor of James Collman of Stanford University. Many thanks to UC for co-sponsoring the event and to Kim Carey for meeting logistics, Heather Trenary for the poster session, Jeff Seeley for the Award plaque, and Mike Baldwin and Roger Parker for representing UC and the Local ACS, respectively.

The following week was National Chemistry Week and Victor Arredondo once again deserves kudos for organizing an outstanding outreach event that connects with numerous young folks around Cincinnati and Northern Kentucky. The theme was, "The Many Faces of Chemistry", and thousands of people attended the presentations at 46 venues.

I am delighted to report that the ACS Undergraduate Programs Office has recognized two local Student Affiliates chapters with awards for their accomplishments. The NKU affiliates won a "Commendable" award and the Xavier affiliate an "Honorable Mention" Award. Congratulations to all the students involved and their faculty advisors, Keith Walters and Heather Bullen at NKU and Barbara Hopkins at Xavier. The Alchemyst club at Xavier supported NCW with demos outside the chemistry building and at local preschools, judged local science fairs, and supported student attendance at ACS meetings.

(Continued on Page 5)

December Monthly Meeting Tuesday, December 11, 2007 Conaton Board Room, Room 201 Schmidt Hall Xavier University

Joint meeting with The National Society for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE)

Featured Speaker Professor Matt Platz, Ohio State University

Program: 5:15 – 6:15	Organic Chemistry Discussion Group Matt Platz, "Ultrafast studies of reactive intermediates" (Albers Hall Room 107)
	Biochemistry Discussion Group Stefan Paula, "Virtual screening for novel calcium ATPase inhibitors by computational docking" (Logan Hall [Chemistry Building] Room 105)
5:30 - 7:00	Registration, Conaton Board Room, 2 nd Floor, Schmidt Hall
6:00 - 7:00	Social (Cash Bar), Conaton Board Room
7:00 – 8:00	Dinner, Conaton Board Room (\$20.00 or \$10.00 for students, emeritus, unemployed & new mem bers). Menu: Pan Seared Chicken Breast with Hunter Sauce, Garden Greens Salad with Italian Vinaigrette, Wild Rice Pilaf, Fresh Seasonal Vegetable Medley, Fresh Baked Bread, Chocolate Mousse with Raspberry Sauce, Whipped Cream and Chocolate Shavings, Coffee, Tea. Vegetarian entrée available upon request when making reservations.
8:00 – 9:00	Speaker, Prof. Matt Platz: "Making the Blood Supply Safer by Applications of Physical Organic Chemistry – Sterilizing Blood Products with Riboflavin and Light"

Directions to Meeting Venue:

The Xavier University Conaton Presidential Board Room is located on the second floor of Schmidt Hall. Parking is provided free with the enclosed Parking Pass (see page 4, bottom) at the F&W Center on Dana Avenue across the street from Schmidt Hall.

- **I-71**: Exit at Dana Avenue exit. Proceed west on Dana Avenue past Ledgewood Drive. As the road begins a slight turn, the F&W parking area will be on the left before you reach Victory Parkway.
- **I-75**: Exit at Mitchell Avenue. Proceed east on Mitchell Avenue, crossing over Reading Road. Continue to Dana Avenue and turn left. Just after crossing Victory Parkway, the entrance to F&W parking area will be on the right.
- **Rt. 562**: Exit the Norwood Lateral at Reading Road. Continue in the left lane of Reading Road to Victory Parkway. Merge left onto Victory Parkway at the light. Continue to Dana Avenue. Turn left onto Dana Avenue. The entrance to F&W parking area will be on the right in about half a block.

Discussion groups – There will be the following two discussion group sessions:

Organic (details on this page) and Biochemistry (details on next page)

Organic Discussion Group:
Matt Platz, Ohio State University
Ultrafast time-resolved studies of reactive intermediates
Dec. 11, 2007, 5:15 PM, Albers Hall Room 107

Abstract: It is now possible to study the photophysics and photochemistry of diazo compounds, diazirines and azides with femtosecond time resolved UV-Vis and Ir methods. This technology can be used to directly observe the excited states of the aforementioned compounds and monitor their fragmentation to form singlet carbenes and nitrenes. The carbene and nitrene species are typically formed with excess vibrational energy. We will report the kinetics of vibrational cooling of the intermediates, chemistry performed by the hot intermediates, and the rates at which either hot or relaxed species undergo solvation, reaction with solvent, intersystem crossing and rearrangement.



About the speaker: Dr. Matt Platz, a Distinguished University Professor at Ohio State University, earned his Ph.D. at Yale in 1977 in Organic Chemistry. After a postdoctoral fellowship at the University of Chicago, Prof. Platz joined Ohio State in 1978. A nationally recognized scholar, Dr. Platz is a recipient of Ohio State's Distinguished Scholar Award, and the Outstanding Teaching Award of the College of Arts and Sciences. He has also been honored with an array of national awards that include a Camille and Henry Dreyfus Teacher-Scholar Award, the American Chemical Society's Cope Scholar Award, and being named to three prestigious lectureships: the Gustafson Lectureship at the University of Denver, the Berson Lectureship at Yale University, and the Ingersoll Lectureship at Vanderbilt University. Throughout his distinguished career, Dr. Platz has authored nearly 300 peer reviewed publications, and he has presented more than 170 invited lectures. He has mentored more than 30 master's degree students, 30 doctoral students, and 20 postdoctoral students, and is an inventor who holds 10 U.S. patents. Dr. Platz is also Vice Provost for Academic Policy and Faculty Resources and was recently appointed Interim Dean of the College of Mathematics and Physical Sciences.

XAVIER UNIVERSITY

Conaton Presidential Board Room Second floor Schmidt Hall

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December 11, 2007

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Biochemistry Discussion Group:

Dr. Stefan Paula, Northern Kentucky University

"Virtual screening for novel calcium ATPase inhibitors by computational docking"

December 11, 2007 @ 5:15 PM, Logan Hall (Chemistry Building) Room 105

Abstract: The sarco/endoplasmic reticulum ATPase (SERCA) is a transmembrane enzyme that utilizes the energy gained by the hydrolysis of ATP to transport calcium ions from the cytosol into intracellular calcium stores. The ion transport activity of SERCA can be



inhibited by a variety of molecules such as derivatives of thapsigargin or of the small molecule 2,5-di-tert-butyl hydroquinone (BHQ). Recently, SERCA has been identified as a potential drug target for anticancer drugs which has spawned widespread interest in the development of novel inhibitors of the enzyme. We have measured the inhibitory potencies of 21 BHQ analogues in ATPase activity assays and compared them to binding affinities predicted by computational docking based on the X-ray crystal structure of SERCA. The results showed a reasonable correlation between predicted and experimental potencies, suggesting that docking could be used for the virtual high throughput screening of large compound libraries for new SERCA inhibitors. So far, a preliminary screen of a compound library (250,000 molecules) maintained by the National Cancer Institute followed by experimental testing of the 20 top-ranked compounds resulted in the identification of six novel SERCA inhibitors.

About the Discussion Group Leader: Dr. Paula received his Diploma in Chemistry from the University of Kaiserslautern, Germany, in 1992. After spending a year as a Fullbright Fellow at the University of California at Davis, he moved to UC Santa Cruz where he received his Ph.D. in 1998. After postdoctoral appointments at the Max Planck Institute for Biochemistry in Munich and at the University of Cincinnati College of Medicine, he joined the faculty at Northern Kentucky University in 2004. The primary goal of Dr. Paula's research is the study of ligand/receptor interactions on the molecular level using a combination of experimental and computational approaches.

(Continued from Page 2)

The NKU affiliate participated in similar activities and had a few other unique events such as an oncampus Human Periodic Table in celebration of Mole Day, and a Pie-in-the-Face fundraising contest (where students have the pie part and faculty have the face part). It's on the web and worth watching!

At our January meeting at the Sharonville Convention Center, we will honor the Cincinnati Chemist of the Year and Research Associate of the Year (be sure to get your nominations in ASAP; see p. 15!). In addition, Tina Engel will conduct a Women Chemists Workshop on communication styles. This topic will be of interest to women and men alike ... everyone is welcome!

-John Janusz

UC and NKU Chemistry Professors Visit District Offices of Kentucky United States Senators

On September 14, members of the ACS Cincinnati Local Section visited the Northern Kentucky offices of the two Kentucky U.S. senators to advocate for funding of physical-science research and K-12 science education.



Pictured left to right: Prof. Allan Pinhas, U. of Cincinnati; Prof. Joel Shulman, U. of Cincinnati; Kentucky Senator Jim Bunning; and Prof. Diana McGill, Northern Kentucky University.

Representing the Section were Diana McGill, Chair of the Northern Kentucky University Department of Chemistry; Allan Pinhas of the University of Cincinnati and a Kentucky resident; and Joel Shulman of the University of Cincinnati and Chair of the Section's Government Relations Committee. They visited with the Northern Kentucky staff of Senator Mitch McConnell and with Senator Jim Bunning himself.

The key point of discussion was the *America COMPETES Act*, which was signed into law in August and which authorizes significant funding increases for research programs at the National Science Foundation, National Institute of Standards and Technology, and the Department of Energy Office of Science. This Act places these agencies on a path to double their funding in the next 5-7 years.

However, *authorization* is different from *appropriation*. Section members urged the senators to vote to provide the authorized funding for the above agencies when the appropriation bill comes to the floor of the Senate.

In addition, the group discussed the importance of the Math and Science Partnership programs at the National Science Foundation and the Department of Education. Both visits elicited general support for our requests. Senator Bunning commented specifically that having a strong foundation in math and science education is critically important for both Kentucky and the entire nation.

ACS Cincinnati Section Committee Chairs / Discussion Groups, 2007-2008

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(ACS Cincinnati Section: Committee Chairs / Discussion Groups, 2007-2008, cont'd.)

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(ACS Cincinnati Section: Committee Chairs / Discussion Groups, 2007-2008, cont'd.)

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(ACS Cincinnati Section: Committee Chairs / Discussion Groups, 2007-2008, cont'd.)

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Xavier University Meeting

Dan McLoughlin

Xavier University

Dan McLoughlin

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Department of Chemistry 3800 Victory Parkway Cincinnati, OH 45207-4221

Younger Chemists Sean Conklin conklinsd@hotmail.com

Sponsors for the 2007-2008 ACS Cincinnati Section Program Year

Here is the listing of the sponsors for the eight monthly Cincinnati ACS meetings in the 2007-2008 program year:

September: Frank Diehl

October: University of Cincinnati, Department

of Chemistry

December: Xavier University, Department of

Chemistry
January: Ted J. Logan

February: Givaudan Flavors

March: Advanced Testing Laboratory, Inc.

April: Procter & Gamble Company

May: Girindus America, Inc.

These companies, universities and individuals have recognized the importance of a strong Cincinnati Section program and have generously contributed money to help the section increase the value of its programs to all ACS members.

These donors will be recognized at their sponsored meeting and in the monthly meeting announcement in each of the 2007-2008 issues of

the CINTACS newsletter.

Ted J. Logan, Chair Sponsorship Solicitations Committee Cincinnati Section, ACS

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Nominations for Outstanding H.S. Chemistry Teacher

Please submit a nomination of your outstanding High School chemistry teacher! They will be considered for both local recognition and for the 2008 "ACS Division of Chemical Education Central Region Award for Excellence in High School Teaching." The latter award consists of \$1,000 plus reasonable expenses (registration, lodging, etc.) to attend the Regional ACS meeting in Columbus OH June 10-14.

The nomination form and instructions can be found on the website (www.cermacs2008.org). Don't delay, submissions (electronic or hardcopy) are due by 31-Dec., 2007. Copy Dr. Jeff Seeley (seeley.ja@pg.com; P&G, SWIC; 11511 Reed Hartman Hwy; Cincinnati OH 45242) on your nomination.



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CERMACS 2008 to be held in Columbus in June

The 40th Central Regional Meeting (CERM) of the American Chemical Society will be hosted by the nearby Columbus Section in June of next year. The meeting will be held in the Hyatt Regency Columbus from the evening of June 10th to the 14th, 2008.

Details of the meeting can be found on the conference website (http://www.cermacs2008.org), which will be updated regularly as plans develop. In addition to an outstanding core scientific program, there will also be a focus on education and selected industry/business topics. Suggestions or questions can be e-mailed to cermacs2008@chemistry.ohiostate.edu.

On behalf of the Organizing Committee, I invite you to mark your calendars now in anticipation of an outstanding meeting.

Regards,

Jimmy Cowan General Chair, CERMACS 2008

Visit the ACS Cincinnati Section On-line:

www.acscincinnati.org



Science Café Serves Up Science and Chemistry Careers

On Saturday October, 6, 2007, Bill Carroll, Vice President of Occidental Petroleum Corporation and former National ACS president, headlined a Science Café style event in the Community Center at Miami University Middletown. About 80 chemists, science teachers, and interested people in the tristate area of southwest Ohio, northern Kentucky and Indiana attended. Bill Carroll's presentation titled "The Evolving Chemistry Enterprise: "Nontraditional" Jobs, Nontraditional Approaches" presented a global view of chemistry and the unique opportunities for chemists and students willing to engage unique challenges. Bill's presentation was followed by an active question and answer period.

Bill Carrolls's inspiring presentation set the tone for lively presentations from local chemists in the tristate area. Ed VonBargen described some of Procter and Gamble's projects. Gloria Story described how infrared spectroscopy and thermal imaging supports consumer products research at Procter and Gamble. The audience was charmed with the pictures from the thermal camera. After lunch, catered by Jeanette's Delicacies, Scott Ulrich shared the sweet smell of chemistry at Givaudan with the creation of strawberry flavor. Tim Cassady presented the "typical chemistry industry" photo, but surprised us by explaining the products were kosher and food grade at Twin Rivers Technologies Natural Ingredients. Gil Pacey of Miami University's Center for Nanotechnology presented pictures and the unique properties of several nano materials like memory

wire, gold nanoparticles, and quantum dots. David Novak's presentation illustrated the importance of lawyers in technology as he shared his past careers and his current career with Inventis Group Ltd. Don Storer, of Southern State Community College shared his inquiry teaching projects which grew from a phosphate fertilizer analysis to following phosphorus from sharks' teeth, through fertilizer, through corn, through milk to your teeth, and another chemistry and archaeology project. Carson Cockayne, an analytical chemist at Emerson Climate Technologies shared his unique position as a chemist in the materials engineering department. In between sessions, Mickey Sarquis and Lynn Hogue shared how teachers might use a hands-on activity using the fortune telling fish to illustrate the career of a packaging chemist. Many of the teachers in attendance were especially interested in teaching their students about emerging careers. The teachers found the day most inspiring as did the chemists in attendance. The café organizers especially appreciate and thank the local presenters who gave up a Saturday to share their careers. The presentations, including Bill Carroll's presentation, are currently available at: www.terrificscience.org.

The Science Café was generously sponsored by the Cincinnati Section of the American Chemical Society, the National American Chemical Society, the Ohio Board of Regents, and Miami's Center for Chemistry Education, Miami University Middletown.





Bill Carroll's presentation at the Science Café on October 6, 2007



Audience at the well-attended Science Café at Miami University Middletown



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Chemical Information Update: Copyright for Chemists

Edlyn S. Simmons, Chair, Chemical Information Discussion Group

In 1999 the U.S. Congress passed the Sonny Bono Copyright Extension Act, named in honor of one of its sponsors, Congressman Sonny Bono of California, a musician and song writer whose heirs will be able to profit from his writings and recordings until 2073 (if anyone is still interested in hearing a performance of "I Got You, Babe"). Unlike Rep. Bono, most chemists don't expect earnings from the copyright on their writings: most journal articles are treated as works made for hire, and the publishers normally require assignment of copyright. Although open access publications are beginning to make inroads into scientific publishing, most chemical publicationss continue to be covered by a publisher's copyright. Even the authors of articles are restricted by the terms of their copyright assignment agreements from making copies of their work, and extended copyright is more inconvenience than benefit for anyone who wants to quote passages from older publications.

Historically, copyright was intended to provide compensation for authors and performers during a fairly limited time. Copies of books and other works (we'll call them works for brevity) were registered with the Copyright Office, and copyright could be renewed only once giving a total of 56 years of exclusivity. If there was no copyright notice on the work, it was in the public domain and anyone could copy, quote or adapt it. That all changed in 1978, when major changes were made in the U.S. law. The new law complied with the Berne Convention for the Protection of Literary and Artistic Works. Under the new law there was no need to register or mark a copyright on a work unless you were planning to sue someone for infringement. Copyright became automatic, even for unpublished works. With the passage of the 1999 act, the term of copyright was extended even further. Copyright expires 70 years after the death of the author, and for works made for hire copyright expires 95 years after the publication date. The basics of copyright are summarized in the copyright module created by the American Chemical Society Joint Board/Council Committee on Publications Subcommittee on Copyright at http://pubs.acs.org/copyright/learning_module/summary.html

Copyright owners can give permission to anyone who wants to copy, quote or adapt their work, and fair use gives a very limited right to noncommercial copying. But how do you know if a there's copyright on a work you want to use? And how do you contact the copyright owner to get permission or pay royalties? Corporate or academic libraries can simplify paying royalties to major publishers through a contract with the Copyright Clearance Center. If the publication isn't covered by a CCC contract, figuring out the copyright expiration date is complicated. If you know when the work was created and/or whether the author is alive, you can figure it out by consulting a handy chart posted on the Cornell University website at http://www.copyright.cornell.edu/training/Hirtle-Public_Domain.htm. But how do you get permission to use or copy a work if the owner of the copyright is dead or out of business? Those are known as orphan works, and they pose a serious and growing problem for people who want to avoid inadvertently infringing copyrights. Publishers are working on a solution, but it isn't here yet.

Footnote:

This year, the Chemical Information Discussion Group is once again offering hints and updates on chemical information resources available to most chemists and techniques for using them. Feedback, contributions, and requests for information you'd like to see in future columns are welcome. If you have any comments, suggestions, or contributions, please email them to simmons.es@pg.com

Nominations for Cincinnati Chemist of the Year & Research Associate of the Year

Please submit a nomination for Cincinnati Chemist of the Year and Research Associate of the Year. Recognize your colleagues and co-workers for their outstanding contributions. The nomination deadline is November 30th, so act fast! The nomination form and instructions can be found on the CINTACS website. Copy Dr. Jeff Seeley (seeley.ja@pg.com; Procter & Gamble, SWIC, 11511 Reed Hartman Highway, Cincinnati OH 45242) on your nominations.

ACS debuts Bytesize Science — A new podcast for young listeners

The ACS Office of Communications has launched <u>Bytesize Science</u>, an educational, entertaining podcast for young listeners. Like the flying car, Anglia, in the Harry Potter films, Bytesize Science transports kids, teachers, and other listeners into a real-life world realm where science is the enchantment. Bytesize Science translates cutting-edge scientific discoveries from ACS' 36 peer-reviewed journals intostories for young listeners about science, health, medicine, energy, food, and other topics. It includes content from ACS's Chemical & Engineering News.

New installments of Bytesize Science are posted every Monday and available without charge. The archive includes items on environmental threats to killer whales, a scientific explanation for why some people love chocolate, some unlikely new uses for compact discs, and a hairy tale about "hairy roots."

The podcaster for Bytesize Science is Adam Dylewski, an ACS science writer and recent graduate of the University of Wisconsin with degrees in genetics and science communication. Dylewski spent his college career immersed in science and journalism, writing down-to-earth explanations of vital discoveries as a weekly science columnist for The Daily Cardinal, UW's student newspaper. Later, he continued to translate science news as a reporter for UW's Communications office and for The Why Files, an award-winning science news site with a witty, fun edge.

Podcasting is an increasingly popular way of accessing news, information, and entertainment content from the Internet. The term was derived from Apple's "iPod," a portable digital audio and video player, and "broadcasting." Podcasts allow users to subscribe to a "feed" and receive new files automatically whenever posted to the Internet. Subscribe to Bytesize Science in iTunes. No iTunes? No problem. Listen to latest episodes of Bytesize Science in your web browser

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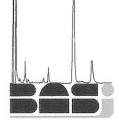
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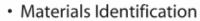
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