IU • CHEMISTRY

Association of Indiana University Chemists Alumni Journal

Vol. 58 • College of Arts and Sciences • Fall 2013

The 246th ACS Meeting Comes to Indianapolis

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Fighting Over Metals

Rationally-designed Chiral Reagents

The Quantum Chemistry Program Exchange

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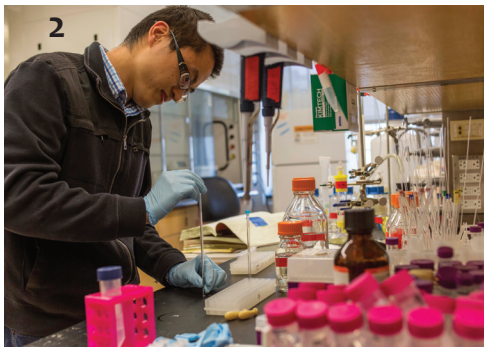

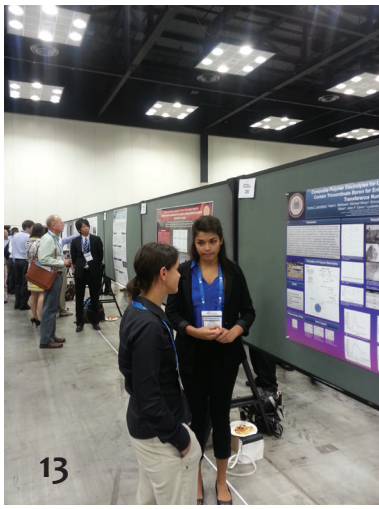

CHAIR'S LETTER

As I peer out the window framing this beautiful campus and write these words, we are well into the Fall semester 2013, my fourth and penultimate year as chair of department.

We've just finished up (I hope!) a run of two weeks or so of unseasonably warm weather (July has finally arrived...in September!!) which also coincides with the last day of a successful 246th National Meeting of the American Chemical Society in nearby Indianapolis. It was a pleasure to meet at least a few of you at our first IU Chemistry Alumni event in years, held at the Indiana State Museum opposite the Convention Center. Stay tuned — we have plans to host an alumni event at least once a year at a national ACS meeting. For all of the latest news, please consult our departmental website (http://www.chem.indiana.edu/) and periodic news releases from the IU Newsroom which showcases recent research breakthroughs by our faculty.

David Giedroc

This past summer, two outstanding chemists joined our department. These are Associate Professor **Jeremy Smith** from New Mexico State University, and Assistant Professor **Thomas Snaddon** from the University of Cambridge in the UK. Prof. Smith is originally from Johannesburg, South Africa and is an inorganic chemist with broad interests in energy-relevant catalysis. Prof. Snaddon is a Scotsman and synthetic organic chemist with interests in organometallic chemistry and catalyst design, synthetic methodologies and the synthesis of complex polycyclic natural products. We warmly welcome these two new faculty to the department. Finally, on the Research Faculty front, we've successfully recruited Dr. **Hongwei Wu** from the National Cancer Institute, NIH, as Assistant Scientist and Specialist in Biomolecular NMR Spectroscopy. Hongwei becomes a member of the staff in the departmental NMR Facility responsible for the 600 and 800 MHz instruments in Simon Hall.

As in past years, our faculty have garnered significant recognition for major university and national awards since the 2012 edition of IU Chemistry. Profs. **Dennis Peters** and **David Giedroc** were elected as Fellows of the American Association of the Advancement of Science (AAAS). Profs. **Erin Carlson** and **Sara Skrabalak** were named 2013 Alfred P. Sloan Foundation Research Fellows as well as Deans Fellows of the IU College of Arts and Sciences. We had another historic first when the Department of Energy announced that Profs. **Megan Thielges** and **Sara Skrabalak** were named 2013 DOE Early Career Awardees. Prof. **Gary Hieftje** is winner of the 2012 Oesper Award while Prof. **Kevin Brown** has received the Thieme Chemistry Journal Award. Profs. **Steven Tait** and **Silas Cook** were recognized as winners of the 2013 IU Trustees Teaching Award while Prof. **Silas Cook** was also honored with receipt of the IU Outstanding Junior Faculty Award.

To top all of this, it was just announced a couple of days ago that two of our faculty were recipients of national awards from the American Chemical Society. Prof. **Ken Caulton** was named winner of the 2014 ACS Award in Organometallic Chemistry while Prof. **Sara Skrabalak** was named winner of the 2014 ACS Award in Pure Chemistry sponsored by Alpha Chi Sigma.

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Fighting Over Metals:

Transition metal chemistry and the host-pathogen Interface

by David Giedroc

Bacterial infections continue to wreak havoc on the human condition. Some are merely annoying, and can usually be cleared by a standard regimen of antibiotics, while other infections can be life-threatening, a situation compounded by developing antibiotic resistance in "super-bugs." The incidence of nosocomial infections, those acquired in a hospital or community health setting, are on the rise and pose a serious threat, again compounded by the failure of drugs of "last resort."Think MRSA, methicillin-resistant *Staphylococcus aureus*, or VRE, vancomycin-resistance *Enterococcus*. As a result, there is an urgent need to discover new antimicrobial targets and develop new strategies to combat infectious disease.

There are a number of research groups in the Department of Chemistry that have taken on this challenge. Prof. **Erin Carlson**'s group is developing new approaches to target an old class of enzymes that are the biochemical targets of the drug penicillin. Her group is also working toward establishing a new route to target a class of enzymes unique to bacteria, called histidine kinases, which allow an organism to "sense" its environment and evade the immune response. The group of Prof. **Mike VanNieuwenhze** is also working in this area, focused on enzymes that build the peptidoglycan layer that provide a protective "coat" around infectious bacteria.

The laboratory of Prof. **David Giedroc** is also interested in how bacteria adapt to a changing environment, but in this case, from the standpoint of a bioinorganic chemist, or someone interested in metals in biology. Giedroc's group hosts a long-standing research program directed toward understanding how microbes that cause significant morbidity and mortality in humans respond to changes in the host-mediated availability and toxicity of essential transition metal ions, including manganese (Mn), iron (Fe), copper (Cu) and zinc (Zn). These metals are central players in human nutrition (all vitamin supplements have them….!) and they largely play roles as cofactors in nature's catalysts, i.e., metalloenzymes, that are responsible for an incredible array of biochemical transformations in the cell. It is estimated that up to one-third of enzymes in the human cell are metalloenzymes. Just as we need these metals, our microbial brethren (or microbiome) as well as unwanted intruders, the infectious pathogens, need them too. "Nutritional immunity" is the term that has been coined to describe the human innate immune response that controls the access of essential metals to invading pathogens.

It has long been established that one of the first things we do upon bacterial infection is to withhold the essential nutrient iron from the organism. As a result, many of those most successful pathogens

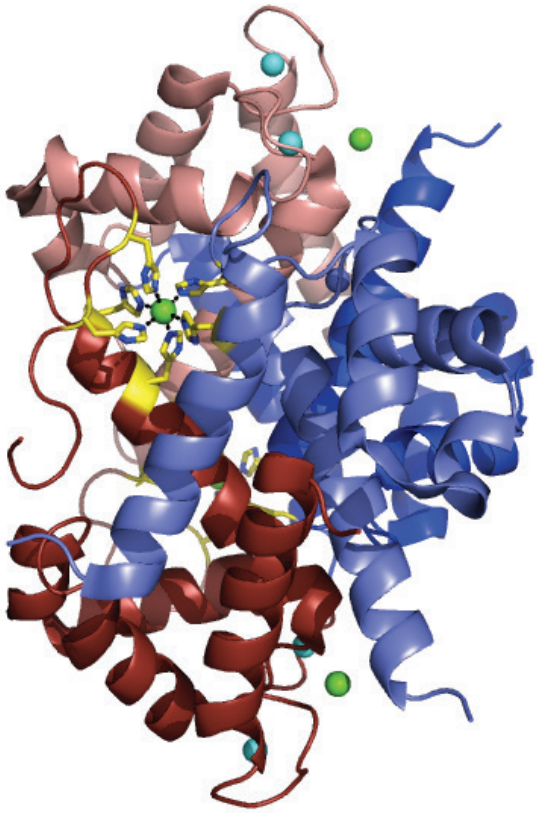
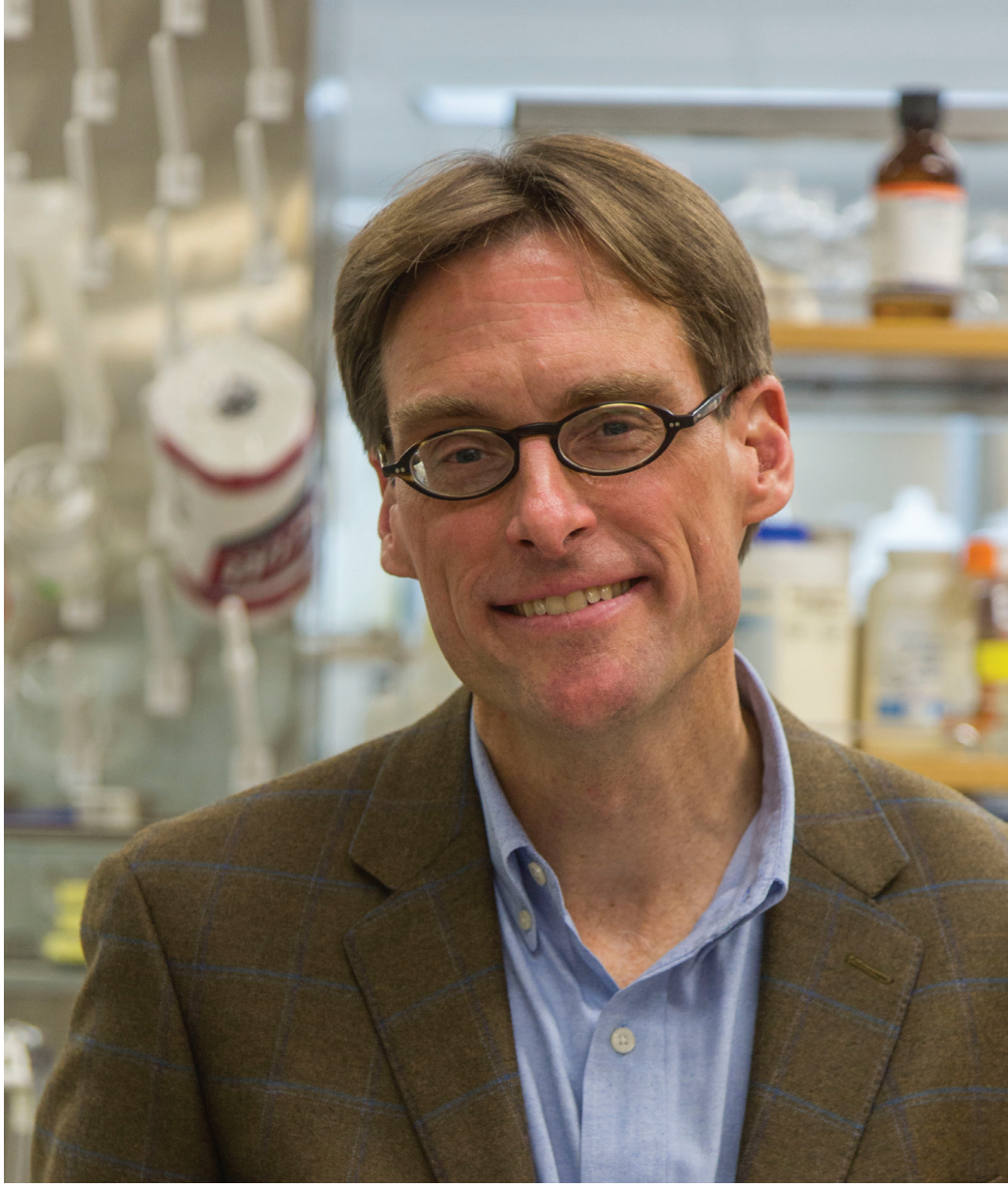


Figure 1. Ribbon representation of the structure of the heterotetrameric form of Ca(II)-bound calprotectin (pdb code 4GGF, Damos *et al.*, **2013**, *Proc Natl Acad Sci U S A* **110**, 3841) emphasizing the coordination chemistry of one of the two Mn(II) chelates.

have multiple ways to extract Fe from us, including stealing it from hemogoblin and from transferrin, the two major Fe-containing protein molecules in the body. Recent work has now established that a similar "tug-of-war" exists for Mn and Zn, with the discovery of a protein called calprotectin (CP) by Eric Skaar'slaboratory at Vanderbilt University (**Figure 1**). CP is a calcium (*cyan* spheres; **Figure 1**)-activated macromolecular chelator that mops up Mn and Zn (indicated by the *green* spheres) and withholds it from the pathogen in a direct competition. The hexa-histidine Mn(II) chelate in CP (*yellow stick*) is unprecedented in biology and presumably ensures that this metal complex will be kinetically and thermodynamically stable.

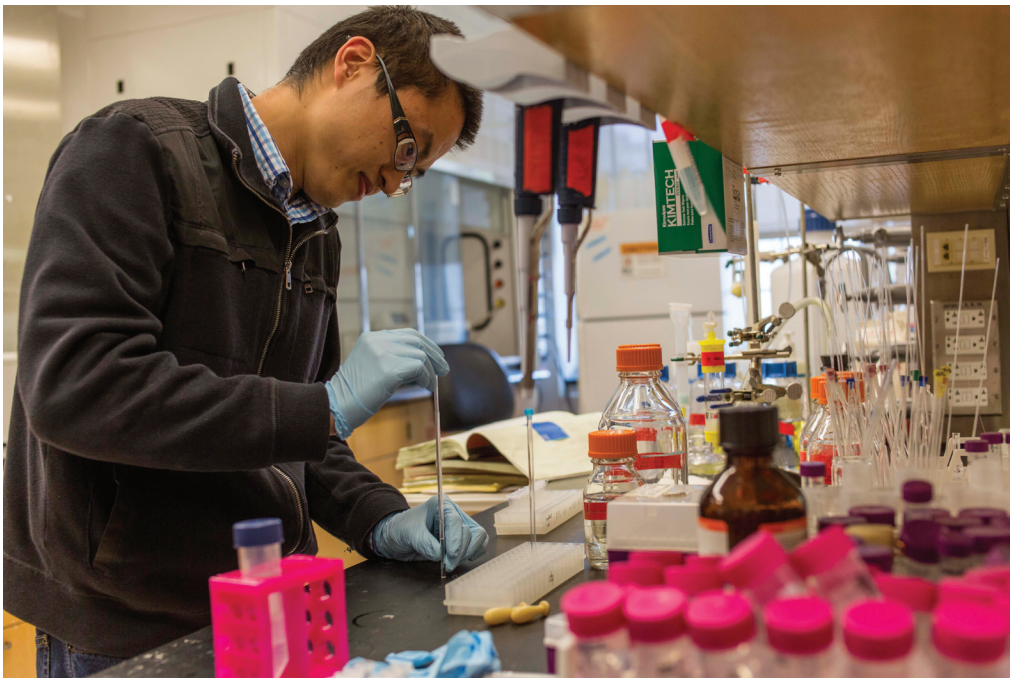
Copper, on the other hand, is a different bird entirely. Cu is an essential cofactor is human enzymes like lysyl oxidase, which crosslinks collagen fibers, and in cytochrome c oxidase, the last enzyme in respiratory electron transfer chain. We are able to breathe air due to cytochrome oxidase. It turns out that most bacteria have very little or no intracellular Cu requirement, and if they respire, this machinery is located on the bacterial membrane facing outside of the bacterial cell. Thus, instead of sequestering this metal from the pathogen, we literally throw copper at the bug. "Copper is a highly reactive metal and is carefully handled by all cells that require it. There is emerging evidence to suggest that human cells use copper toxicity as a weapon to kill microbial pathogens," Giedroc says. Copper is a redox-active transition metal due to its ability to reversibly access reduced Cu(I) and oxidized Cu(II) states, and if left free in the reducing environment of the cytoplasm, reduced copper will interfere with the bioactivity of Fe-containing enzymes, while possibly potentiating the effect of oxidative stress, another major weapon of our immune systems. As a result, literally all bacteria have evolved resistance to Cu-mediated killing even if they never encounter a human host.

In 2007 in *Nature Chemical Biology*, the Giedroc group discovered and characterized a protein they named CsoR (copper-sensing operon repressor) from *Mycobacterium tuberculosis*, which is now known to be representative of a very large family of bacterial regulatory proteins. CsoR is a Cu(I)-sensing repressor that controls the expression of Cu(I) efflux pump in response to copper toxicity. In 2011, they identified and characterized CsoR from *Staphylococcus aureus* as well as a CsoR paralog they named CstR, which controls toxicity toward inorganic sulfur and selenium compounds, including sodium sulfite and hydrogen sulfide. Hydrogen sulfide of course is a poisonous gas that attacks cytochrome oxidase metal-complexes directly and leads to asphyxiation; more recently, H_2S in low concentrations has been established to function as a signaling molecule in higher organisms including humans. The physiological significance of this regulatory pathway in the human pathogen *S. aureus* is currently being dissected by the Giedroc laboratory.



Professor Giedroc shown in his lab.

In a new paper published earlier this year in *Nature Chemical Biology,* the Giedroc group teamed up with Prof. **Charles Dann III** in Chemistry, Prof. **Malcolm Winkler** in the Department of Biology and Prof. Michael Maroney of the University of Massachusetts, and described a previously unknown function of a protein they now know is responsible for protecting a major bacterial pathogen, in this case, *Streptococcus pneumoniae*, from toxic levels of copper. *S. pneumoniae*, commonly known as the pneumococcus, is a commensal organism that lives asymptomatically in the upper respiratory tract; however, upon infection of deeper sterile tissues of the lung and ultimately the bloodstream, becomes the causative agent of a number of life-threatening diseases including pneumonia, meningitis and sepsis.



Yue Fue, a Ph.D. student in Biochemistry and member of the Giedroc group, is shown loading an NMR tube with sCupA for solution structural analysis on the 800 MHz NMR instrument.

Giedroc states that "The novel copper trafficking system that we describe in this paper represents a new functional twist on an evolutionarily ancient family of proteins that opens up a potential new antibacterial strategy." Giedroc and coworkers describe the structure and function of the protein CupA (see **Figure 2**) as a chaperone that buffers copper to very low concentrations, in turn protecting *S. pneumoniae* from cellular damage. "We're proposing that the primary role of CupA in S. pneumoniae is to bind copper ions near the plasma membrane as soon as they enter the cell and, after diffusion of copper-bound CupA in the membrane, delivers copper directly to the exporter CopA, which extrudes copper out of the cell," Giedroc said.

Copper chaperones are known to exist in all cells from bacteria to humans. In this report, the Giedroc group describes a completely novel way in which a copper chaperone and a domain of a copper recipient target protein, CopA, bind copper. Using biomolecular nuclear magnetic resonance (NMR) spectroscopy — a technique to obtain mechanistic and structural information about large molecules — they were able to determine the pathway by which copper is transferred from CupA to CupA. Giedroc states that "The Cu(I) coordination chemistry that we have identified in CupA (**Figure 2**) and in the Cu(I) efflux pump CopA is completely unprecedented in the Cu(I) trafficking literature, and provides a stunning example of how nature has exploited an ancient fold, the cupredoxin fold, to do entirely new biology."

"This work represents an excellent example of collaborative science that works so well on the Bloomington campus, teaming up structural biologists from the Department of Chemistry, a microbiologist and an inorganic chemist." Giedroc said. "This allowed us to quickly grasp the biological significance of what is novel coordination chemistry that bacteria use to protect themselves from copper-mediated killing." ■

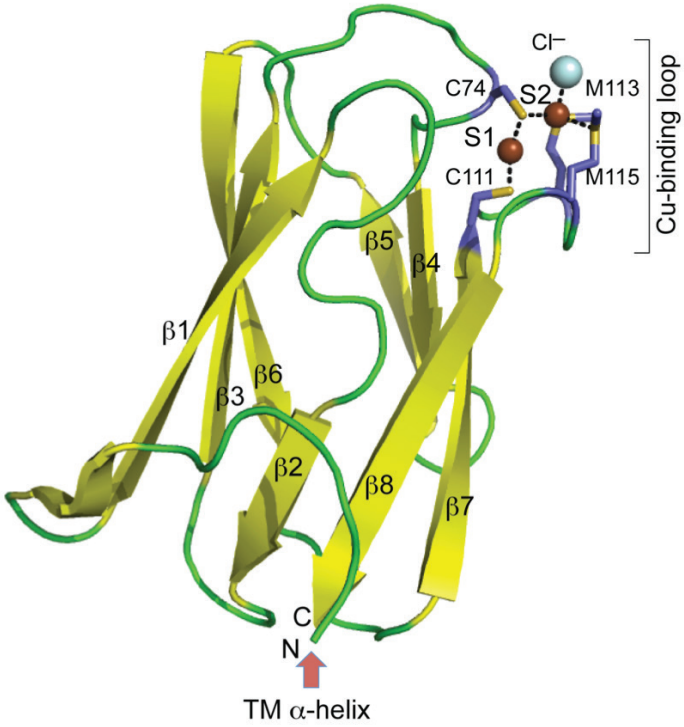
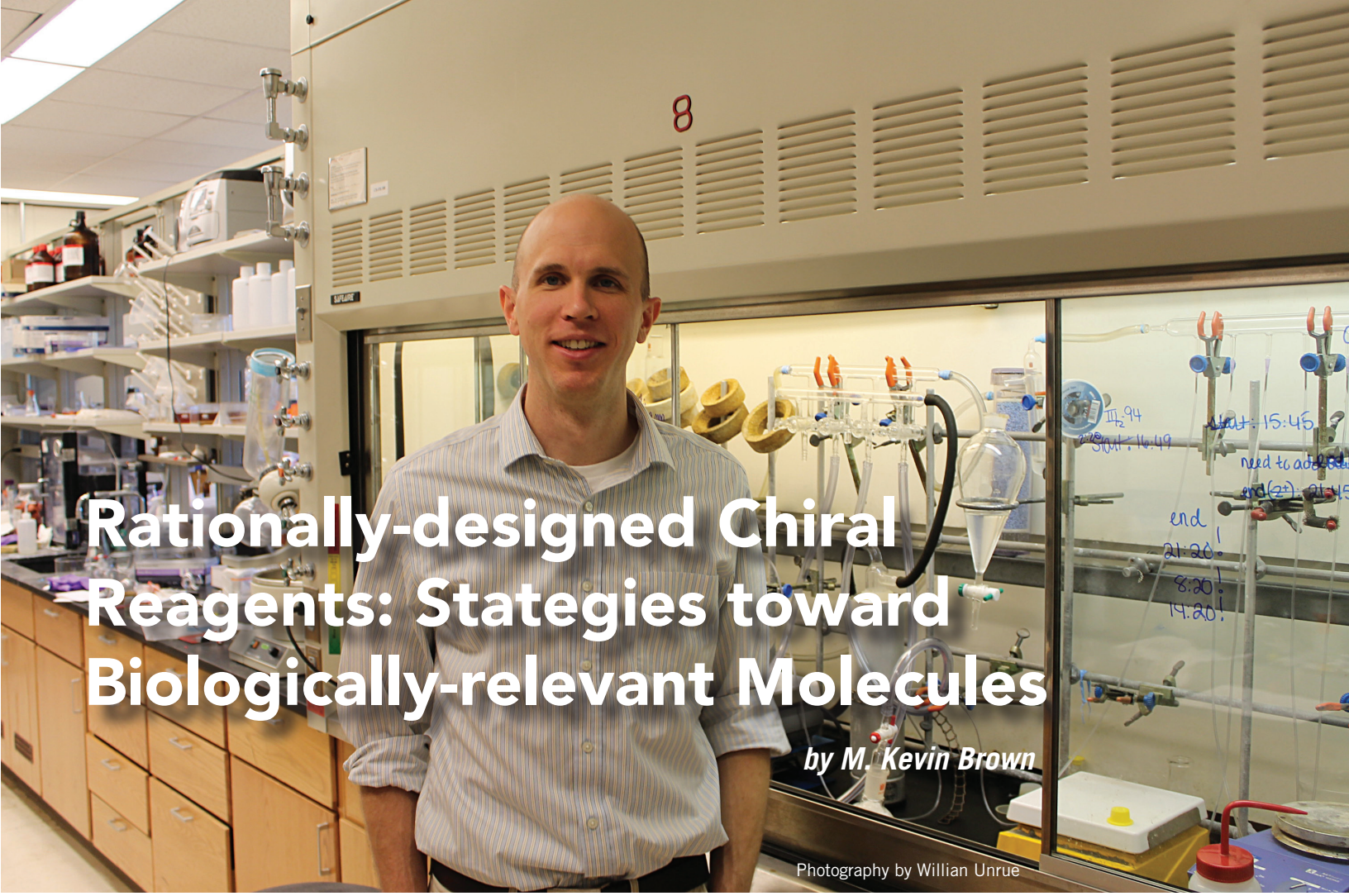


Figure 2. Ribbon representation of the structure of the soluble domain of Cu(I)-bound CupA (pdb code 4F2E, Fu *et al.*, *Nat Chem Biol* **9**, 177). The two Cu(I) ions are represented as *bronze* spheres denoted S1 and S2; TM, transmembrane.

David Giedroc earned a B.S. in Biochemistry from Pennsylvania State University in 1980. He earned a Ph.D. in Biochemistry at Vanderbilt University in 1984, followed by an NIH postdoctoral fellow from 1984-1988, where he worked on zinc-containing DNA binding proteins. From 1988-2007, Dr. Giedroc was a member of the faculty in the Department of Biochemistry and Biophysics at Texas A&M University. In 2007, he became Professor of Chemistry at Indiana University where he has continued his studies of transcriptional metalloregulatory proteins, with a particular focus of zinc- and copper-specific metal sensor proteins from bacterial pathogens, translational frameshifting, and RNA structure and function in mammalian coronavirus replication. The research in Prof. Giedroc's laboratory is supported by funding from the National Institutes of Health and the Lilly Endowment.



Rationally-designed Chiral Reagents: Stategies toward Biologically-relevant Molecules

by M. Kevin Brown

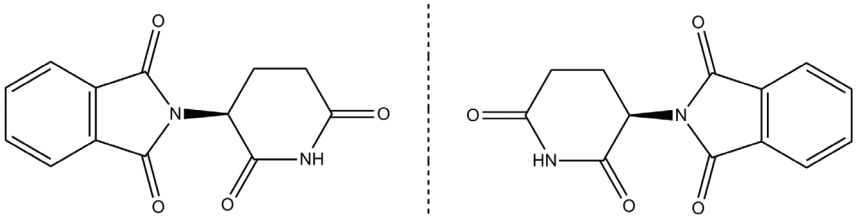
Photography by Willian Unrue

Professor Brown in his lab.

A mirror image is likely encountered by each of us, every day, as we admire our own reflections. You may notice that, for example your right ear is now the left ear of the person looking back at you. What you may not have noticed, however, is that you and your mirror image are non-superimposable (unless you are perfectly symmetrical!). You can illustrate this concept by considering your hands. Simply place your right hand on top of your left hand (e.g., tops of the hands facing up). You will find that your two hands cannot be superimposed on one another; hence they are non-superimposable mirror images. Objects that are not superimposable with their mirror image are defined as chiral. In fact, the word chiral derives from the Greek word *kheir*, which literally translates to *hand*.

In chemistry, a great deal of work is done with *molecules* that display this characteristic of chirality. Two chiral molecules which are non-superimposable mirror images of one another are referred to as a pair of enantiomers. The seemingly subtle structural difference between the two molecules in an enantiomeric pair can, and often does, have critical significance in the context of complex biological environments, and specifically in the drug discovery process.

The identification of new drugs is a lengthy and time-consuming process that consumes millions of dollars and requires ~10 years. The likelihood that any potential drug candidate is approved by the FDA is a whopping



S - thalidomide *R* - thalidomide

Enantiomers of thalidomide

~0.01%. Despite these discouraging statistics, the pharmaceutical industry has created a multi-billion dollar enterprise that provides much needed new medicines to the general public. The importance of single enantiomer molecules to the pharmaceutical industry lies in the difference in biological effects that each enantiomer might have in the body.

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This significance of enantiomeric molecules and their effect on the human body was tragically displayed by the use of a now infamous molecule called thalidomide. In Europe during the 1950's, thalidomide was prescribed to alleviate the symptoms of morning sickness in pregnant women. Shortly after the drug's release, severe birth defects were observed in the children of some of the women that had taken the drug, and a causative connection was quickly established. Only later was it determined that one of the enantiomers of thalidomide alleviated morning sickness while the other had severe teratogenic effects. Due to this unfortunate tragedy, the FDA now requires that any chiral molecule seeking approval as a new therapeutic must either be a single enantiomer, or the "other" enantiomer must be shown to be benign. Due to the high cost associated with evaluation of new molecules in humans, pharmaceutical companies most often opt for producing and marketing chiral drugs as single enantiomers. A major hindrance to this is that many simple reactions form both enantiomers in a *racemic mixture* (i.e. 50:50 mixture of both products), aggravated by the fact that enantiomers are not easily separated from each other. Both enantiomers exhibit the same physical properties, making it non-trivial to separate them analytically, leading to higher drug development costs.

"The likelihood that any potential drug candidate is approved by the FDA is a whopping ~0.01%."

These restrictions have led, in part, to the direction of a significant portion of the field of organic synthesis towards identifying methods to prepare chiral molecules as a single enantiomer. Early efforts resulted in the identification of numerous chemical reactions that favor the formation of one enantiomer over the other. While these contributions are certainly important, one issue with many of these reactions is that formation of single enantiomer compounds required the use of an excess of costly chiral reagents or starting materials. More recent efforts have focused on identifying reactions that generate single enantiomer molecules through the use of *chiral single enantiomer catalysts*, which are used in significantly lesser quantities. This field, deemed *enantioselective catalysis*, offers the potential to generate large quantities of single enantiomer molecules from small quantities of catalyst. Achievements in this field were so significant that the Nobel Prize was ultimately awarded in 2001 to several of the field's pioneers. [The 2001 Nobel Prize in Chemistry was divided, one half jointly to William S. Knowles and Ryoji Noyori "for their work on chirally catalysed hydrogenation reactions" and the other half to K. Barry Sharpless "for his work on chirally catalysed oxidation reactions".]

Despite substantial progress in the field of catalytic enantioselective chemical synthesis, many significant challenges remain unsolved. In particular, there is a lack of generally effective methods for the enantioselective chemical synthesis of chiral single enantiomer molecules that contain a 4-membered ring (cyclobutane) functionality. Many current therapeutics as well as many potential drug candidates contain cyclobutanes, but are only available in small quantities from their natural source. Our research group is actively working to provide practical solutions to this problem.

In developing a strategy for solving this problem, we decided to employ a well-known class of chemical reactions called cycloadditions. We have identified a chiral catalyst that is capable of promoting the fusion of two carbon-carbon double bonds (or alkenes) in a single step to generate a chiral cyclobutane-containing molecule with nearly perfect selectivity for one enantiomer over the other (Figure 1). Current efforts in our lab are aimed at utilizing this newly developed reaction toward the chemical synthesis of several of the biologically important molecules. ■

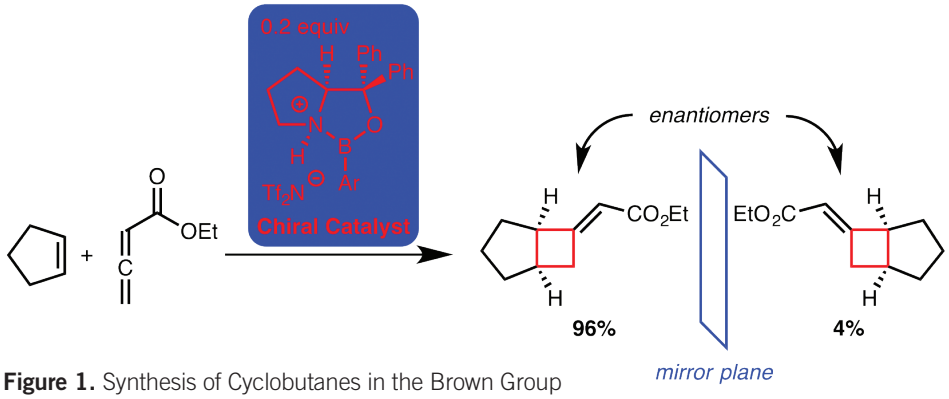

Figure 1. Synthesis of Cyclobutanes in the Brown Group

Professor Brown earned an bachelor's degree at Hamilton College (Clinton, NY) and a Ph.D. in organic chemistry at Boston College with Professor Amir Hoveyda in 2008. After completion of his graduate studies, he began a Ruth L. Kirschstein National Institutes of Health funded postdoctoral fellowship in the laboratories of Nobel laureate E. J. Corey at Harvard University. In 2011, Professor Brown joined the faculty at Indiana University. Research in the Brown lab is directed toward the development of new and important chemical reactions (which includes new chiral catalysts/reagents) for the enantioselective preparation of chiral molecules. All of our research goals have direct application toward the synthesis of biologically relevant molecules, contribute to our fundamental understanding of reaction mechanism, and introduce new concepts in organic chemistry.

The Quantum Chemistry Program Exchange of IU

by Donald Boyd

How many IU chemistry graduates are aware that all though the 1970s, 1980s, and 1990s the Chemistry Department at Indiana University was responsible for providing software to a worldwide audience? ***The Quantum Chemistry Program Exchange*** (QCPE) was a service conceived by an IU professor in 1962 and that started operating on the Bloomington campus in 1963. Its purpose was to provide an inexpensive mechanism for theoretical chemists and other research scientists to exchange computer programs. QCPE reached its zenith in the 1980s when computational chemistry was growing rapidly and becoming widely recognized by the scientific community. Computational chemistry utilizes the power of computers to shed new light on the properties of molecules. The field has become a powerful partner in the quest to discover useful medicines.

As the name implies, the Quantum Chemistry Program Exchange started with the purpose of being a distribution hub for software tools used by quantum chemists. Most of the leading names in theoretical chemistry — and later computational chemistry — became members of QCPE. Unlike most commercial software companies, QCPE expedited science by distributing source code at nominal cost and providing free guidance to users.

Figure 1. Professors Shull (left) and Hagstrom.

QCPE was founded at the inspiration of Professor **Harrison G. ("Harry") Shull**, a quantum theoretician and research professor at Indiana University, Bloomington in the years 1955-1979 (**Figure 1**). Shull has been described as the sort of person from whom ideas bubbled forth. He had a knack for inspiring people around him to gladly work on his ideas. Shull did not mind letting his associates get credit for the achievements they accomplished.

Many theoreticians could see the advantage of exchanging computer programs. It was inefficient for graduate students at one university to have to write a program to do the same calculations that had already been programmed elsewhere. It made sense to have these widely needed programs available in order to avoid "reinvention of the wheel."

A second motivation for setting up a library of shared software was to create a more or less permanent repository. So, if a graduate student finished a thesis and left a university, or if a professor changed research interests, the fruits of their labors — in terms of software written — would not be lost or forgotten.

A third motivation for a central repository was to create an intermediary between the code writers/owners and users. Quantum chemistry professors whose students had created useful programs could directly share copies with other research groups. However, the users in the other groups might not understand all the requirements of operation or the limitations for getting useful results. The new program might be minimally or unclearly documented. Hence the users would frequently be asking the developers for help. For widely used programs, such requests could consume time and distract the original developers from other work. So, someone at a central depository could field some of these routine questions from the users.

There was a fourth motivation. Depositing programs with QCPE could be regarded as a form of "publishing" the code. There were few or no means of publishing codes in the vetted scientific literature. In this regard, academic traditionalists were just beginning to think about the fact that creating a significant computer code was, in effect, a form of intellectual writing.

QCPE thus served as a conduit through which individual researchers could donate their programs.

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Before the programs were distributed, the QCPE staff or volunteers would check programs to make sure the software performed as claimed. Some of the deposited programs ran without problem, but others were written specifically for one machine or one operating system, and they had to be modified. With an appointment in the IUB Computing Center, Dr. **Stanley A. Hagstrom** (**Figure 1**), an assistant professor at the time, had the expertise for porting programs to other machines. He was also an early donor of programs and provided direction to the endeavor. Recall that QCPE started in the days when computer code was written on so-called IBM punch cards. The cards were read into the room-filling mainframe computers of that era. The machines seemed marvelous at the time but were slow by today's standards.

The person who first set up the mechanics of the QCPE operation was Dr. **Keith M. Howell**, a postdoctoral associate from England in Shull's group. When Howell returned to England, Dr. **Franklin (Frank) Prosser**, another postdoctoral associate in Shull's group, was recruited to continue the operation.

Figure 2. Mr. Counts ca. 1980.

In 1967, **Richard W. Counts** (**Figure 2**), with a physics background and a Master's degree, was hired from the National Aeronautics and Space Administration (NASA) office at IUB to run QCPE. Counts' title was Project Supervisor. Under his leadership, QCPE continued growing and serving the community of theoretical chemists with an ever-expanding library of programs.

Upon the advice of Prof. Hagstrom, Counts assembled a board of advisors in 1979 consisting of Shull (then at Rensselaer Polytechnic Institute), **Max M. Marsh** (then with Eli Lilly and Company), and other prominent practioners. Marsh (**Figure 3**) was one of the first people in the pharmaceutical industry to foresee the possibility of computer-aided drug design. After Marsh retired from Lilly, he joined IU to share his wealth of knowledge in advisory roles.

One of the first topics the Advisory Board addressed in January 1980 was a proposal by Counts to organize workshops on applications of quantum chemistry. Counts and the board anticipated that a workshop would be a new revenue stream for QCPE and would enhance the image of IU. With a green light from the chemistry department and the advisory board, Counts organized annual summer workshops starting in 1980.

Figure 3. Dr. Max Marsh.

Most of these weeklong courses were held at IUB, but one was held in La Jolla, California, another in Marlboro, Massachusetts, and others were held in Europe. The QCPE workshops were taught by practicing computational chemists including ones from industry. Computational chemists in industry had experience dealing with research questions that may not be ideally suited to any of the available methods, but nevertheless required the best possible answers, immediately if not sooner. In contrast, academic users could be more selective in choosing research problems where available methods can be expected to give something publishable at some point down the road.

The QCPE workshops turned out to be great successes financially and in training more scientists in the techniques of computational chemistry, as well as in bringing new people to Bloomington and increasing awareness of IU and its chemistry department. The workshops were so effective at training users and generating revenues that other universities and organizations emulated them.

Starting from an original library of 23 programs in 1963, QCPE's holdings grew steadily. For the period April 1980 to April 1981, 451 copies of programs were distributed to the United States, 212 to West Germany, 138 to Great Britain, 106 to Japan, and 77 to Switzerland.

As business at QCPE increased, Counts hired temporary graduate student assistants, work-study students, and part-timers to assist him. Such a beneficent policy created jobs and helped students who needed to work their way through college. In 1973, he hired **Margaret (Peggy) Edwards** who worked at QCPE until her retirement in 1999.

For a number of years, Counts operated essentially independently of the chemistry department hierarchy. However, some faculty members and especially the chairmen of the department recognized that QCPE benefited and supported the department as a magnet for government research grants and as a stimulus for donations of computer hardware to be used by the department and university. Although QCPE was not part of the core mission of educating undergraduate students in Bloomington, it was an asset to the university and thus benefited everyone.

In 1984 Professor **Ernest R. Davidson** (**Figure 4**) was enticed to move his group from the University of Washington in Seattle to IUB. Davidson did his undergraduate training as a chemical engineer at what is now called Rose-Hulman Institute of Technology in Terre Haute, Indiana. With light guidance from Shull

and occasional mentoring from Hagstrom, he had obtained his Ph.D. at IUB in just three years. In addition to his faculty position at IUB, the chairman of the department at the time, Professor **Paul Grieco**, named Davidson to replace Hagstrom as director of QCPE. The appointment helped win approval for Davidson's pending proposal for purchasing his own large IBM computer. In its heyday, the QCPE "brand," as we say nowadays, carried with it prestige and the aura of a worthwhile service to the community.

Figure 4. Prof. Davidson.

Although the QCPE was originally conceived as a service to theoreticians, the variety and scope of its software holdings expanded naturally over the years. QCPE came to service computational chemistry in general, not just quantum chemistry. Even experimentalists contacted QCPE for assistance when they needed a program to address a research problem.

During its lifetime, QCPE occupied several different offices at IU. The spaces allotted to QCPE were characterized by being filled with a variety of computers so that programs could be tested on machines prevalent in the user community at the time. Also, the offices had many piles of mimeographed and later photocopied documentation corresponding to each program in the

Figure 5. The QCPE office was on the second floor of the Quonset hut situated between the Chemistry Building and the Indiana Memorial Union.

catalog. This paperwork was needed because a copy of the documentation was shipped with the computer cards or magnetic tape to each requestor.

After the QCPE office vacated the Chemistry Building at Indiana University, it was located in a temporary structure called the Quonset hut (**Figure 5**), which stood in a nearby parking lot. Such structures with corrugated metal roofs were popular during and after World War II because of their low cost and quick construction.

QCPE's next move was upward: it "moved up" to the top floor of one of the towers of the nearby Indiana Memorial Union (IMU, **Figure 6**) in the 1980s. The top floor was once occupied by an IU president who enjoyed the expansive view. Still later, QCPE moved to a university building on Indiana Route 46 Bypass, which circled part of the perimeter of the campus. This building has since been torn down to make way for a large new information technology building.

In October 1999, QCPE operations were moved back to the Chemistry Building where they were spread over four rooms. In the period 2001-2011, QCPE operations were conducted in the small-molecule X-ray crystallography laboratory on the fourth floor of the chemistry department annex, which is the large laboratory building behind the older chemistry building.

Figure 6. The central tower of the Indiana Memorial Union (IMU).

In the 1990s a number of factors started to undermine the important role QCPE was playing in the scientific community. A significant factor was the emergence of the Internet in the 1990s. This major technological advance gave individuals an independent way to distribute software. The healthy flow of new programs being deposited in QCPE gradually diminished as some had predicted. The number of programs being requested also slowed. Software had been deposited by American chemists as well as by researchers in other advanced countries. However, distribution of programs in the 1990s was largely to places outside the United States. Interestingly, the Japanese remained some of the main customers of QCPE's holdings.

The 1980s and 1990s witnessed the commercialization of software by relatively large companies in the computational chemistry business. In order to obtain the latest versions with the most features and with the most recently fixed bugs, customers had to buy commercial versions of popular programs. The software companies often had large staffs of Ph.D. computational chemists who could both continually improve their products and respond to queries from their customers.

The commercial programs tended to be written (or rewritten) in current program languages according to what were the current standards. In contrast, some of the QCPE holdings had been hastily written in older languages as part of a Ph.D. thesis and lacked sufficient comment cards to explain the detailed thinking of the programmers.

Yet another trend impacting QCPE was the fact that users wanted and expected technically supported software, i.e., they wanted to be able to call up a toll-free telephone number or send an email to ask questions about the operations of a program. Mr.

Continued on page 10

Counts provided support to QCPE customers on an ad hoc basis His efforts at keeping QCPE running are to be applauded, but it was hard to compete with large software companies. These changes in attitudes and expectations, as well as other factors, slowly diminished the important role QCPE had been playing.

The older QCPE software holdings became less relevant as the expectation of user-friendly input to software became more and more popular. By 1990, the QCPE library had started to acquire some programs with modern graphical user interfaces. The library also had some elaborate programs qualifying for the name "system" or "package."

As members of the computational chemistry community saw the changing landscape, they realized it was time to honor the service that IU had provided. The only major tribute to QCPE was a symposium organized in honor of Counts for his impact on the field of computational chemistry. The symposium was held by the Division of Computers in Chemistry (COMP) of the American Chemical Society (ACS) at their spring meeting of 1994. These meetings typically draw thousands of chemists from across the United States and the world to partake of a rich assortment of concurrent symposia.

Counts' talk pointed out that one of the important achievements of QCPE was that it brought the creation of an important computer code to a level of respectability in the academic world. Many institutions started to accept the contribution of a successful computer code as similar to having publications. In some cases, the publicity that came to a programmer could be the determining factor in a tenure decision.

Figure 7.
Dr. and Mrs. Huffman.

Counts also spoke about two events that shook the computing landscape and changed the nature of user support. In 1978 the VAX superminicomputer came onto the scene and that was followed a few years later by the IBM desktop minicomputer. Up to that time, computers had been confined to one isolated computer center on each campus. Each center was controlled and maintained by a powerful bureaucracy and its staff. The users carried their computer cards to the centers and picked up their printouts a day or two later. The VAX broke the monopoly that the administrators of central computer centers had on computational resources. A group or a department could afford to buy its own VAX. The IBM personal computer (PC) moved the resource to the desktop of each user.

For an ACS book chapter the author (**Boyd**) recently published (2013), the positive effect that QCPE had on the growth of computational chemistry was measured by the number of times QCPE had been cited in the scientific literature. More citations corresponds to more interest by the scientific community. The number of citations grew steadily over the decades and peaked in the early 1990s when QCPE was cited over 1100 times per year.

Whereas at one time 2000 members were receiving the quarterly QCPE Bulletin, the membership slipped toward 1000 in the 1990s. The issues of the QCPE Bulletin became thinner. Fewer programs were being deposited and announced. Many people thought that QCPE had fulfilled its role and was simply no longer needed after scientists could conveniently exchange programs over the Internet.

In the late 1990s, the chair of the IUB chemistry department asked Dr. **John Huffman** (**Figure 7**), to be the faculty supervisor over QCPE. Huffman's official title was Director of Technical Services, which included responsibility for the machine shop, glass shop, mass spectrometry, duplicating, etc. Even in 1999 when Counts retired, software continued to be deposited in — and distributed by — QCPE, but at a slow and declining pace. The QCPE library was approaching 775 programs for mainframes and workstations, plus about 200 additional programs for desktop computing.

Around 1999 Mrs. **Carolyn Huffman** was hired to assume the day-to-day operation of QCPE. Among the responsibilities she assumed, she started converting the paper records to electronic Portable Document Files (PDFs) by scanning. It is a process that continues but is nearing completion. Her goal is to deposit the PDFs in the Indiana University Archives. The purest and noblest form of service is working not for recognition, riches, or requirement, but doing it because it needs to be done.

We end by reviewing the current status of some of the key players in QCPE's history. **Dr. Shull** went on to a successful career as an administrator in higher education. He died in July 2003 at the age of 79. His obituary mentions his idea for QCPE as one of his major accomplishments. **Dr. Hagstrom**, **Dr. Prosser**, **Mr. Counts**, **Ms. Edwards**, and **Dr. and Mrs. Huffman** are retired and still live in Bloomington. **Dr. Howell** is retired in England. **Dr. Davidson** retired in Seattle, Washington. The scientific community owes much to these people who made IU a hub for the advancement of computing in chemistry. ■

Prof. **Donald Boyd** has been a Research Professor of Chemistry at Indiana University Purdue University Indianapolis (IUPUI) since 1994. Prior to that he was a scientist involved in drug discovery at Eli Lilly & Company for 25 years. He did his undergraduate studies at Penn State (1963), obtained a Master's (1965) and PhD (1968) from Harvard, and was a postdoctoral fellow at Cornell (1967-68) before joining Lilly. Boyd served on the Advisory Board of QCPE in the 1980s. His research continues to probe relationships between structure and properties of molecules. They are interested in all sorts of molecules, but have a special interest in pharmaceutically relevant molecules. In particular, the economics of drug discovery has led to a prominent role for computer-aided drug design (CADD) methodologies in pharmaceutical companies. CADD helps determine which structures are more promising as drug candidates.

Global flame retardant levels indicated in tree bark samples

by Ron Hites

Chemicals used as flame retardants are present as environmental pollutants at locations around the globe, including remote sites in Indonesia, Nepal and Tasmania, according to a study by researchers from Prof. **Ron Hites**' Group.

The study, published in the journal Environmental Science and Technology, makes use of a novel but highly effective sampling technique: measuring concentrations of the chemicals in the bark of trees, which absorbs compounds in both vapor and particle phases.

"These findings illustrate further that flame retardants are ubiquitous pollutants and are found all around the world, not only in biota and humans but also in plants," said **Amina Salamova**, a postdoctoral research associate in Prof. Hites' Group and co-author of the study.

The study measured concentrations of brominated and chlorinated flame retardants collected in tree bark samples at 12 locations around the globe: three sites in Canada and single sites in Iceland, Ireland, Norway, Czech Republic, South Africa, Nepal, Indonesia, Tasmania and American Samoa.

The highest concentrations were found at an urban site: Downsview, Ontario, Canada, near Toronto. However, the second-highest concentration of one type of flame retardant, Dechlorane Plus, was found at a remote site at Bukit Kototabang in Indonesia. Salamova and Hites do not know the cause of the relatively high concentrations at the site but suspect it may be near a source.

Brominated and chlorinated flame retardants have been used for several decades in consumer products made of plastic, foam, wood and textiles to prevent combustion and slow the spread of fire. They persist in the environment and bio-accumulate in ecosystems and in human tissues. Exposure to the compounds has been associated with thyroid and other endocrine system disruption and with adverse neurological development. As a result, the production and use of certain flame retardants has been restricted in North America and the European Union.

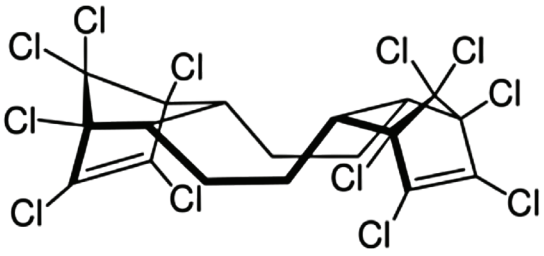

Figure 1. Structure of decachlorane plus.

Salamova and Hites measured a variety of flame retardants, including widely used polybrominated diphenyl ethers as well as non-regulated compounds such as Dechlorane Plus and "older" flame retardants that were used in the 1980s. Most of these compounds were detected at all the locations, with concentrations varying widely. Concentrations were associated with population density, suggesting the compounds most likely entered the environment through their use in nearby homes and offices.

Higher concentrations of flame retardants in bark and atmosphere have been found by Hites and others in previous studies of the Great Lakes region, especially urban areas near Chicago and Cleveland, and also at cities in China. Even higher concentrations were found in southern Arkansas and at Niagara Falls, New York, near the sites of manufacturing facilities for polybrominated diphenyl ethers and Dechlorane Plus, respectively.

The study also confirms the effectiveness of using tree bark as a sampling medium, a technique that Hites and colleagues have used in previous studies of persistent organic pollutants (POP) such as flame retardants. Bark makes an effective sampling medium because of its

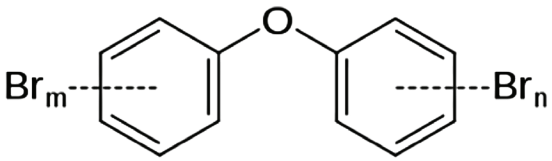

Figure 2. Polybrominated diphenyl ethers.

large surface area and high lipid content. The samples are easy and inexpensive to collect, an advantage in developing countries that lack funding for extensive environmental monitoring programs. Tree bark also collects both vapor and particle phase pollutants, while other samplers collect one or the other.

Support for this study came from the Great Lakes National Program Office of the United States Environmental Protection Agency. ■

Professor Hites received his B.A. degree from Oakland University (1964), and a PhD in organic analytical chemistry at the Massachusetts Institute of Technology (1968). He was a Postdoctoral Fellow at the U.S. Department of Agriculture (1968–1969). Dr. Hites was a professor at MIT in chemical engineering from 1972–1979 before coming to Indiana University. Dr. Hites is a Distinguished Professor at the Indiana University School of Public and Environmental Affairs. The Hites' research group applies organic analytical chemistry to the understanding of environmental problems. Most of their work uses mass spectrometry for the analysis of trace levels of potentially toxic environmental pollutants. Specific research areas include the global scale transport of halogenated compounds, the reactions of pollutants with the hydroxyl radical and ozone, and anthropogenic organic pollutants in the Great Lakes.

Example of a sampled tree located in Sleeping Bear Dunes, Michigan in the Great Lakes basin.

The 246th ACS Meeting Comes to Indianapolis

On September 8 –12, 2013, over 10,000 chemists, academics, students, and other professionals met in Indianapolis, IN for the 246th ACS National Meeting & Exposition. If you missed this meeting, highlights included a live appearance by celebrity chef Alton Brown and the ACS Board of Directors featured special featured guest — actor, author, and director Alan Alda — who is a vocal spokesperson for the necessity of communicating science to the general public. Many of us were in meetings, but perhaps you had time to stick your head in the exposition hall to get a peek at the new equipment or newest textbook.

Sunday started off the meeting at the Indianapolis Speedway to *rev up* their theme of "*Chemistry in Motion*." Our Outreach Team (thanks **Norman Dean, James Clark**, **Chris Chatelain** and **Aulaire Schmitz**!) was on hand to work with kids of all ages with hands-on demonstrations, including making their own *Cartesian Diver* that the kids took home with them.

Indiana University took advantage of the close proximity of the meeting, and the Department of Chemistry organized or presided several symposia, including:

- Electroanalytical Measurements (Organizer: Prof. **Lane Baker**)
- Developments in Mass Spectrometry (Organizer: Dr. **Steve Ray**)
- High Resolution Microscopy for Bioanalysis (Organizer: Prof. **Yan Yu**)
- 75 Years of Analytical Chemistry (Organizer: Prof. **Dennis Peters**)
- Current Topics in Glycobiology (Organizer: Prof. **Nikki Pohl**)
- Monodisperse Inorganic Nanoparticles for Catalytic and Biomedical Applications (Organizer: Dr. **Lyudmila Bronstein**)
- Nuclear Reactions (Organizer: Prof. **Romualdo DeSouza**)
- Supramolecular Nanomaterials (Organizer: Prof. **Amar Flood**)
- Optical Spectroscopy of Proteins (Organizer: Prof. **Megan Thielges**)
- Micro/Nanofluidics: Fundamentals and Applications (Organizer: Prof. **Stephen Jacobson**)
- The Science of Separation (Organizer: Grad. student **Zachary Harms**)
- Advances in Capillary Electrophoresis (Organizer: Grad. student **Indranil Mitra**)
- New Techniques and Methods in Proteomics (Organizer: Grad. student **Michael Ewing**)
- Analysis of Living Systems: in vivo and in vitro (Organizer: Grad. student **Celeste Morris**)
- General Poster Session for Analytical Chemistry (Organizer: Grad. student **Kirstin Morton**)

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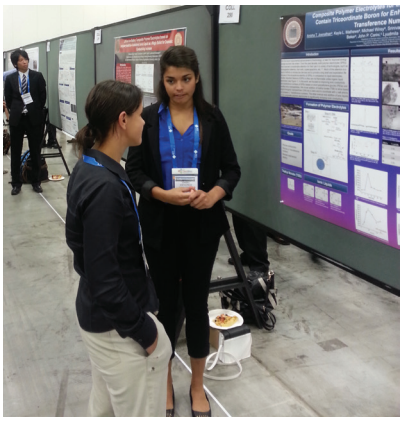
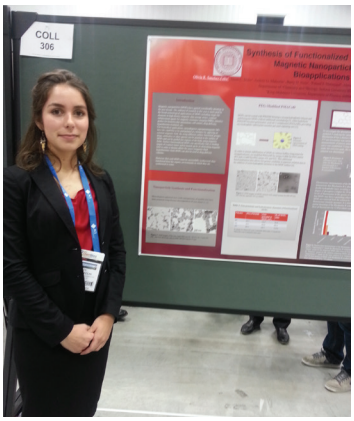
From left to right: **Milos Novotny** (IU), **Gary Hieftje** (IU), **Dennis Peters** (IU, and symposium organizer), William Heineman (University of Cincinnati), and Graham Cooks (Purdue University) at the 75 Years of Analytical Chemistry symposium.

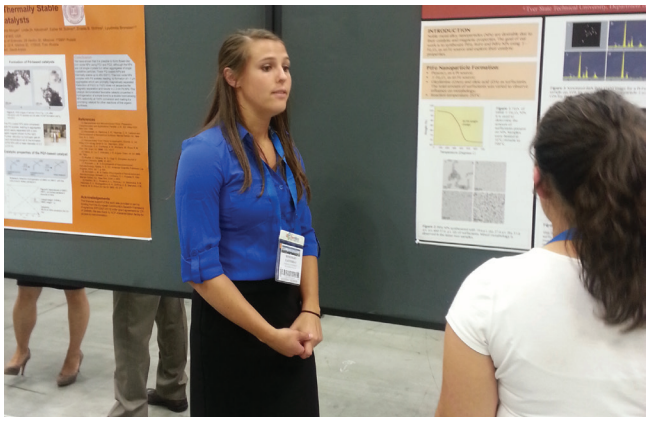
All of our sessions were well attended, but one of the highlights on the meeting was the celebration of the 75th Anniversary of the founding of the Division of Analytical Chemistry (organized by **Dennis Peters**). After an introduction and recount of the history of the division by Prof. Peters, highlights from the last 75 years of mass spectrometry, electrochemistry, spectroscopy and chromatography were recounted to a standing room only crowd by Graham Cooks (Purdue), Bill Heineman (Cincinnati), **Gary Heiftje** (Indiana) and **Milos Novotny** (Indiana), respectively.

Metal and metal oxide nanoparticles (NPs) received considerable attention because of their numerous applications and these were highlighted in the symposium organized by Senior scientist **Lyuda Bronstein**. Monodisperse NPs are of particular interest because many NP properties are size dependent. This symposium focused on syntheses of such NPs, their functionalization and applications. In particular biomedical and catalytic applications have been addressed. The symposium included three oral sessions and a poster session. Of special note, six undergraduate students from the **Bronstein group** presented posters. Additionally, the Ortoleva group presented six lectures on nanosystems, mostly related to nanomedicine.

The Department of Chemistry hosted an *Indiana University Chemistry Alumni* Event Tuesday, September 10, at 6:30 p.m. at the Indiana State Museum, one block from the Indiana Convention Center. Alumni socialized with current and past members of our department in a gorgeous environment. Our department intends on making this a yearly event at the fall meetings — look for the date, time and location at the ACS meeting in San Francisco in 2014! ■







Clockwise: Poster presentations by **Anisha Joenathan**, **Olivia Sanchez-Felix**, and **Rosemary Easterday**.

Graduate students **Chris DeSantis**, **Andjela Radmilovic**, **Becca Weiner** and **Nancy Ortiz** (Skrabalak students) in front of chemistry undergraduate Andjela's poster at the Colloidal Chemistry poster session.

FACULTY NEWS

The **Bronstein** group continues development of novel hybrid composite polymer electrolytes for flexible Li ion batteries. This project has two major aspects: fundamental studies of complex multicomponent materials, their interactions and morphology and applied studies of structure-property relationships for fabrication of competitive polymer electrolytes for use in Li ion batteries. The electrolytes were made of a polymer component, a Li salt, an organic-inorganic component (OIC) and an ionic liquid (IL) as a plasticizer. It was demonstrated that the addition of an ionic liquid allows an increase of conductivity by at least two orders of magnitude, while the material retains good mechanical and electrochemical stability and flexibility. This project is a collaborative effort of Bronstein's group and Prof. Marcus Hunt's group from Bennett College (NC). The research is carried out by two IU undergraduate students, **Michael Wirey** and **Anisha Joenathan**, and two visiting student from Bennett, Jessica Ayivi and Rayonna Purvis.

The **Flood Group** has created a novel star-shaped macrocycle that is easy to synthesize and has characteristics that may find use in biology, chemistry and materials sciences. **Amar H. Flood** continually challenges the group members to generalize the previous discovery of strong CH hydrogen bonds by creating new molecules with similar properties. In response, **Semin Lee** designed and synthesized a "star"-shaped macrocycle with "cyano"-stilbene repeating units, so-called cyanostar. Surprisingly, it was possible to produce this compound in multigram scales by a simple one-pot reaction followed by easy purifications, which is promising for future industrial scale usage.

While cyanostar has a neutral charge overall, the electron-withdrawing cyano-groups cause it to exhibit electro-positive properties and bind very strongly with weakly coordinating anions that were once thought to be incapable of being captured by molecular receptors. The types of anions captured by these compounds have many roles in chemistry and biology. For example, widely used Li-ion batteries carry a phosphate counter anion, and cyanostars could advance the clean-up of spent batteries. Furthermore, perchlorate, which is an environmental contaminant in the Colorado River arising from rocket fuel, could be cleaned up using the large supplies of cyanostars.

In addition, cyanostar can be assembled into a dialkylphosphate rotaxane, a wheel-on-axle assembly in which a pair of macrocycles is threaded with an anionic molecular rod, which is then capped on both ends by a "stopper." Rotaxanes are precursors of molecular machines and motors. This work was published in the August 2013 issue of *Nature Chemistry*. (http://www.nature.com/doifinder/10.1038/nchem.1668)

The **Hieftje** group has developed and is evaluating a new system for elemental analysis of solution samples. Unlike the popular and widely used method of inductively coupled plasma atomic-emission spectrometry (ICP-AES), the new emission source requires no compressed gases, nebulizer (sprayer) or spray chamber. Further, it requires less than 100 W of dc power, rather than the 1500 W of radio frequency power needed for ICP operation. Lastly, the emission spectra of the new source are surprisingly uncomplicated, and contain mainly spectral lines of neutral atoms. As a result, spectral interferences are far less likely than in ICP-AES, and even moderate-resolution spectrometers or interference filters can be used to isolate the emission lines of interest. Perhaps surprisingly, the new source yields detection limits that are at least as good as those achievable with ICP-AES, and precision reaches the 1% rsd level. Termed the Solution-Cathode Glow Discharge (SCGD), the source is compact and seems ideally suited for elemental analysis in remote sites, and for unattended operation. It is also being explored as a detection method for separation methods, particularly ion chromatography. Group members active in the project include **Andy Schwartz** and Dr. **Steven Ray**.

At the Electrochemical Society meeting in Toronto, Canada, in May, 2013, **Elizabeth Wagoner**, **Jonathan Karty**, and Dennis Peters were coauthors of an invited oral paper on the nickel(I) salen-catalyzed reduction of 4,4′-(2,2,2-trichloroethane-1,1-diyl)bis(chlorobenzene) (DDT); a publication describing this work has appeared (*J. Electroanal. Chem.* **2013**, *706*, 55–63). **Angela Peverly** completed her Ph.D. degree in April, 2013, and has moved across campus to be a postdoctoral fellow in environmental chemistry as a member of **Ronald Hites**' research group. Other recent publications from the Peters' group describe studies of the electrochemical reduction of Lindane at silver cathodes (**Angela Peverly**, **Jonathan Karty**, and **Dennis Peters**, *J. Electroanal. Chem.* **2013**, *692*, 66–71), the electrocatalytic reduction of 1,1,2-trichloro-1,2,2-trifluoroethane (CFC-113) at silver cathodes (**Elizabeth Wagoner** and **Dennis Peters**, *J. Electrochem. Soc.* **2013**, *160*, G135–G141), the reductive intramolecular cyclization of halophenylalkynes at silver electrodes (**Lauren Strawsine**, **Mohammad Mubarak**, and **Dennis Peters**, *J. Electrochem. Soc.* **2013**, *160*, G3030–G3037), and the reduction of decabromodiphenyl ether at carbon and silver cathodes (**Angela Peverly**, **Erick Pasciak**, **Lauren Strawsine**, **Elizabeth Wagoner**, and **Dennis Peters**, *J. Electroanal. Chem.* **2013**, *704*, 227–232). The August, 2013 issue of the *Journal of The Electrochemical Society* (co-edited by **Dennis Peters**, who continues to serve as one the Associate Editors of that journal) was devoted exclusively to 28 papers dealing with organic and biological electrochemistry. In August, 2013, three undergraduate research students left the group to pursue graduate work: **Clark Baumberger** (to Texas A & M University for chemical engineering), **Nathan Buehler** (to University of Utah for organic chemistry), and **Kent Griffith** (to Cambridge University in the United Kingdom for analytical–physical chemistry).

Jill Robinson, a senior lecturer, continues to improve active learning strategies in analytical chemistry lecture and laboratory courses. A new learn-lab classroom in Cedar Hall was used to facilitate collaboration and discussions by using tables and multiple projection screens instead of auditorium style seating. To demonstrate relevance in laboratory work, two projects were developed in collaboration with local businesses. The first was the evaluation of precision and accuracy of a microplate protein assay in the context of pharmaceutical product analysis. Wendy Clemmer, Director of Research at Baxter Biopharma Solutions, served as an industry expert and visited our class to answer questions that students had while working on the project. The second was quality control analysis of important flavor and aroma components in various types of beer for the Upland Brewery. The Upland recently moved to a new production facility on Bloomington's west side in order to increase production and improve uniformity in batches. The

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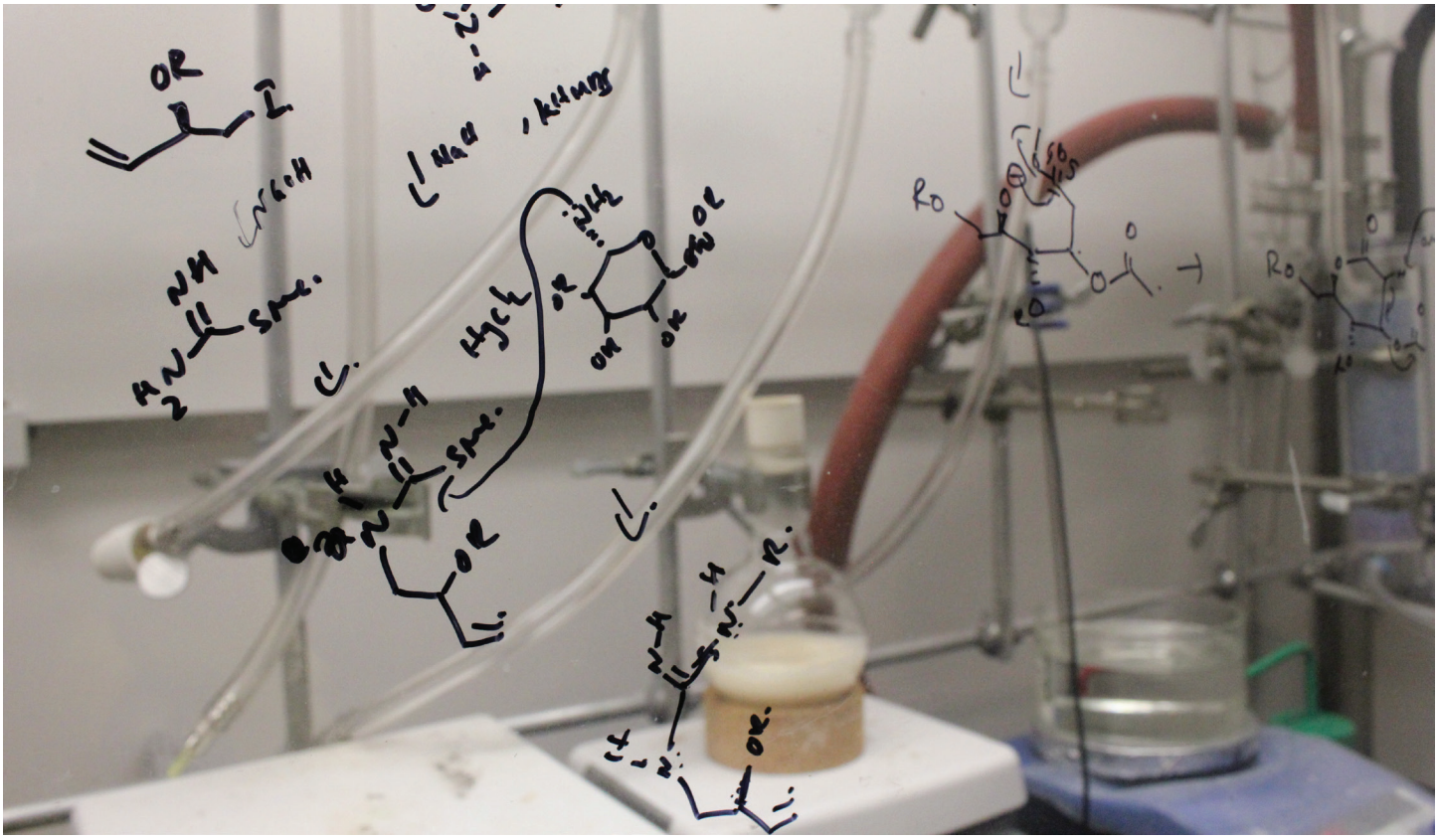
students' data will help the staff at the brewery evaluate processes over time. The brewery project has been published in the ABC's of Teaching Analytical Science Column (Anal Bioanal Chem, 2013, 405:7-13) and on the Analytical Digital Sciences Active Learning Website- a peer reviewed site currently being developed with NSF funding. (http://community.asdlib.org/activelearningmaterials/category/laboratory-activities/).

Analytical chemistry students working in groups in the new learn-lab in Cedar Hall.

This last year has been marked with a lot of travel for many members of the **Skrabalak** Laboratory. Professor Skrabalak organized a special symposium "Advanced Metal Nanocrystals for Catalysis" for the Division of Inorganic Chemistry at the Fall National ACS Conference in Philadelphia, where graduate students **Chris DeSantis**, **Moitree Laskar**, and **Nancy Ortiz** all presented their results on metal nanomaterial synthesis and their applications to catalysis and chemical sensing. Nancy Ortiz received an ACS GREET award, which provided her with resources to travel to Victoria University, New Zealand where she started a collaboration with Professor Richard Tilley's laboratory. This program paid for Professor Skrabalak to visit New Zealand for two weeks. During that time, Professor Skrabalak gave seminars at both Victoria University and the University of Auckland. She and Nancy also traveled a bit through the beautiful country and caught up with IU Chemistry Professor **Amar Flood** who was visiting his home country and also giving a seminar at Victoria University. With the skills gained from this visit, Professor Skrabalak and Nancy are now conducting scattering experiments at various synchrotrons in order to monitor nanomaterial formation in real time. In addition to this new research direction, a collaboration with the Dragnea laboratory has begun and is spearheaded by new graduate student **Alison Smith**, where she is using tools built in the **Dragnea** Laboratory to understand the light scattering properties of individual nanoparticles. In 2013, Professor Skrabalak was also selected as a Sloan Research Fellow and a recipient of an Early Career Award from the Department of Energy.

Professor **Yan Yu** is an assistant professor of Chemistry who joined in July 2012. Research in the Yu laboratory focuses on using chemical and material approaches to understand and manipulate cell-cell and cell-materials interactions, with potential applications in developing novel therapeutic materials to treat cancer and infectious diseases. With multidisciplinary approaches from chemistry, materials engineering, and biophysics, researchers in her laboratory are current working on the following problems: (1) How to use surface chemistry of micro- and nano-particles to control immune cell functions? (2) How do immune cells use protein arrangements in their cell membranes to control the "on" and "off" of the immune responses? (3) Can we reproduce the various shapes of cellular organelles using chemistries of artificial cell membranes? Research in the Yu laboratory brings multidisciplinary approaches from materials engineering, biophysics, and cell biology to modern chemistry. ■



FACULTY PROFILE: Carolyn Jarrold

by Kate Reck

While many of our colleagues are still sleeping, Caroline Jarrold is already in the building in the wee hours of the morning getting work done. A native from Michigan, Caroline grew up in Detroit, and later, Saginaw, Michigan. The daughter of a piano teacher, Caroline was encouraged to pursue her artistic inclinations. Starting in college, her intention was to become a biological illustrator to unite her love of drawing and science. However, the early coursework in biology did not suit her as much as she had anticipated.

Luckily for us, honors freshmen chemistry piqued her interest. She found herself qualified with her strong math and physics background, and the field of chemistry fit like a glove. While in college, she enjoyed a wide variety of courses from the sciences to music composition, and earned her B.S. in Chemistry at the University of Michigan, Ann Arbor, in 1989.

She left the Midwest for the west coast to pursue her Ph.D. in Physical Chemistry from the University of California, Berkeley, where she worked on ZEKE spectroscopy of negative ions in the laboratory of Daniel Neumark. After earning her Ph.D. in 1994, she became a University of California President's Postdoctoral Fellow at UCLA, where she synthesized and measured photophysical properties of semiconductor nanoparticles in the laboratory of James Heath (now at Cal Tech). Finally, she joined the Chemistry faculty at the University of Illinois, Chicago in 1997, where she receive tenure just prior to her move to the Indiana University Chemistry Department in 2002. Prof. Jarrold's research involves applying a combination of gas-phase reactivity, mass spectrometry, anion photodetachment spectroscopies, and computational chemistry. Since coming to the department, her research has taken on a strong multidisciplinary and collaborative focus.

All research projects in the Jarrold group are motivated by problems associated with *energy* and the *environment*. One such project involves probing the electronic, structural and chemical properties of homonuclear and heteronuclear transition metal oxides and sulfides. In particular, the group attempts to correlate structural and electronic features of metal suboxide (oxygen-deficient) species with chemical activity toward small molecules such as H_2O (for H_2 production), CO_2 (for CO_2 reduction) and CH_4 (for value addition). The primary goal is to understand the molecular scale metal oxide/reactant interactions that govern overall reactivity. The results can inform efforts to design and optimize low-temperature, robust heterogeneous catalysts for important processes, such as H_2 production from water decomposition. For this broad project, the Jarrold group has a very synergistic and productive collaboration with the theory group of Prof. Krishnan Raghavachari, who approach the same systems with high-level computational studies. The result of the interplay between theory and experiments is a much deeper understanding of the underlying chemical and physical principles that can then be generalized to a variety of metal oxide systems, and larger, applied systems.

Another research thrust in the Jarrold group is atmospheric reaction complexes leading to the oxidation of volatile organic compounds. Starting with relatively stable negative ions, e.g., OH^- or O_3^-, X^-·(isoprene) molecular clusters can be readily generated and mass selected. Photodetachment of the ions allows direct access to a neutral system at an energy associated with species deformed in a collision. Shifts in neutral energy levels that cannot otherwise be readily observed by standard spectroscopic techniques allow the Jarrold group to draw conclusions about the relationship between molecular collisions and, for example, the consequent sensitization of atmospheric species to photolysis while undergoing collisions.

Around ten undergraduates have found a good home in the Jarrold lab. These undergraduates get a valuable experience in how research is accomplished. Surrounded by electron guns, lasers, molecular beams and differentially pumped vacuum chambers, undergraduates work with a graduate student, they watch and learn, ask questions, and keep the graduate students on their toes. Several graduate students who have matriculated from the Jarrold group have found a variety of employment opportunities, such as AK Steel, Intel and academic positions.

Prof. Jarrold has been a good member of the department. She served as Director of Graduate Studies from 2010–2013. As DGS she helped make the graduate office a more welcoming environment. Her philosophy was to encourage inclusiveness and diversity. During her tenure as DGS, the graduate students in the department at the grass-roots level founded the Chemistry Graduate Representative Committee (GRC), with whom Jarrold met to ensure the graduate students had a voice in departmental concerns.

Prof. Jarrold's pioneering involvement with Prof. **Martha Oakley** to initiate the Women in Chemistry program has also brought a more supportive environment to our department. As a strong role model, this department has hired five more tenure-track women faculty (four at the assistant level, one at the senior level) bringing our number to seven women in chemistry. Jarrold also was involved in the formation of the Women in Science Program, facilitated by the (former) Office for Womens' Affairs. WISP introduced the annual Research Day for graduate and undergraduate women in STIM departments. Continuing her commitment to the department, she is currently chairing the new Diversity Affairs Committee.

Prof. Jarrold's accomplishments have been recognized, and she has risen to the rank of Full Professor. But that has not slowed her down. In fact, she is busier than ever I can barely keep up with her — *literally, she walks faster than anyone I know!* ■

STAFF NEWS

by Cheryl Johnson

Marcia Brown has been hired as a Supplies Coordinator in the Chemistry Scientific Storeroom (replacing Devon Underwood). Marcia has 16 years of experience working at Sunrise Greetings as a Shipping Clerk, Manifest Operator/Operations Specialist and Order Prep Clerk. In 1997 she received an Associated Degree in Conservation Law and Law Enforcement from Vincennes University.

Margit Campos was hired as an Office Assistant working under the direction of Dr. Jay Levy. She graduated from Academy Plus High School in 2004, then attended Ivy Tech Community College (Studies in Education).

Chris Chatelain has been hired as a Lecture Demo Technician in the undergraduate teaching labs (replacing Oscar Judd). Chris has a BS in Biochemistry and has experience in performing chemistry demonstrations at the Boys and Girls Club events and at IU Chemistry Open House. He also worked as the Preparatory Laboratory Assistant for the Chemistry Undergraduate Program since August 2010.

Shelly Dodson was hired as the Student Services Assistant in the Undergraduate Office (replacing Amanda Ellis) Shelly received an A.A. in Liberal Arts from Saint Cloud State University (Saint Cloud, MN) in 2002, and a B.S. in Community Health Education from Portland State University (Portland, OR) in 2010. She recently relocated back to the Bloomington area to be closer to family.

Pavle Kirilov was hired as a Senior Electronics Engineer Specialist in the Chemistry Department. Pavle came to Bloomington from the Atmospheric Sciences Department at the University of North Dakota, Grand Forks, ND. He received his M.Sc. in Electrical Engineering (1983) from the Faculty of Electronic Engineering, University of Nis, Yugoslavia. Pavle has over 20 years of experience on higher education research and in industry.

Tania Koontz was hired as the Office Services Assistant Senior in the Chair's Office (replacing Kathy Fields after she retired). She comes to us with an Associate Degree in Business Administration from Ivy Tech Community College. Tania brings 17 years of experience from Sunrise Publication, Inc. where she held positions with increased responsibility such as Assistant Buyer to Senior Inventory Controller.

Kristina McReynolds was hired as Grant Specialist (replacing Kelly Clark). Ms. McReynolds has over nine years of institutional experience in the field of research administration. Most recently she worked as a Grant and Contract Administrator at Northern Arizona University where she was responsible for finding extramural/intramural funding opportunities, developing proposal applications, drafting/approving budgets, and advising faculty on pre and post award compliance management.

Matthew Polley was hired as a Research Machinist III in the Chemistry Department (replacing Jeremy Boshears' machinist position vacated due to his promotion to Machine Shop Manager). Matthew is from Bloomington, Indiana. He received an AAS degree in Machine Trades Technology Injection Mold and Advanced CNC Manufacturing in April 2012. His work experience includes welding and machining at Carlisle Brake and Friction and at MCD Machine, as well as the repair, maintenance and operation of farming equipment at the Polley Ridge Farm.

Service Recognition

10 years – **Stephen Creps, William Unrue**
20 years – **Brian Ferguson, Rebecca Hanson, Judi Roberts**
25 years – **John Poehlman, Amy Van Pelt**
30 years – **Brian Crouch, Stacy Felton**
35 years – **Delbert Allgood**

2012 Staff Award Recipient

Becky Wilson
James Clark

In Memoriam

Robert Addleman, 70
May 9, 1942 - December 23, 2012
Robert Edward Addleman passed away on December 23, 2012 in Bloomington Hospice House. He was the son of Edward and Grace Marie (Jones) Addleman and was born in Pittsburgh, PA. Robert worked for I.U. Chemistry as an electronics engineer for 34 years and was an avid Boy Scout leader. He had a passion for antique cars and tractors. Robert was a very loving husband and father who leaves behind his wife, Carole (Dierker) Addleman; son, Hans (wife Jennifer) Addleman; daughter, Elisabeth (husband Brandon) Sturgis; grandson, Logan Addleman; his brother, Terry (wife Dianne) Addleman and five nephews.

Patricia Ann Stapleton, 80
April 7, 1932 – January 31, 2013
We note with sadness the death of Pat Stapleton on January 31, 2013 in Aurora, Colorado, where she had moved upon her retirement in 2002 to be near her son Jeff, his wife Terri and her grandsons, Tyler and Kiefer. Pat joined the Chemistry Department in 1975, initially as a secretary in the Graduate Office, but she was rapidly promoted to the position of Administrative Assistant for Graduate Affairs, a post she held with distinction until her retirement.

During most of her long tenure, Pat was the key staff person involved with the recruitment and subsequent administration of the graduate careers of approximately a thousand advanced degree candidates. Many alumni will no doubt remember Pat's invaluable advice and encouragement as they navigated the complex and frequently challenging pathways leading to their graduate degrees. She clearly contributed substantially behind the scenes to the growth in size and reputation of the graduate program in Chemistry at IU.

Pat was a consummate professional who always showed great concern and sensitivity for the needs of the students and the image of the Department and the University. Her energy, tenacity and capacity for hard work were legendary, as were her standards for accuracy and attention to detail in her work product. In recognition of her outstanding service, Pat was selected for the *Chemistry Staff Award* in 1980 and for the prestigious Leo F. Solt Distinguished Service Award of the Graduate School in 1998.

Outside of Chemistry, Pat was active in local politics and served on the Monroe County Alcoholic Beverage Commission during a time when liquor licenses were rare and highly sought after. Pat was an extraordinarily gifted and prolific knitter, a hobby that she no doubt practiced on the cross-country train trips she loved so well and during televised sporting events involving either IU or Purdue, where her son studied engineering and played football. ■

CONFERENCES, SPECIAL LECTURES & SYMPOSIA

Over the last calendar year, IU Chemistry was treated with over 130 seminar speakers presenting their recent research efforts in our department. These speakers included fifth-year graduate students and defending Ph.D. students, present IU faculty and staff, including faculty visiting IU from around the world, representing all areas of chemistry and biochemistry. A few major highlights of this past year's lectures and symposia are provided below.

September 29, 2012: *Watanabe Symposium in Biotechnology*

The Watanabe Symposium honors the late August "Gus" Watanabe, a renowned physician, researcher and professor who led research and development at Eli Lilly and Company for nearly a decade, and who was a pioneer in the study of the cellular mechanics of the heart. In 1994, Watanabe assumed the role as President of Lilly Research Laboratories and is responsible for launching eleven new and pivotal pharmaceutical products. IU hosted the 3rd annual Watanabe on September 29, 2012, and the list of speakers is below.

- **Professor Kate Carroll**, Associate Professor, Department of Chemistry, The Florida Scripps Research Institute, *"Painting the Cysteine Chapel: New Tools to Probe Oxidation Biology"*
- **Professor Peter Schultz**, Professor of Chemistry, Scripps Research Institute, Director of the Genomics Institute of the Novartis Research Foundation, *"Synthesis at the Interface of Chemistry and Biology: From Stem Cells to the Genetic Code"*
- **Professor Stephen Jacobson**, Associate Professor, Indiana University, *"Micro- and Nanofluidic Devices for Cancer Screening and Virus Sensing"*
- **Professor Tom Kodadek**, Professor, Department of Cancer Biology Faculty, Kellogg School of Science and Technology, The Florida Scripps Research Institute, *"Chemical Tools to Monitor and Manipulate the Immune System"*
- **Professor Scott McLuckey**, John A. Leighty Distinguished Professor, Department of Chemistry, Purdue University, *"Bioconjugation in the Gas-Phase: An Exploration of New Directions in Tandem Mass Spectrometry"*
- **Professor JoAnn Stubbe**, Novartis Professor of Chemistry & Biology, Massachusetts Institute of Technology, *"Clofarabine Nucleotides: Potent Inhibitors of Human Ribonucleotide Reductase via an Unexpected Mechanism"*

October 2, 2102: Gill Symposium – "Model systems for studying human disease"

The Linda and Jack Gill Center for Biomolecular Science (GCBS) was established to advance the understanding of complex biological processes and to train next generation scientists in state-of-the-art biomolecular measurements, especially in the field of neuroscience. Collaborations include Indiana University's world-class Departments of Biology, Chemistry, Molecular and Cellular Biochemistry, Physics, Psychological and Brain Sciences, Neuroscience, and the School of Medicine.

- **Dr. Hugo Bellen**, HHMI, Baylor College of Medicine, 2012 Gill Award recipient, *"Molecular Mechanisms Underlying Lou Gehrig's Disease (ALS)"*
- **Dr. Guoping Feng**, Massachusetts Institute of Technology, 2012 Gill Young Investigator Award recipient, *"Probing Synaptic and Circuitry Mechanisms of Psychiatric Disorders"*
- **Dr. Craig Montell**, The Johns Hopkins School of Medicine, *"Control of Animal Behavior and Decision Making through TRP Channels"*
- **Dr. Ulrike Heberlein**, HHMI, Janelia Farms Research Campus, *"Flies, Sex, and Alcohol: How Social Experience Affects Ethanol Consumption"*
- The symposium culminated with a graduate student poster session, 5:30 - 6:30 p.m., in the Frangipani Room, Indiana Memorial Union.

Graduate student poster session at the Gill Symposium.

October 13, 2012: Inorganic Annual Alumni Symposium

- **Dr. Brad Bailey,** (Ph.D. 2007, Professor **Daniel Mindiola**), Associate Scientist, Dow Chemical, Midland, MI, *"Selling Out to Industry and Loving It"*
- **Dr. Sibaprasad Bhattacharyya**, (post-doctoral 2003-2005, Professor **Jeffrey Zaleski**), Senior Scientist, Frederick National Laboratory for Cancer Research, NIH/NCI, *"Translating Radiolabeled Biomolecules – From Bench to Bedside"*
- **Dr. Falguni Basuli**, (post-doctoral 2003-2005, Professor **Daniel Mindiola**), Research Chemist, Imaging Probe Development Center (IPDC), National Heart, Lung, and Blood Institute, National Institutes of Health, Rockville, MD, *"Fluorine-18 Labeled Radiotracers for Positron Emission Tomography (PET) Imaging"*
- **Dr. Xiaofan Yang**, (Ph.D. 2008, Professors **Mu-Hyun Baik** and **Kenneth Caulton**), Staff Chemist, BASF Corporation, Iselin, NJ, "*Catalysis, from Air Free to Air Rich"*

Other Special Seminars

October 12, 2011 ACS *Student Selected Seminar* was delivered by Professor **Michael Summers**, Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD, *"Insights into the Mechanism of HIV-1 Genome Packaging and Virus Assembly"*

November 2, 2011 *Frank C. Mathers Lecture* was delivered by Professor **Samuel Stupp**, Board of Trustees Professor of Materials Science, Chemistry and Medicine, Departments of Chemistry, Materials Science and Engineering, and Medicine, Northwestern University, Evanston, IL, *"Self-Assembly in Materials Chemistry"*

March 21, 2012 *ACS Student Selected Seminar* was delivered by Professor **Fred McLafferty**, Peter J. W. Debye Professor Emeritus, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, *"Gas-Phase Protein Chemistry: Unfolding and New Folding Pathways in Electrosprayed Native Ubiquitin"*

April 4, 2012 *Chemistry of Everyday Life Series* was delivered by Dr. **Joe Schwarcz**, Director, Office for Science and Society, Department of Chemistry, McGill University, Montreal, Quebec, Canada, *"Hey! There Are Cockroaches in my Chocolate Ice Cream"*

April 25, 2012 *Raymond Siedle Distinguished Lecture* was delivered by Professor **Guy Bertrand**, Distinguished Professor of Chemistry, University of California, Riverside, CA, *"Novel Families of Carbon- and Boron-based Ligands, Novel Catalytic Reactions"*

November 7, 2013 *ACS Student Selected Seminar:* Professor **Daniel Nocera**, Patterson Rockwood Professor of Energy, Harvard University, Cambridge, MA, "The Artificial Leaf"

January 16, 2013 *Harry G Day Distinguished Lecture:* Professor **Kevan M. Shokat**, Professor and Chair, Department of Cellular and Molecular Pharmacology, University of California San Francisco, CA, *"Chemical Genetic Dissection of Oncogenic Signaling Pathways"*

February 6, 2013 *Student Selected Seminar Speaker:* Professor **Timothy M. Swager**, Timothy M. Swager, John D. MacArthur Professor, Department of Chemistry, MIT, Cambridge, MA, *"Synthesis of Polycyclic Aromatics for use as High Performance Electronic Materials"*

March 6, 2013 *ACS Chemistry of Everyday Life Seminar:* Professor **Kent Kirshenbaum**, Associate Professor, Department of Chemistry, New York University, New York, NY, "A Taste for Science: Adventures at the Interface of Chemistry and Cuisine"

March 27, 2013 *Raymond Siedle Lecture:* Professor **Jacqueline K. Barton**, Jacqueline K. Barton, Arthur and Marian Hanisch Memorial Professor and Chair, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, *"DNA Signaling by Metalloproteins"*

April 10, 2013 *Student Selected Analytical Seminar:* Professor **Allen Bard**, Department of Chemistry, University of Texas at Austin, Austin, TX, *"Electrochemistry of Single Molecules and Single Nanoparticles"*

August 23, 2013 *Frank C. Mathers Distinguished Lecture:* Professor **Trevor Douglas**, Regents Professor, Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT, "Packing Them In: Using Self-Assembled Protein Cages to Direct the Synthesis and Packaging of Polymers, Minerals, and Proteins."

Professors (left to right) Amar Flood, Bogdan Dragnea, Frank C. Mathers Distinguished Lecturer Trevor Douglas, David Giedroc, and Srini Iyengar.

Chair's Letter

Continued from page 1

I note with regret that two inorganic chemists have left the department in the past year, including Profs. **Dan Mindiola**, to the University of Pennsylvania, and **Dongwhan Lee**, to Seoul National University in Korea. As significant contributors to the faculty, we're sorry to see them go; however, we wish them the best of success in their new locales. Finally, I note with sadness that Prof. Emeritus **Earnest E. Campaigne** passed away this past spring in his late 90s. A scientific symposium is planned in the late Prof. Campaigne's honor for Saturday, October 26, 2013, with three outstanding organic chemists most familiar with Campaigne's work to come to Bloomington to lecture in his honor.

In closing, let me again express my gratitude for your continued support of the department. Please stop by during your next trip to Bloomington — you're always welcome here.

— David Giedroc

STAFF PROFILE

by Norman Dean

James Clark, Freshman Chemistry Coordinator

If you ask **James Clark** what his duties in the chemistry department are, don't expect a quick answer. As Freshman Chemistry Coordinator, he oversees the operation of the 100-level chemistry lab courses: C103, C118, C121, C122, and C127. He helps hire, train and schedule 15-20 undergraduate workers a semester and is supervisor to the two demonstration technicians. As part of his responsibilities he makes sure that chemicals are prepped for the courses, equipment is available and in "good" working condition, and has a major role in enforcing the safety policies for the labs.

Blowing off a little steam before a demonstration.

As Outreach Coordinator, he serves as a resource for local teachers by lending them equipment and other supplies to enrich their courses and by serving as the contact person in the department for other agencies. In the last year he gave more than 30 demo shows, both on and off campus for local schools and community organizations; coordinated departmental tours for visiting high schools; participated in six different summer camps and programs; and coordinated chemistry activities for Family Science Nights at all the local Bloomington area elementary schools. As if that isn't enough he is also the coordinator for the department's annual chemistry open house during National Chemistry Week and teaches a course in chemistry, *G201: Service Learning in Chemistry: Community Outreach*.

In G201 students learn to plan, prepare, and present hands-on science activities with children. They then put their skills into action around Bloomington working with after school programs at the Boy's and Girl's Club, Girl's Inc., and the Banneker Center. In 2013 James was co-winner of the staff award (along with glassblower Don Garvin) for his outreach work on behalf of the department.

James came to the department in 2007 after teaching Chemistry, AP Chemistry, and Physical Science at Edgewood High school in Ellettsville IN for 3 years. He graduated from Ball State University in Muncie in 2003 with a BS degree in Chemistry and Secondary Education. Although he was born in Illinois, from 3rd to 5th grade he attended University Elementary School when his parents Jeff and Sue and his sisters Rachel and Christine lived in Bloomington. Although his family also lived in New Albany, he primarily considers Muncie his 'Hometown" as it is where he went to high school and college while his parents were Professors of Physiology and Health Science at Ball State.

He has been married for 9 years to his wife Erin, who is the H1B scholar advisor for the Office of International Services at IU. While he loved being in the classroom and watching his students mature through their four years of high school, the opportunity to work on campus with his wife was one of the benefits that convinced James to leave teaching high school. He also admits that getting to blow things up regularly when giving demo shows was a big part of the reason as well. He had some very big shoes to fill in taking over the demo shows as they had previously been run by Prof. **Dennis Peters**. If one of the requirements for engaging young people in science is to always have a bit of little kid inside you, then James easily passes the test. This is apparent to anyone who has seen the extensive collection of science (and other) toys found in his office.

Surprisingly James somehow has time to devote to several hobbies. He enjoys participating in triathlons, and he both plays and referee's soccer. He comes from a family of swimmers so swimming remains an activity he enjoys, and he has also coached swimming both at Edgewood High school and for fellow triathletes. He and a group of friends have been known to (*allegedly for fun?*) bike from Muncie to Indianapolis the morning of the Indy Mini marathon and then run the race. He enjoys travelling having visited Hawaii, San Francisco, and France in recent years and would be described by most of his friends and colleagues as something of a foodie. He also finds time, along with his wife, to volunteer at the No Limits Diabetes camp each summer. We are not sure what we did before we had James here, and we hope we don't find out! ■

GRADUATE NEWS

by Toni Lady

During the 2012-2013 school year, Professor **Caroline C. Jarrold**, was the Director of Graduate Studies. Serving with her on the Standards Committee were professors **Mu-Hyun Baik**, **Richard DiMarchi**, **Amar Flood**, **Dennis Peters**, and **Michael Van Nieuwenhze**.

Daniel Mindiola chaired the Graduate Admissions Committee. Evaluating the hundreds of dossiers submitted to the department were professors **Mu-Hyun Baik**, **Kevin Brown**, **Erin Carlson**, **Silas Cook**, **Charles Dann III**, **Steven Tait**, **Megan Theilges**, and **Yan Yu**.

Fellowship Award Winners for 2012-2013

- **Christopher DeSantis** was awarded the Raymond Siedle Materials Fellowship. Chris joined the lab of Dr. **Sara Skrabalak** in the fall 2009.
- **Benjamin Gamoke** was awarded the Richard Slagle Fellowship. Ben joined the lab of Dr. **Krishnan Raghavachari** in the fall 2009.
- **Semin Lee** was awarded the Chester Davis Organic Fellowship. Semin joined the lab of Dr. **Amar Flood** in the fall 2009.
- **Katie Leslie** was awarded the Raymond Siedle Inorganic Fellowship. Katie joined the lab of Dr. **Martin Jarrold** in the fall of 2009.
- **Qiqi Li** was awarded the Paget Organic Fellowship. Qiqi joined the lab of Dr. **Liang-shi Li** in the fall of 2010.
- **Sarah Lindahl** was awarded the Chester Davis Inorganic Fellowship. Sarah joined the lab of Dr. **Jeffery Zaleski** in the fall 2009.
- **Daniel Skomski** was awarded the Richard Siedle Materials Fellowship. Daniel joined the lab of Dr. **Steven Tait** in the fall 2010.
- **Elizabeth Wagoner** was awarded the Robert & Marjorie Mann Fellowship. Lizzy joined the lab of Dr. **Dennis Peters** in the fall 2009.
- **Sarah Waller** was awarded the E.M. Kratz Fellowship. Sarah joined the lab of Dr. **Caroline Jarrold** in the fall 2009.

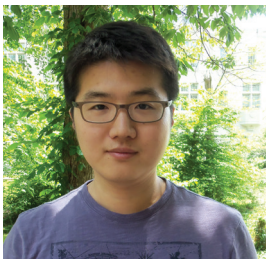
Other Fellowship Recipients:

- **Scott Curtis**, Chester Davis add-on Inorganic/Organic Fellowships
- **Jonathan Dilger**, Crane Fellowship
- **Ethan Harak**, Chester Davis add-on Inorganic/Organic Fellowships
- **Zachary Harms**, QCB Training Grant Fellowship
- **Andrew Johnson**, QCB Training Grant Fellowship
- **David Keifer**, QCB Training Grant Fellowship
- **Rachel Lecker**, Baxter Fellowship
- **Ziran Li,** Mann Fellowship, Paget add-on Organic Fellowship
- **Kaitlyn Logan**, Chester Davis add-on Inorganic/Organic Fellowships, Berk Fellowship
- **Keevan Marion**, Mays Fellowship
- **Erin Martin**, Mann Fellowship
- **Fese Mokube**, NIH-Pre-doctoral Fellowship
- **Kevin Schwarz**, Mann Fellowship, Paget add-on Organic Fellowship
- **Elizabeth Siegel**, QCB Training Grant Fellowship
- **Alison Smith**, Crane Fellowship
- **Jonathan Snider**, Paget add-on Organic Fellowship
- **Mitchell Stadler**, Lanterman Fellowship
- **Alison Vickman**, Berk Fellowship, Paget add-on Organic Fellowship
- **Kaelyn Wilke**, QCB Training Grant Fellowship

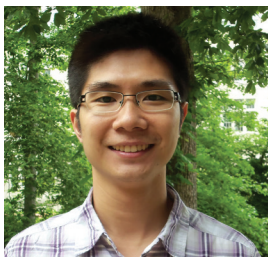

Christopher DeSantis


Benjamin Gamoke


Ozden Kocaoglu


Semin Lee


Katie Leslie


Qi Qi Li

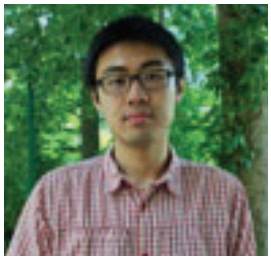

Sarah Lindahl


Shivnath Mazumder


Megan McCormick


Nancy Ortiz

Aylssa Pirinelli


Bo Qial

Christ Rasik

Jonathan Rittichier

Keith Searles

Akshay Shah

Daniel Skomski

Elizabeth Wagoner

Sarah Waller

Anna Weber

Annual Chemistry Department Award Winners

E. Campaigne C500 Award: **Christopher Rasik**, Professor Kevin Brown lab

Jack K. Crandall Award: **Akshay Shah**, Professor David Williams lab

Wendell P. Metzner Memorial Award: **Shivnath Mazumder**, Professor Mookie Baik lab

William H. Nebergall Memorial Award: **Keith Searles**, Professor Mu-Hyun Baik lab

Felix Haurowitz Award: **Zachary Harms**, Professor Daniel Mindiola lab

Felix Haurowitz Award: **Benjamin Gamoke**, Professor Krishnan Raghavachari lab

Henry R. Mahler Award: **Ozden Kocaoglu**, Professor Erin Carlson lab

David A Rothrock Award: **Daniel Skomski**, Professor Steve Tait lab

Charles H. Stammer Award: **Semin Lee**, Professor Amar Flood lab, **Qiqi Li,** Professor Liang-shi Li lab

Associate Instructor Awards: **Anna Weber**, Professor Lane Baker lab; **Meghan McCormick**, Professor Mookie Baik lab; **Bo Qiao**, Professor Amar Flood lab; **Jonathan Rittichier**, Professor Mike Van Nieuwenhze lab; **Alyssa Pirinelli**, Professor Nicola Pohl lab

Congratulations to recent graduates!

Ph.D. Degree Recipients

Natalya Atlasevich, Analytical, November 2012, Professor **David Clemmer**

Bruce Atwater, Organic, May 2013, Professor **David Williams**

Indrani Bhattacharyya, Materials, November 2012, Professor **Martin Jarrold**

Randall Binder, Organic, May 2013, Professor **Michael Van Nieuwenhze**

Angela Carrillo, Organic, August 2012, Professor **Michael Van Nieuwenhze**

Chiao-Chen Chen, Analytical, December 2012, Professor **Lane Baker**

Shujiang Cheng, Chemical Biology, December 2012, Professor **Richard DiMarchi**

Ramkrishna De, Organic, November 2012, Professor **David Williams**

Soumya Ghosh, Inorganic, February, 2013, Professor **Mookie Baik**

Alfredo Guerra, Chemical Biology, September 2012, Professor **David Giedroc**

Yuran Hua, Materials, August 2012, Professor **Amar Flood**

Junyong Jo, Inorganic, April 2013, Professor **Dongwhan Lee**

Pucheng Ke, Organic, April 2013, Professor **David Williams**

Sarah Keane, Chemical Biology, August 2012, Professor **David Giedroc**

Matthew Lauber, Chemical Biology, July, 2012, Professor **James Reilly**

Wenjun Liu, Inorganic, June 2012, Professor **Dongwhan Lee**

Benjamin Mann, Analytical, January 2013, Professor **Milos Novotny**

Amanda Mann, Inorganic, November 2012, Professor **Sara Skrabalak**

Byung Gyu Park, Inorganic, April 2013, Professor **Dongwhan Lee**

John Perry, Analytical, October 2012, Professor **Stephen Jacobson**

Angela Peverly, Analytical, April 2013, Professor **Dennis Peters**

Abhishek Singha Roy, Physica, January 2013, Professor **Peter Ortoleva**

Nichole Stewart, Chemical Biology, June 2013, Professor **Martha Oakley**

Benjamin Wicker, Inorganic, August 2012, Professor **Daniel Mindiola**

Xin Yan, Materials, May 2012, Professor **Liang-shi Li**

MS Degree Recipients

Irma Hamilton, Materials, December 2012, Professor **Liang-shi Li**

Oscar Judd, Analytical, December 2012, Professor **Martin Jarrold**

Continued on page 24

GRADUATE NEWS

Continued from page 23

Special Recognition Awards

Alexander Gundlach-Graham (Hieftje's Group) was chosen to receive the **2013 Gordon F. Kirkbright bursary award**. The bursary award is a prestigious annual award that enables a promising student/non-tenured young scientist of any nation to attend a recognized scientific meeting or visit a place of learning. The fund for this bursary was established in 1985 as a memorial to Professor Gordon Kirkbright in recognition of his contributions to analytical spectroscopy and to science in general.

Alexander Gundlach-Graham (Hieftje's Group) was the recipient of the **2013 ACS Division of Analytical Chemistry Graduate Fellowship Award** sponsored by Agilent Technologies.

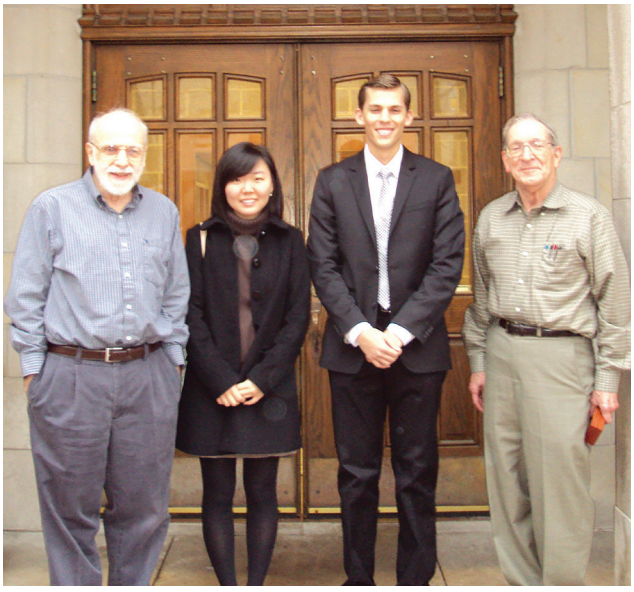
Nancy Ortiz for being the recipient of the **2013 Distinguished Graduate Student Award** sponsored by the Latino Faculty and Staff Council. These awards were given to individuals whose efforts have contributed to a positive campus environment in tandem with helping support retention of Latinos at Indiana University. It is also meant to highlight exemplary academic and professional work.

Raghunath O. Ramabhadran (Raghavachari's Group) is the recipient of a Research Excellence Award by the Computers in Chemistry division of the ACS. He received the award at the New Orleans National ACS meeting.

Andrew Schwartz (Hieftje's group) is the recipient of a **Society for Applied Spectroscopy (SAS) 2013 Graduate Student Award**. This award was given based on Andrew's outstanding work in the area of atomic emission spectroscopy, leadership role within the research group and exceptional productivity evidenced by multiple first-author papers published in excellent journals. He will receive the award at the national meeting, SciX, this fall in Milwaukee, WI.

Kaelyn Wilke (Carlson Group) is the recipient of a **2013 Aldrich Graduate Student Innovation Award** sponsored by the Sigma-Aldrich Company. Aldrich typically gives eight to ten GSIA awards annually to students who have completed three years of graduate study for work that focuses on the "de-velopment and creative use of current or new reagents, catalysts, and ligands in methodology or syn-thetic chemistry projects." The recipients receive a $1K cash award, an iPad 3, and expenses for a trip to the 2013 GSIA Symposium. All Awardees give a short presentation on their research.

Undergraduate News: Fall 2012 and Spring 2013 G410 Symposium Students



Fall 2012 G410 Symposium Students and their PIs; from left, Professor **Peter Ortoleva**, **Yeiji Im**, **Clark Baumberger** and Professor **Dennis Peters**.

Spring 2013 G410 Symposium Students. Front row, from left: **Clayton Brown**, **Rebecca Schwab**, **Emily Renzi**, **Michelle Gray**; back row, from left: **Joseph Dempsey**, **Nathan Buehler**, **Kent Griffith**, **Ian Norden**, and **Joseph Thomas**.

UNDERGRADUATE NEWS

by Carly Friedman

This past year brought us 95 new alumni to the IU-Chemistry family after December 2012 and May 2013 commencements. Our department conferred 11 chemistry BS degrees, 28 biochemistry BS degrees, 38 chemistry BA degrees, and 18 biochemistry BA degrees to our students.

One highlight of the undergraduate experience is our *Undergraduate Research Program* which serves to acquaint students with the nature of chemical research and to provide rewards for creativity and good scholarship. Students conducting undergraduate research work closely with a faculty advisor and with the graduate students, post-doctoral fellows, and other scientists in a group. They participate in all aspects of the research program including studying the original research literature, designing projects, and interpreting results. This year there were 55 students participating in the Undergraduate Research Program, and 13 students concluded the program with a thesis and oral presentation. Students frequently comment that their research experience was the best part of their academics at IU and is what really prepared them for their future endeavors We want to showcase two current student researchers: **Paige Matthews** from the **Dann lab** and **Jonathan Schmidt** from the **de Souza lab**.

Paige Matthews is a fourth-year student who is pursuing a Biochemistry BS. Paige is currently working on discovering biological mechanisms of proteins that produce cyclic-di-GMP (c-di-GMP), an important second messenger molecule in bacteria that has a role in various bacteria processes, such as promoting biofilm formation and virulence. In particular, she is studying a class of proteins called diguanylate cyclases, which are metabolic enzymes that convert two GTP to c-di-GMP and generally have a conserved GGDEF domain. Eventually, at least one of the protein structures will be determined for all three diguanylate cyclases. The research on diguanylate cyclases is important because these metabolic factors have great clinical applications as novel antibiotics drug targets. This could lead to development of a drug that inhibits c-di-GMP formation, leading to decreased formation of biofilms, a bacterial "coating" that imbues bacterial resistance to antibiotics and antiseptics.

Paige became interested in the Dann lab after she heard Dr. Dann discuss his research in *CHEM-C107: Frontiers of Chemical Research*. Throughout her three years in the Dann lab, Paige has earned three summer scholarships and one merit scholarship (this year she was awarded the *Robert & Marjorie Mann Scholarship* and the *Enola Rentschler Van Valer Trafford Scholarship*) which have allowed her to remain in Bloomington during the summers to focus on research and refining her skills. Her experience in the Dann lab has taught her not only lab techniques but, by solving research problems, she has also learned how to think in new ways that she can apply to her coursework and other academic pursuits. She is developing perseverance and determination which will help her reach her goal of becoming an excellent doctor. Her career aspirations have realized, as Paige just recently learned she was admitted to Indiana University School of Medicine for the entering class of fall 2014!

Jonathan Schmidt is also a fourth-year student pursuing a Biochemistry BS. Jonathan's research project involves the creation of a new detector which, when completed, should allow the group to image particle beams in accelerators with little to no beam tuning abilities. Specifically, the group intends to utilize it to image beams comprised of neutron-rich oxygen isotopes in an experiment which measures the fusion cross section of a number of these different isotopes and carbon-12. The detector itself uses scintillating fibers and silicon photomultipliers operated near breakdown at reverse bias to give an avalanche of electrons corresponding to an incident photon generated by an incoming particle. Jonathan is working with Dr. de Souza to implement his idea for the detector and is engineering the majority of the detector components and systems used for testing.

Although Jonathan was in Dr. de Souza's *S117: Honors Principles of Chemistry and Biochemistry* class, he did not get a good notion of de Souza's research until he heard him discuss it in the *C107: Frontiers of Chemical Research* course in the spring semester of his first year. He has learned many valuable things from his research experience, but most notable and enjoyable is the ability to use a variety of tools and thought processes in order to be directly involved in the engineering of a detector and various testing setups. Not only does he face academic and intellectual challenges, but he must also constantly be aware of logistical issues with designs such as cost, spatial requirements, and the efficiency of one method over another. Jonathan was awarded both the *Robert and Marjorie Mann Scholarship* for summer research and the *Grim Scholarship* for the academic year.

The department was able to award summer research scholarships to 20 students, including Paige and Jonathan, so that they could remain in Bloomington for the summer to continue their research.

Oftentimes, the culmination of this research experience is the *G410: Chemical Research Capstone*. After students have pursued at least two semesters of undergraduate research, students may elect to take this 2-credit course in which they finish up any final research details, write a senior thesis, and give a 25-minute oral presentation before their peers and the department to honor their accomplishments. This opportunity has existed for five years now, and we have had 61 students participate in this symposium.

Students who participated in the *G410: Chemical Research Symposium* this past academic year (see photos on previous page):

Fall 2012

- **Clark Baumberger**
- **Yeiji Im**

Spring 2013

- **Matthew Bower**
- **Clayton Brown**
- **Nathan Buehler**
- **Joseph Dempsey**
- **Michelle Gray**
- **Kent Griffith**
- **Ian Norden**
- **Emily Renzi**
- **Rebecca Schwab**
- **Tyler Stanage**
- **Joseph B. Thomas**

Continued on page 26

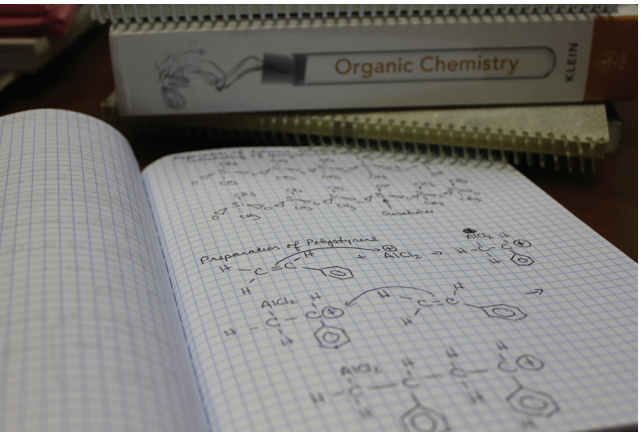
UNDERGRADUATE NEWS

Continued from page 25

Chemistry Honor Roll

The following chemistry and biochemistry majors attained an overall and in-major grade point average of 3.75 or better through the fall 2012 semester.

Senior Honor Roll: **Radhika Agarwal, Sukriti Bansal, William Berry, Wenjing Cai, Divan Chauhan, Kevin Chaung, Ryan Clodfelter, Caleb Cooper, Matthew Colin, Alexander Elias, Kent Griffith, Ethan Hamer, Shannon Harvey, Hailey Holland, Mary Hon, Jonathan Hourmozdi, An Huynh, Stephanie Iden, Ryan Kabi, Y-Lan Khuong, Joseph King, Alex Lazar, Chloe Mangas, Christopher Mattson, Zachary Moon, Stephen Overcash, Adam Richter, Jonathon Rogers, Jonathan Schmidt, Rebecca Schwab, Keith Scott, Supriya Shah, Joseph Thomas, Emily Tisma, Yilun Wang, Yueren Wang, Ethan Wappes, Audrey Welklin, Anirudh Yalamanchali, Evan Yanni, Michael Zimmerman**



Junior Honor Roll: **Kyle Baugh, Donald Brake, Ha Eun Cho, Matthew Coghlan, Lily Delalande, Ryan DesCamp, Ian Emmons, Robert Gassert, Adam Given, David Haak, Connor Hannon, Taylor Hero, Kristin Hunter, Evan Jameyfield, Madeline Jones, Luke Kurowski, Samantha Mayhew, Keerthana Mohankumar, Laura Oehlman, Grace Park, Brooks Platt, Trevor Poplewko, Andjela Radmilovic, Stephanie Ross, Jared Salisbury, Elizabeth Schueth, Molly Scripture, Juan Serna, Allyson Shambaugh, Samyuth Subramanian, Emma Winkler, Michael Wirey**

Sophomore Honor Roll: **Tyler Barnes, Grant Gornick, Samantha Harvey, John Hauber, Devin Jones, Kevin Kuo, Mary LaFleur Connie Lu, Kyle O'Malley, Priya Parikh, John Rose, Lauren Wahle, Joseph Wendt, Evan Zehr**

Freshman Honor Roll: **Kyle Hardwick**

Chemistry Honors Program

The following students are BS majors in chemistry or biochemistry, have maintained a minimum grade point average of 3.3, and have completed a research project and thesis.

Clark Baumberger, Clayton Brown, Joseph Dempsey, Kent Griffith, Yeiji Im, Ian Norden, Rebecca Schwab, Tyler Stanage, Joseph B. Thomas

Phi Beta Kappa Fall and Spring Inductees

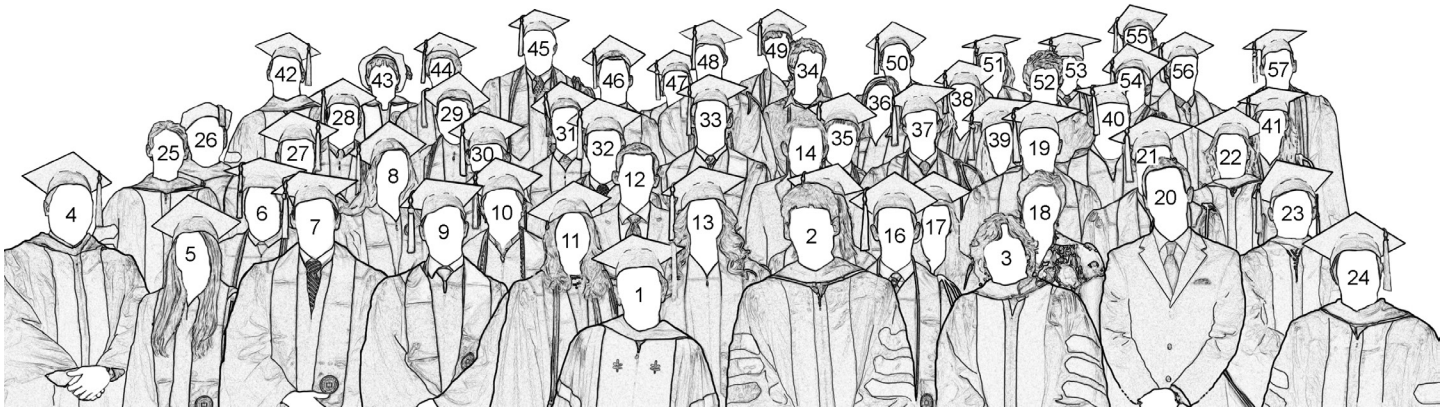
Michael Andreas, Clark Baumberger, William Berry, Stacey Blank, Matthew Bower, Maxwell Breitinger, Kevin Chaung, Ryan Clodfelter, Matthew Colin, Trevor Crafts, Liron Ganel, Kent Griffith, Logan Guckien, Ethan Hamer, Nicolas Hidalgo, Mary Hon, Jonathan Hourmozdi, Joseph King, Christopher Mattson, Zachary Moon, Stephen Overcash, Raymond Parrish, Adam Richter, Keith Scott, Adam Schafer, Supriya Shah, Joseph B. Thomas, Yilun Wang, Evan Yanni

Departmental Scholarships and Awards

- C117: **Stephen Hartman, Lauren Wahle**
- S117: **Kevin Kuo, Connie Lu**
- Organic Chemistry Course Award: **Eric Pan**
- American Chemical Society Award: **Sukriti Bansal, William Berry, Hailey Holland**
- Keith Ault Scholarship: **Anisha Joenathan**
- William H. Bell Award: **Alexander Doran, Andrea Patterson, Audrey Welklin**
- The John H. Billman Scholarship: **Tyler Barnes**
- Harry G. Day Summer Research Scholarships: **Alexander Doran, Rosemary Easterday, An Huynh, Evan Jameyfield**
- Leroy Dugan Scholarship: **Tyler Werner**
- Harlan English Scholarship: **Evan Jameyfield, Michael Wirey**
- Courson Greeves: **Patrick Gamache**
- Grim Scholarships: **Wenjing Cai, Caleb Cooper, Chloe Mangas, Ethan Wappes, Jonathan Schmidt, Ben Ryan**
- Russell & Trula Sidwell Hardy Scholarship: **Luke Kurowski**
- Ira E. Lee Summer Research Scholarships: **Wenjing Cai, Lily Delalande**
- Eli Lilly Organic/Williams: **Andrea Patterson**
- Andrew Loh Scholarship: **Ian Walker**
- Robert & Marjorie Mann Scholarships: **Luke Kurowski, Paige Matthews, Jonathon Rogers, Olivia Sanchez-Felix, Jonathan Schmidt, Michael Wirey**
- Frank Mathers Undergraduate Summer Research Scholarships: **Yeuren Wang, Ethan Wappes**
- Dennis Peters Scholarships: **Tyler Barnes, Olivia Sanchez-Felix, Lauren Wahle**
- William G. Roessler Scholarship: **Priya Parikh**
- Joseph B. Schwartzkopf Award: **Kent Griffith**
- Raymond Siedle Scholarship: **Patrick Gamache, Andjela Radmilovic**
- Sturdevant Summer Scholarships: **Adam Spitz**
- Lee J. Todd Chemistry Memorial Scholarship: **Matthew Bower**
- Enola Rentschler Van Valer Trafford Scholarship: **Paige Matthews, Yeiji Im**
- Viola Scholarship in Nuclear Chemistry: **Kent Griffith**
- Votaw Undergraduate Summer Research Scholarship: **Brooks Platt**
- Forrest L. Warner Scholarship: **Joseph Wendt, Devin Jones**
- Francis and Mildred (Eckerty) Whitacre Scholarship: **Jeff Rytlewski, An Huynh**
- James C. White Award: **Joseph B. Thomas**
- Mary Frechtling White Memorial Chemistry Scholarship: **Rebecca Schwab**

GRADUATION 2013

Photograph courtesy Chadon Photography.



Graduation "outline" made by William Unrue

1) Professor **Dennis Peters**, 2) Professor **David Giedroc**, 3) Professor **Martha Oakley**, 4) Professor **Todd Stone**, 5) **Stacy Blank**, 6) **Jonathan Hourmozdi**, 7) **William Tilbury**, 8) **Emily Renzi**, 9) **James Rizkalla**, 10) **Clayton Brown**, 11) **Mary Hon**, 12) **Clark Baumberger**, 13) **Jessica Bostic**, 14) **Matthew Colin**, 15) **Melissa Rosa** (behind David Giedroc), 16) **Matthew Bower**, 17) **Supriya Shah**, 18) **Sukriti Bansal**, 19) **Brian Andersen**, 20) **Lucas Berghoff**, 21) **Drake Everson**, 22) Professor **Sara Skrabalak**, 23) Professor **Debashis Adhikari**, 24) Professor **Erin Carlson**, 25) Professor **Laura Brown**, 26) Professor **Norman Dean**, 27) **Trevor Crafts**, 28) **Adam Richter**, 29) **Faiz Kidwai,** 30) **Joseph B. Thomas**, 31) **Craig Michael**, 32) **Nathan Duncan**, 33) **Brice Brookshire**, 34) **Ian Norden**, 35) **Ryan Clodfelter**, 36) **Sarah Bottomley**, 37) **Joseph King**, 38) **Amanda Holt**, 39) **Jennifer Campi**, 40) **Adam Schafer**, 41) **Rebecca Schwab**, 42) Professor **Charles Dann, III**, 43) Professor **Kate Reck**, 44) **Rodney Richardson**, 45) **Christopher Mattson**, 46) **Evan Yanni**, 47) **Michelle Gray**, 48) **Kent Griffith**, 49) **Nicholas Hidalgo**, 50) **Christopher Gast**, 51) **Crystal Heim**, 52) **Nathan Buehler**, 53) **Joseph Dempsey**, 54) **William Berry**, 55) **Logan Guckien**, 56) **Nathan Keesler**, 57) **Tyler Stanage**

LIBRARY NEWS

by Roger Beckman

Tiea Julian continues as our branch coordinator and takes care of the day to day operations. She has developed impressive computer and reference skills over the years and is a real asset to the patrons of the Chemistry Library. I split my time between the Chemistry Library and the Life Sciences Library. I also have responsibility for collection development and some reference for the IU Optometry Library and the IUB Nursing Program. I will be retiring in April 2014 and a search for my replacement should start soon after that.

The Chemistry Library has an "apprenticeship" program that helps train students enrolled in the School of Library and Information Science (SLIS) in the finer points of chemical librarianship. Our new SLIS GA is **Meg Knapke** who has a Bachelor of Science in Public Horticulture degree from Purdue University. Our previous GA, **Margaret Janz**, accepted a position in the Science and Engineering Library at Temple University. Another previous GA, **Elsa Alvaro**, was offered a chemistry library position at Northwestern University and started in September.

Library budgets always seem to be tight but we were able to add some useful library resources this year. The major additions were the backfiles for several Wiley titles: *Chemische Berichte* (now called *European Journal of Inorganic Chemistry*) 1868-present, *Liebigs Annalen* (now called *European Journal of Organic Chemistry*) 1832-present, *Comprehensive Organic Name Reactions and Reagents*, 1999-2013, and *Organic Reactions*, 1942-present (vols. 1-80). The good news going forward is that the campus has agreed to increase the collections budget for the IUB Libraries substantially in the next two budget years. The collections budget for the IUB campus for the last few years was one of the lowest among our peers and not sufficient to keep the collection adequate for the faculty and students' research needs. Good news indeed.

We continue to expand our offering of electronic books and get most of the electronic titles published by Springer e-books (2005 to 2013) and Elsevier (2008 to 2013). For Wiley e-books we own most of what they published between 2007 and 2010 and then I select the important titles recently published. The e-book environment is still in flux so it will be interesting to see what happens in the next few years. ■

NECROLOGY 2011–2013

Due to changing staff positions last year, the Necrology was missing from the Magazine. We anticipate this will catch up as we remember all those in the IU-Chemistry family who have passed away since 2011. Included here are deaths of which we learned since 2011.

Herman L. Auerbach, M.D., BA '44, Sept. 21, 2012
Roy J. Ault, M.D., BA '43, June 4, 2011
Robert W. Bedwell, BS '42, Sept. 6, 2011
Col. Daniel J. Benefiel, BS '50, Dec. 19, 2012
Frank R. Berson, D.D.S., BA '41, Jan. 30, 2012
Robert B. Bourne, BA '51, May 5, 2012
James P. Brennan, Ph.D. '73, Oct. 21, 2011
Arthur Chovnick, Ph.D., BA '49, Sept. 5, 2011
Richard E. Cline, Ph.D. '51, May 7, 2012
Guy R. Collins, Ph.D. '65, Dec. 15, 2012
Hollace L. Cox, Jr., Ph.D. '67, Oct. 1, 2011
William E. Creek, BS '45, May 29, 2012
William J. Cron, M.D., BA '51, March 24, 2011
Lt. Col. J. Alan Davidson, Ret., BA '51, Dec. 24, 2011
Russell H. Davis, M.D., BA '42, Sept. 11, 2011
Robert J. Detamore, D.D.S., BA '43, Sept. 20, 2012
Paden F. Dismore, Ph.D. '48, September 29, 2011
Richard L. Doerr, BS '48, May 4, 2012
Harry Dolyniuk, MA '53, March 26, 2012
Robert D. Donaldson, BS '42, Nov. 2, 2011
Monnie Dotlich, BA '42, Aug. 20, 2011
Donald G. Earl, BA '60, Aug. 29, 2011
Merrill T. Eaton, Jr., M.D., BA '41, Feb. 19, 2011
John T. Esmon, D.D.S., BA '42, March 28, 2012
John R. Feferman, BA '78, July 17, 2012
Henry L. Feffer, M.D., BS '39, May 9, 2011
Allan F. Fehlandt, Jr., BA '84, Aug. 6, 2012
Ernest G. Flint, Jr., MA '59, April 12, 2011
A. Ronald Garber, Ph.D. '74, Aug. 14, 2012
Stanley J. Gasior, Jr., BA '65, Nov. 27, 2012
Reid G. Gibson, BA '79, Dec.31, 2012
Stephen B. Givens, BA '63, Sept. 13, 2012
Jeffrey L. Gordon, BS '81, Sept. 8, 2011
Herschel G. Grose, Ph.D. '51, Dec. 30, 2012
Peter M. Hamang, II, BS '08, Jan. 1, 2011
Rudiger D. Haugwitz, Ph.D. '66, July 18, 2011
Lowell L. Henderson, M.D., BA '38, Jan.7, 2012
Leland G. Howard, BS '50, March 31, 2011
Lloyd G. Hyndman, M.D., BA '55, Jan. 16, 2011
Charles E. Jackson, M.D., BA '44, Dec.30, 2012
Michael G. Johnston, BS '79, Dec. 22, 2011
Quan Ju, Ph.D. '99, April 22, 2012
Leonard E. Koenig, D.D.S., BA '37, Jan. 8, 2012
George N. Konrad, BA '50, Sept. 15, 2011
William A. Koontz, M.D., BA '42, June 30, 2011
Richard S. Kubiak, BA '49, April 16, 2011
Larry M. Kuhlenschmidt, D.D.S., BA '68, Dec.13, 2011
Edmund K. Lai, MS '75, June 10, 2012
Sanford H. Lawrence, M.D., BA '41, Jan. 4, 2012
George R. Long, Jr., Ph.D., BA '61, Oct.11, 2012
Earl J. Mason, Jr., Ph.D., M.D., BA '47, Nov. 2, 2011
Michael S. Matta, Ph.D. '66, Jan. 3, 2011
Helen E. McClelland, BA '57, June 22, 2012
Ralph W. McCullough, BA '48, Feb.14, 2011
Kenneth F. McKee, M.D., BA '74, Dec.10, 2012
Donald L. McMasters, Ph.D. '59, Sept. 28, 2011
Wendell W. Meyer, Ph.D. '62, Feb.10, 2012
Charles G. Miller, Ph.D., BA '63, April 15, 2012
Jerry A. Miller, Ph.D. '84, May 12, 2012
J. Weir Mitchell, D.D.S., BA '43, April 20, 2011
Harlan B. Moss, M.D., BA '42, Feb. 26, 2012
Rodney D. Moss, Ph.D. '51, April 13, 2011
Frances F. Murray, BS '45, May 7, 2011
Stanley S. Murzyn, BA '50, March 17, 2011
F. John Naples, Ph.D. '36, Nov.6, 2011
Leonard A. Neubert, Ph.D. '69, Oct. 31, 2012
Betty J. Nichols, BA '41, Nov. 17, 2011
James R. Overman, BA '63, May 18, 2012
John S. Peake, Ph.D. '35, December 12, 2011
John D. Pera, Ph.D. '60, March 29, 2011
Eric L. Peterson, BA' 96, Aug. 26, 2011
Virgil A. Place, M.D., BA '44, March 14, 2012
Charles N. Purlee, D.D.S., BA '47, Jan. 13, 2012
Ronald L. Reynolds, BA '64, Sept.17, 2012
T. Ben Rhinehammer, Ph.D. '53, July 28, 2012
Mac M. Robinson, Ph.D. '44, May 17, 2012
Roger W. Rodgers, M.D., BA '68, March 28, 2012
Eugene F. Rodman, BA '43, Jan. 11, 2011
John M. Ruddell, Jr., BA '42, Dec.17, 2011
Keith B. Ryther, BA '88, June 28, 2011
Fred Sanders, M.D., BA '49, March 28, 2012
William J. Schenck, Jr., BS '54, Jan. 3, 2011
Julius Schneiderman, M.D., BA '36, Aug. 24, 2011
Maurice E. Selzer, BA '36, March 21, 2011
John L. Shively, M.D., BA '44, June 23, 2011
George W. Simpson, D.D.S., BA '42, Aug. 4, 2012
Walter T. Smith, Jr., Ph.D. '46, Sept. 25, 2012
Jo Ann Spencer, BA '46, Jan. 4, 2011
Robert H. Stahlschmidt, BS '50, Dece.r 19, 2012
Edward F. Steinmetz, M.D., BA '50, May 27, 2011
Lawrence A. Stone, M.D., BA '68, Dec. 5, 2011
Lane E. Strock, BA '44, April 16, 2012
William T. Thanholt, BA '49, Dec. 19, 2012
Wesley L. Tharp, BA '48, June 17, 2011
Lee J. Todd, Ph.D. '64, March 22, 2011
James F. Vasil, BS '48, April 11, 2011
Robert H. Walsh, Ph.D. '54, Jan. 25, 2011
Douglas H. White, Jr., M.D., BA '46, Jan. 11, 2012
Mary F. White, BA '43, Dec.7, 2011
David Williams, BS '65, Nov. 8, 2011
Bernard Wolnak, Ph.D. '43, June 11, 2011
Jay A. Young, Ph.D., BS '39, Oct. 13, 2011

Ernest E. Campaigne

FEB. 13, 1914 — MAY 5, 2013

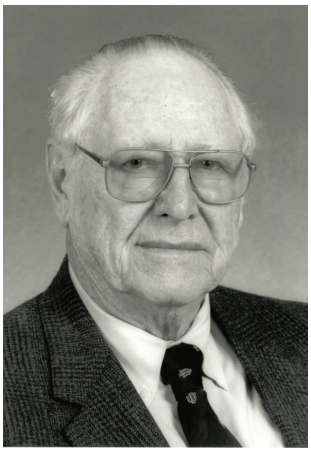
Ernest E. Campaigne was born in Chicago, IL, on February 13, 1914, to Nellie and Herbert Campaigne. Professor Campaigne was a true Chicago-native, earning his BS (1936), an MS (1938) and a Ph.D. (1940) from Northwestern University. Besides obtaining his vast education, it is the location that he met and married his wife, Jean, in 1941. They were married for 72 years.

In 1943, Professor Campaigne came to Indiana University as an Instructor in the Army Specialized Training Program after early teaching and research experience at Northwestern University Dental School, Bowdoin College, the M.D. Anderson Hospital for Cancer Research, and the Medical School of the University of Texas. His earliest teaching and research experiences in the environment of a dental school and a cancer hospital perhaps influenced his entire career, for Professor Campaigne combined his principal interest in organic chemistry with a search for new therapeutic agents.

Professor Campaigne's rise through the ranks from Instructor to Professor concluded in 1953. During his years at Indiana, he taught a variety of courses in general chemistry, biochemistry, and organic chemistry, and contributed to joint efforts in the teaching of pharmacology. He was consistently concerned with the quality of teaching by taking responsibility for the organization and reorganization of many courses, by authoring several textbooks of chemistry, by serving on the Committee on the Improvement of Teaching of the College of Arts and Sciences, by acting as Graduate Advisor of the Chemistry Department and as a member of the Chemistry Department's Policy Committee. He directed the dissertation research of nearly 60 Ph.D. students and 20 M.S. candidates. He followed the careers of his students with close and helpful interest. During his varied pedagogic activities, Professor Campaigne published more than 275 research papers, reviews, and books.

Campaigne's work at IU involved antiviral agents, cancer-producing hydrocarbons and antidepressant drugs. He also worked with the synthesis of naturally occurring compounds, including serotonin, an agent in the central nervous system related to the development of schizophrenia, and melatonin, the substance which controls skin color changes in some fish and amphibians.

Professor Campaigne had a busy professional life at the state, national, and international levels. He was an active member and often a chief administrative officer of numerous scientific and professional societies, where his extremely effective organizational skills were widely recognized. He devoted years of service to the American Chemical Society, beginning with the Southern Indiana Section, as Chairman and Circuit Lecturer and later as a national Councilor. This activity led him to a series of increasingly responsible administrative positions, including that of Chairman, with the Division of Medicinal Chemistry of the American Chemical Society. From these national activities he became Chairman of the newly created Section on Medicinal Chemistry, Division of Organic Chemistry, of the International Union of Pure and Applied Chemistry. Dr. Campaigne was the holder of fifteen commercial patents including the commercially successful antihistamine, *Thenfadil*.



Campaigne continued his research even after his retirement in 1979. Most drugs produced by medicinal chemists are discovered accidentally, according to Campaigne. "You make it, and you test its properties. It is wildcat work. You're always taking chances." With 43 years of active research Campaigne has seen many seemingly useless compounds result in valuable, marketable chemicals. "When I got into medicinal chemistry, it was the most important area of scientific research. The public thought we could prolong life indefinitely," he said, pointing out that human life expectancy had increased dramatically in the years between 1935 and 1955.

Since retirement in 1979, he has been active in the Indiana Academy of Science serving as president in 1986, the University Club, the Indiana University Retirement Community, and the I.U. Annuitants Association. He served on the Board of Science Advisors, American Council on Science and Health since its inception in 1979, and was elected to the honorary Indiana Academy in 1988.

On a University level, Professor Campaigne twice served as President of the Men's Faculty Club, as a member of the University Athletics Committee, and a member of the initial University Patent Policy Committee. He was awarded the Indiana University President's Medal for Excellence in Teaching and Research by President Thomas Ehrlich, and The I.U. Laboratory of Organic Chemistry is named for him and his longtime colleague, **Marvin Carmack**. He was the longest holder of I.U. faculty/staff season football tickets, beginning long before records of such things were kept.

Professor Campaigne's wide circle of former students, faculty and professional colleagues found in him a generous source of wise advice, encouragement, and unfailing good humor.

Ernest E. Campaigne passed Sunday, May 5, 2013, at the Meadowood Health Pavilion in Bloomington. He and Jean White were married in Chicago on January 1, 1941. He is survived by Jean as well as a son, David of Bloomington, and two daughters, Claudia Campaigne Burrus (Tony) of Ft. Wayne, IN, and Barbara Campaigne (Larry Boot) of Bloomington. He is also survived by four grandchildren, Barbara Koch of Columbus, OH, Ron Buskirk II of Ft. Wayne, Gillian Overly of Bloomington, IN, and Christian Campaigne of Mt. Pleasant, SC, and five great-grandchildren. ■

This memoriam was compiled and edited by Kate Reck based on archival information in the Chair's office.

Kaci M. Alexander, BA/BS'10, writes that she married fellow medical student Matt Smith in June. In July, she moved to Akron, Ohio, to begin her third year of medical school.

In January 2013, **William F. Carroll Jr.**, PhD'78, a vice president at Occidental Chemical Corp. in Dallas was re-elected chairman of the board of directors of the American Chemical Society. The organization is the world's largest scientific society and a global leader in providing access to chemistry-related research. An ACS member since 1974, Carroll has served on and chaired numerous committees and task forces, and he served as ACS president in 2005. His areas of interest in industry have included combustion science, plastics recycling, and chemistry and the environment. In addition to his position at Occidental, Carroll is also an adjunct industrial professor of chemistry at IU Bloomington. He lives in Dallas with his wife, Mary.

In December 2010, **Charles H. Davis**, BS'60, MA'66, PhD'69, was elected a senior member of the Association for Computing Machinery, the world's largest educational and scientific computing society serving to advance computing as a science and a profession. Davis, IU Bloomington School of Library and Information Science senior fellow and adjunct professor, lives in Bloomington.

In December 2012, then-Indiana Gov. Mitch Daniels honored IU chemist **Richard D. DiMarchi**, PhD'79, with the 2012 *Dr. Phillip E. Nelson Innovation Award* for his demonstrated excellence in the laboratory, his leadership as an executive administrator, and his tenure as a distinguished teacher. Daniels created the award in 2007 to recognize outstanding Hoosier scientists for their unique discoveries, research, and inventions and to encourage young people to consider careers in science. DiMarchi is the Linda and Jack Gill Chair in Biomolecular Science and Standiford H. Cox Professor of Chemistry at IU Bloomington.

Maury L. Fisher, BA'80, is an orthopedic surgeon and partner in the Florida Joint & Spine Institute in Winter Haven, Fla. His wife, Joni Esser Fisher, BA'80, is an author, book editor, and private pilot, who also teaches online writing workshops. She has published a science fiction novel, *Phobos: Manned Mission*, under the pen name J.M. Fisher. The couple lives in Auburndale, Fla.

Dustin R. Masser, BS'10, is working on a Ph.D. in biomedical sciences at Penn State College of Medicine. He lives in Hershey, Pa.

Eric D. Morrell, BA'03, MA/MD'08, married Laura Townsend in Indianapolis in May 2012. He is an internal medicine resident at the University of Pittsburgh Medical Center. After graduating from the IU School of Medicine, Morrell became a medical officer with the U.S. Marines and served in Afghanistan. While there, he treated more than 2,300 civilians, over 200 Marines and sailors, and was awarded the Bronze Star. Morrell plans to become a physician-scientist in the field of pulmonary and critical care medicine.

Alexandra Lipps Sylvia, BA'93, JD'96, a partner in the Indianapolis law firm Plews Shadley Racher & Braun, has been elected to the *Fellows of the American Bar Foundation*. The Fellows is a select, honorary organization of attorneys, judges, and legal scholars who have demonstrated exceptional dedication to the welfare of their communities and to the highest principles of the legal profession. Membership is limited to one-third of one percent of lawyers admitted to practice in each state. Sylvia lives in Indianapolis.

Sarah A. Webb, PhD'04, contributed a chapter to the new book, *The Science Writers' Handbook: Everything You Need to Know to Pitch, Publish, and Prosper in the Digital Age*, published by Da Capo in May. Webb writes about science, health, technology, and policy for researchers, for the general public, and for children. Her work has appeared in *Discover*, *Science News*, *ScientificAmerican.com*, *Science*, *Nature Biotechnology*, *National Geographic Kids*, *Science News for Kids*, and many other publications. She has reported on the Mars Rovers Spirit and Opportunity, the science and policy of stem cell research, and the acoustics of carbon fiber cellos. Webb also served as the research coordinator for the award winning astronomy exhibits at Griffith Observatory in Los Angeles. She lives in Chattanooga, Tenn., with her husband, two cats and a Senegal parrot. Webb is the editor-in-chief of *pitchpublishprosper*.com.

Mansukh Wani, Ph.D. '62, emeritus principal scientist at RTI International, was inducted into the American Chemical Society Division of Medicinal Chemistry Hall of Fame for his outstanding contributions to medicinal chemistry, specifically his efforts in the discovery of two anti-cancer agents Taxol and Captothecin, recognized as a National Historic Chemical Landmark by the American Chemical Society.

The Medicinal Chemistry Hall of Fame recognizes individuals who have contributed to medicinal chemistry through research, technology and service to the American Chemical Society. The induction ceremony was held Sept. 10 during the society's fall meeting in Indianapolis, Indiana.

With more than 50 years of experience in medicinal chemistry, Wani is an internationally-recognized leader in natural products research His research focuses on the isolation and characterization of biologically active natural products and synthesis of anticancer and antifertility agents.

WHAT'S NEW WITH YOU?

The IU Chemistry Department is now is charged with maintaining records for all IU alumni. Please print as much of the following information as you wish. Updates are used as class notes and help keep IU's alumni records accurate and up to date. Attach additional pages if necessary. Mail to the IU Chemistry Department or update online by visiting **http://whatsnewwithyou.chem.indiana.edu**.

Publication carrying this form: IU • Chemistry Date _____

Name _____

Preferred name _____

Last name while at IU _____ IU degree(s)/year(s) _____

Univ. ID # (PeopleSoft) or last four digits of Soc. Sec. # _____

Home address _____ Phone _____

City _____ State _____ Zip _____

Business title _____ Company/institution _____

Company address _____ Phone _____

City _____ State _____ Zip _____

E-mail _____ Home page URL _____

Mailing address preference: ❒ Home ❒ Business

Spouse name _____ Last name while at IU _____

IU degree(s)/year(s) _____

Your news: _____

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CHEMISTRY HONOR ROLL 2012

The Indiana University Department of Chemistry thanks and honors the alumni, friends and companies who supported the Department of Chemistry with financial contributions from January 1, 2012 through December 31, 2012.

Aleyamma Abraham
Robert and Terri Agan
Robert and Joyce Ake
Kent Alleman
Robert Ammlung
Robert Anders
Mark and Ann Anderson
Deon and Lisa Anex
Peter Arvan
Paul Asmus
Timothy and Irene Ayers
Mary Bacon
Ann Bailey
Lane and Maurie Baker
Donald Ball
Thomas Bannister
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