CHEMISTRY, COMPLEXITY, LIFE

Chemical research is crucial for understanding the complex molecular interactions that form the basis of life, and such research holds great promise for addressing the variety of ailments that afflict us. Thus, a major research thrust in our Department is “The Chemical Basis for Disease.” Chemistry is at the heart of all biological processes, and an ever important goal for our discipline is to understand the complex molecular interactions that give rise to biological function. In this sense, chemistry is the key to addressing human health and diseases.

Revolutions in chemical methods and instrumentation are now enabling us to focus on problems of increasing complexity. Some of the big challenges facing chemists who try to understand biological processes include finding the links between biological and environmental signals and gene expression, developing diagnostic methods for early detection of diseases, such as cancer, and discovering the molecular basis for diseases such as dementia.

The following stories summarize how researchers within our department are addressing the chemical complexity of biological processes.

TOOLS FOR DISCOVERY

New Tools for Discovery
Human cells have many inter-connected pathways, ensuring health. But throw one of these pathways out of balance, and you develop cancer, inflammation, or an infection. Oftentimes the key to discovering a new treatment is to identify the role of each protein in that biochemical pathway. A great strength of chemical approaches is that they can lead to new tools for discovering the key players in these pathways and for identifying novel drug targets.

DIAGNOSTICS AND TREATMENT

Detection of Disease
Sensitive, accurate, and precise methods for detecting disease biomarkers are crucial for early disease diagnosis and treatment. Biomarker detection is incredibly challenging, however, as molecular indicators of disease are chemically diverse and are present amongst a background of significant chemical complexity.

Nanomaterials and protein recognition. Most molecular recognition processes in biology occur via specific interactions between a single
Dear Alumni and Friends of the Department of Chemistry,

I hope you enjoy this latest issue of the Goessmann Gazette. The Department of Chemistry has had another outstanding year, and our research prominence continues to grow. Your donations have helped tremendously as we rebuild our faculty, and I am pleased to welcome two new Assistant Professors to our department, Nate Schnarr and Jim Chambers, both organic chemists. Nate and Jim are developing cutting-edge research which is a mixture of organic chemistry and biology. Over the past year our faculty and staff have been recognized with various awards, including the 2007 NSM Outstanding Researcher Award (Paul Lahti), the NIH Pioneer Award (Lila Gierasch), a Discovery Corps Fellowship (Julian Tyson) and a Chancellor’s Citation Award (Margaret Snape-Kolodzinski). Congratulations also to Profs. Thayumanavan, Hardy, Auerbach and Venkataraman for bringing a highly prestigious Chemical Bonding Center to our department.

We continue to be deeply grateful to all of you who have contributed so generously to our department over the years. In addition to improving our teaching and research facilities and providing scholarships to students, your gifts help us to provide startup packages for new faculty. I thank you all again for your generous support.

Sincerely,

Bret Jackson, Department Head

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alumniNEWS

• **Kathleen Gorski** (PhD ’94) is a 2007-8 Fellow of the Albert Einstein Distinguished Educator Program that is associated with the National Science Foundation Polar Programs Office. For more information see http://www.triangle-coalition.org/fellows/2007/eingorski.htm.

• **Assistant Prof. Atitaya Siripinyanond** (PhD ’02) was awarded the Thailand National Young Scientist Award 2007 from the Foundation for the Promotion of Science and Technology under the Patronage of His Majesty the King. An outstanding achievement! To read more about Atitaya please visit http://www.sc.mahidol.ac.th/award/atitaya.htm.

• **George Epstein** (’48) was sports editor of the Collegian when Mass. State College became UMass Amherst. A poker author and columnist for the Poker Player newspaper, he teaches poker classes and conducts a Poker Lab for the City of Los Angeles.
The featured theme for the 2007 Reunion was Energy. **Professor Venkataraman** discussed global energy demand and the associated economic, environmental and geopolitical factors. **Professor Thayumanvan** described the newly formed Massachusetts Center for Renewable Energy Science and Technology (MassCREST) and provided an overview of the energy related research at UMass Amherst. The reunion was well-attended and evoked passionate discussions among the audience about energy problems and solutions.

**Don’t miss this year’s alumni reunion on June 7, 2008, entitled “HEALTH & DISEASE: Diagnostics and Treatment.”** See page 28 for more details.

**ISB UPDATE**

The ISB project is moving along quite nicely, and on schedule to open in January 2009. We have recently witnessed the start of lab cabinetry being installed in the lab wing, and several interior areas have already been painted making the building feel cozy. We recently identified the necessary equipment needed to outfit the new expanded teaching labs, and are making progress with the building furniture and signage.

We encourage you to take a look at the building through our web cam at: http://umassamherstisb.webcam.chilmarktech.com/

Please also visit the following link for additional ISB information: http://www.umass.edu/fp/projectmanagement/constructioninformation/integratedsciencebuilding/
In the Adams lab ...
I continue to teach the main stream and honors general chemistry courses, act as the departmental honors coordinator, advise chemistry majors, and serve on the Undergraduate Program Committee. I chair the Undergraduate Awards Committee and organize the annual Senior and Awards Dinner. I also serve on the NSM Scholarship Committee and chaired the faculty University Distinguished Teaching Award Committee.

My research activities include researching and writing biographical essays and interviews of famous chemists for the New England Association of Chemistry Teacher’s Journal. I also continue to assemble information for the comprehensive history of the UMass Amherst Chemistry Department, and have co-authored a book on UMass Amherst history with Lynne E. Adams.

In the Auerbach lab ...
The Auerbach group continued its theoretical chemistry research in the interface between nanotechnology and renewable energy. This has been a very exciting year with much fundraising success. We are supported by 1 old and 3 new federal grants: (i) NSF grant to model the spectroscopic properties of new, functionalized zeolites that show promise in biofuel production; (ii) NSF center grant (Chemical Bonding Center on Fueling the Future) to model proton transfer in new fuel-cell materials; (iii) Department of Energy (DOE) grant to simulate self-assembly of zeolites and other ordered, nanoporous solids; and (iv) DOE grant to study solid basic catalysts for biofuel production. Auerbach group research was featured during seminar visits at U. Florida and U. Cincinnati, and also at the 20th North American Catalysis Society meeting in Houston. Senior graduate students Karl Hammond and Usha Viswanathan had their latest research published in Langmuir and J. Phys. Chem. C, respectively.

Regarding Auerbach alumni, Dr. Chandra Saravanan (1st PhD student) will be moving back to India after he accepts one of his many job offers in industry. Leanna Toy is back at UMass Amherst working on her masters in education to become a high school chemistry teacher. Aldo Combariza left for Spain to continue his graduate work with Avelino Corma in Valencia. Matt Ford changed jobs, leaving AER Inc. in Lexington MA, moving to Telvent, Inc in Columbia MD, which is much closer to Matt’s home in both location and type of work – Matt is back to doing simulations relevant to chemical engineering.

In the Barnes lab ...
In the past year, Prof. Mike Barnes received a $25,000 Supplemental Equipment Grant from the U.S. Department of Energy, and was a co-investigator in the newly funded NSF-Chemical Bonding Center (Fueling the Future) at UMass Amherst. Our group has continued participation in the NSF-Center for...
Hierarchical Manufacturing as well. As part of the Targeted Research Group 2–Molecular Electronics, our research group is exploring electronic and photonic properties of nanoscale materials and assemblies. Prof. Barnes gave four invited seminars this year at the American Chemical Society Spring National Meeting in Chicago II, Optical Society of America Frontiers in Optics National Meeting in San Jose, CA, at the 11th International Circular Dichroism Meeting in Groningen, The Netherlands, and the Chemical Engineering Department Seminar at UMass Amherst. He also served as a panel reviewer for the NSF-IGERT program.

Our group members and research news: Kevin Early, a third-year graduate student in the group received a highly competitive IGERT Fellowship this year, with a stipend of $30,000/year for 2 years plus funding for a 2-month study overseas. Kevin has discovered a novel polarization-driven directionality in surface-derivatized quantum dot systems—an effect that is potentially important for next-generation nanostructured optoelectronic devices. Kevin McCarthy, a postdoctoral fellow with a PhD in Physics from UMass Amherst last fall, has focused on experimental and theoretical modeling of photophysical properties of surface-derivatized quantum dot systems and individual chiral molecules. Michael Odoi, a 4th year graduate student from Ghana has had some spectacular success investigating the photon-pair correlation statistics from individual quantum dot systems which may be important for single-photon applications such as quantum cryptography. Ruthanne Hassey, also a 4th year student, has made great progress in exploring chiroptical properties of single molecules in collaboration with the Venkataraman group. A full paper on the experimental observations as well as computational modeling has been accepted for publication in a special issue of Chirality and will appear later this year. Ellen Swain (BS ’08) who made a significant contribution to our single-molecule chiroptics research under the support of the Bates Summer Research Fellowship at UMass Amherst, is now a graduate student in the Chemistry Department at Northeastern University. We also had several of undergraduate researchers working with us this past year who contributed to our research efforts: Francois Jean-Charles (BS ’09), BJ Odusami (ChE ’08), Tim Mortsolf (BMB ’09), and Samuel Bearg (BS ’09).

In the Bianconi lab ...
This year Prof. Bianconi received a Massachusetts Technology Transfer Center “Technology Investigator Award” of $25,000. She was also appointed as a visiting professor at The Johns Hopkins University Applied Physics Laboratory, where she gave an invited seminar on her “polymer precursor to diamond carbon” research. She presented her work at the 9th International Applied Diamond and Nanocarbon conference, and at two DARPA conferences by invitation.

This year Prof. Bianconi’s laboratory is collaborating with Hexcel Corporation on producing next-generation super carbon fibers with an award of $278,000. The lab is also collaborating with Johns Hopkins Applied Physics Laboratory on diamondizing plastic substrates.

In the Chambers lab ...
Professor James Chambers joined the faculty in January 2008. He is looking forward to setting up his chemical biology/neuroscience lab where he will be studying new FACULTY

James Chambers as a lad growing up in Hicksville, NY (Long Island), was fascinated by hockey and truck driving. Instead, he majored in medicinal chemistry as an undergraduate at SUNY Buffalo. This was followed by his PhD in medicinal chemistry and molecular pharmacology from Purdue University. Following postdoctoral appointments at University of California San Francisco and University of California Berkeley, he joined our department in January 2008. Jim brings a unique mix of chemical intuition and electrophysiology expertise to shed new light on problems in neurobiology.
protein trafficking, signaling, and memory formation by using small molecules, photochemistry, and single cells.

In the Dubin lab ...  

The Dubin research group graduated its first UMass Amherst PhD this August, Basak Kayitmazer. With postdoc offers from Rutgers, Delaware, Johns Hopkins and Northwestern, she made a good choice of the last one, and is working with Messersmith on mucin biomaterials. She's currently seeking an academic job in Turkey. Joining us this year were Burcu Baykal (joint with Igor Kaltashov); Malek Mazzawi and Elaine Foun (undergraduates) joined Maragita Antonov and Erin Sutherland (continuing). Burcu's project involves mass spectroscopy of glycosaminoglycan-protein interactions, featured on the cover of Analytical Chemistry in August. Malek and Elaine are working on polyelectrolyte-surfactant interactions, as described in a paper just published in Langmuir.

In the Gierasch lab ...  

This was a very stimulating and busy year in the Gierasch laboratory. There were several passages: Chemistry graduate student Annie Marcelino recently defended her PhD (March 2008) with great success. Annie will pursue post-doctoral studies at RPI with Peter Tessier on protein aggregation mechanisms. After many years of fruitful collaborative research and teaching, former Research Assistant Professor Joanna Swain moved ‘East’ to keep her family in one home, as her husband took a faculty job at the University of Southern New Hampshire. Joanna joined the young pharmaceutical company Adnexus in August 2007 and is doing great work. Undergraduate researcher Jeff Bombardier successfully defended his thesis and graduated last May. He is now working as a research technician at Massachusetts General Hospital, planning to go to graduate school in the near future. We wish Joanna, Jeff and Annie the best of luck.

New faces in the lab include three new postdoctoral researchers who are studying different aspects of protein folding in the context of the cell (Harekrushna Sahoo and Ivan Budyak) and the mechanism of allostery in Hsp70 proteins (Anastasia Zhuravleva).

We are very pleased to have successfully renewed our long-running NIH grant that supports our research on Hsp70 molecular chaperones. The project is now funded for four more years. Also, senior postdoctoral fellow Beena Krishnan received a grant from The Alpha One Foundation to study the mechanism by which serpin proteins fold and function.

Professor Gierasch and the Gierasch crew have been traveling quite a lot. Most of the lab attended the Protein Society Meeting held in Boston in July 2007, where Lila gave a major lecture. Molecular and Cellular Biology program graduate student Jenny Maki attended the Gordon Research Conference on ‘Protein Transport Across Cell Membranes’ in Lucca, Italy in June 2007, and during the annual MCB retreat (March 2008) she received a poster award. Lila Gierasch and postdoctoral fellow Eugenia M. Clerico presented a talk and a poster respectively at the 63rd Harden Conference on “Protein folding and assembly in vivo and in vitro,” in Ambleside, England in August 2007. Lila gave a number of other seminars and talks throughout the year. Additionally, we published five papers and three review articles and book chapters last year in the period since the last Gazette.

In the Hardy lab ...  

It has been a terrific year for the Hardy Lab. We have added two new graduate students to our crew, Samantha Bernard, a native Vermonter, and Elih Velazquez, a native Puerto Rican. Three of our graduate students, Kristen Huber, Sravanti Vaidya and Witold Witkowski have all advanced to candidacy after successfully completing the defense of their Original Research Proposals in December. Sravanti Vaidya managed to win not just one, but two poster prizes–at the Chemistry-Biology Interface Retreat and at the departmental Posterfest–for her work to engineer allosteric sites in caspase. Kristen Huber was awarded a National Institutes of Health Chemistry-Biology Interface training fellowship for her work to develop allosteric inhibitors of caspases. During the summer, the Hardy lab hosted two National Science Foundation Undergraduate REU Fellows. Jessica Bauer from Knox University worked on a project to make proton transporting membranes for hydrogen fuel cells out of proteins. Kevin Olsen, a UMass Amherst undergraduate member of the lab, developed a system for rapid generation of caspase blocking agents.

Research is also moving along well. Hardy received an $825,000 five-year grant from the National Institutes of Health to design allosteric regulatory sites into caspasas-proteases that regulate cell death in diseases such as cancer, heart attack and stroke. She was also part of the team that was awarded the Fueling the Future grant for work on proton transport and received an Excellence Fund Award from the Dean.
Peter Khalifah, our much admired instructor for the undergraduate inorganic laboratory, departed at the end of 2007 for a tenure-track position at SUNY-Stony Brook, where he will split time between the Chemistry Department and Brookhaven National Lab. This move is a tremendous opportunity for Peter, as it will allow him to devote full energy to his research interests in solid-state materials chemistry. In addition to his teaching, Peter also worked at UMass Amherst as a crystallographer and materials-science researcher. Peter trained at Princeton University, learning solid state synthesis techniques from one of the leaders in solid-state chemistry, Robert Cava. His postdoctoral training was with the Correlated Electronic Materials group at Oak Ridge National Laboratory, under the leadership of Dr. David Mandrus. While there, Peter built expertise in the electronic and magnetic properties of extended solids. Peter’s new position at SUNY-Stony Brook will allow him to develop his research for solving problems in renewable energy and microwave communications. We wish him much success in his new location, and look forward to future visits.

In the Jackson lab ...
Professor Jackson, now in his sixth year as Department Head, continues his vigorous research in theoretical chemistry. In addition to serving as Chair for last summer’s Dynamics at Surfaces Gordon Research Conference, Prof. Jackson gave several invited lectures last year, including a plenary lecture at the US-China Partnership Workshop for Heterogeneous Catalysis and Surface Science in Dalian, China, and an invited talk at the Workshop on Elementary Reactive Processes at Surfaces, in San Sebastian, Spain. Much of Prof. Jackson’s research focus has recently turned to the reactions of methane on Ni and Pt catalysts. In other Jackson group news, Zuleika Medina defended her PhD in September 2007, has two papers out in J. Chem. Phys., and is currently a postdoc at Penn State. Also, former postdoc Dmitrii Shalashilin is now a Professor of Chemistry at the University of Leeds, in the UK.

Hui Xiao (PhD ’04) became an assistant professor at the Department of Pathology, Albert Einstein School of Medicine (Bronx, NY) and Wendell P. Griffith (PhD ’05) became an assistant professor at the Department of Chemistry, University of Toledo (Toledo, OH).

In the Knapp lab ...
The Knapp group enjoyed a great year working at the intersection of oxidation chemistry and biochemistry. The central question we are addressing is how oxidation reactions depend on the inherent reactivity of both the metal cofactor and protein conformational changes. This has led us to employ a wide variety of biophysical and spectroscopic techniques, which makes for a rich training environment.

Recent group honors include a Graduate School Fellowship for Halil Bayraktar’s work on protein/nanoparticle reactivity, and the William E. McEwen Fellowship for Meaghan Germain’s presentation on fluorescence sensing of explosives. For more information, see http://www.umass.edu/knappchem/

In the Lahti lab ...
The Lahti group had a good year for published articles in 2007, thanks to the hard work of recently graduated former students. PML was honored with a College of Natural Sciences and Mathematics Outstanding Research Award.

On the alumni side Jacqueline Ferrer sends word that she is continuing to work with Dr. Karl Hostetler at UCSD Medical School (Veterans’ Medical Research Foundation). She is also teaching part time at Southwestern Community College. Nibedita Sanyal sends word that she is working as a postdoctoral research associate in Knoxville, TN. Martha Baskett seems to have settled in well for her new faculty job at University of Arkansas Montville. She has already has
had a proposal funded by the Arkansas Space Grant
Consortium (NASA link) for a project “Functionalized
Cotton Smart Fabric: an Ammonia Detector Test Case.”
Good luck with the work, Martha! Hidenori Murata
sends word from Japan that he has been promoted.
His work on the quasi-1D ferromagnet F4BImNN has
been published in full detail in J. Am. Chem. Soc. (see
the group publications site), and even featured on the
Chemistry Department WWW site. Congratulations,
Hidenori, on the well-deserved recognition of your hard
work at UMass Amherst and at Tokyo University of
Science!

In the Maroney lab ...
To paraphrase Mark Twain, rumors of my demise
were greatly exaggerated. The department was able
to significantly renovate a suite of labs for my group;
we are moving into remodeled labs on the fifth floor
of LGRT as I write this. It is good to be back, even
without leaving. I finished my sabbatical semester
(Spring ’07) with a trip to the International Conference
on Biological Inorganic Chemistry in Vienna, Austria
(it was about 100 °F) where I gave a talk on nickel
trafficking proteins and managed not to pass out.

In the Martin lab ...
Professor Craig Martin’s laboratory continues to
produce talented graduates (and has been rebuilding
with new, young talent). Han Gang (PhD ’07), a joint
PhD student with Vincent Rotello, finished up in the
summer and has moved on to a postdoctoral position
at the University of California at Berkeley, while Selase
Enuameh (PhD ’08) successfully defended his PhD in
March and is wrapping up manuscripts as he looks for
a position in industry.

This has been an exciting year scientifically. Yi Zhou
(PhD ’06), saw the publication in Proc. Natl. Acad.
Sci., USA of his manuscript detailing how an RNA
polymerase that is topologically “locked” onto the
(double) helical train track can fall off the track – it
must first slide forward, dethreading the lock, before
the RNA can be released. Yi is now in Cambridge, MA,
doing pharmacokinetics with Altus Pharmaceuticals.

Rosemary Turingan (PhD ’06), currently with
Network Biosystems, saw the publication of two
important papers using fluorescence energy transfer to
measure intramolecular distances in RNA polymerase
transcription complexes. In the first paper published in
Biochemistry, she confirmed a model for the complete
initiation complex, showing that the DNA is bent,
with an eight base bubble. In a follow-up paper, also
in Biochemistry, she provided very strong evidence
confirming a new model proposed earlier by the lab
that presents a “new twist” on how this protein is
driven to undergo a large structural rearrangement as it
reconfigures itself from the requirements of a de novo
initiation complex, to the very different requirements of
a stably elongating complex.

In the Metz lab ...
Murat Citir defended his PhD dissertation on July
12, 2007. To complement his graduate studies of the
spectroscopy of intermediates of C-O and C-H bond
activating reactions, he is doing a postdoc with Prof.
Armentrout (Utah) studying reactions of metal ions.
An invited review article in Advances in Chemical
Physics by Prof. Metz highlights the group’s studies of
the spectroscopy of the potential energy surfaces for
C-H and C-O bond activation by transition metal and
metal oxide cations. These studies are being extended
to longer wavelengths and with improved sensitivity by
Gokhan Altinay and Geoff Austein-Miller (freshman
undergraduate), who have recently set up a multi-pass
infrared excitation for vibrational studies from 600-
4000 cm⁻¹. Manori Gunawardhana and Paul Ganssle

new FACULTY

Nathan Schnarr was trained as a peptide chemist at Colorado State University (PhD ’04), where
he learned to test protein stability and molecular recognition with synthetic peptides. As a NIH
Postdoctoral Fellow at Stanford University he decided to let enzymes called polyketide syntheses,
which synthesize medicinal compounds from peptide building blocks, to do the dirty synthesis
work. Nate joined us in September 2007, and is embarking on his independent career to develop
novel polyketide-like natural products through the combined approach of protein design and
organic synthesis.
(senior undergraduate) have obtained exciting results on solvation of multiply charged ions by aprotic solvents by looking at the spectroscopy and photodissociation dynamics of ions such as $M^{2+}(CH_3CN)_n$ where $M =$ Co and Ni; $n = 2-5$. They have also studied mixed acetonitrile-water clusters, complementing previous work in our group on solvation of $M^{2+}$ by water and methanol. Manori wrapped up these studies just in time to (briefly) return to Sri Lanka to marry Thushara Perera, who is a postdoctoral associate with Prof. G. Wilson, UMass Amherst Astronomy. She will be presenting a poster on her work at the American Society for Mass Spectrometry meeting, where Prof. Metz will also be giving a talk.

**In the Rotello lab ...**
The Rotello group focuses on the synthesis and application of nanomaterials. A key issue in the use of nanomaterials is controlling the interfacial interactions of these complex systems. Our research program focuses on the tailoring of interfaces through the atomic-level control provided by organic synthesis. Using these tailored monolayers, we have developed particles for biological applications, including highly effective gene and drug delivery agents. Our most recent move is into the area of sensors, where we have created new sensor systems for proteins and bacteria. The bacteria sensor is particularly promising, enabling the identification of both species and strains of pathogens.

We are concurrently using nanoparticles as building blocks for the creation of new functional materials. In our research we couple synthetic capability with nanomaterials characterization and top-down fabrication techniques, providing access to materials an devices structured on all length scales. These studies use the resources available through the NSF-funded Center for Hierarchical Manufacturing, including electron-beam and nanoimprint lithography.

On the alumni side Angelika Niemz has been promoted to associate professor at the Keck Graduate Institute. Catherine Goodman has been promoted to Associate Editor at Nature Chemical Biology. News from more recent alums: Hao Xu is working at Brewster Scientific, Gang Han is out at the Molecular Foundry. Chang-Cheng You is sorely missed and is working at WMR Biomedical.

**In the Schnarr lab ...**
Professor Schnarr joined the faculty in Fall 2007 and began filling every square inch of lab space with new, shiny equipment. Recently, he joined the Chemistry-Biology Interface (CBI) program and presented his research plans to diverse crowds at both CBI and Molecular and Cellular Biology (MCB) events.

The Schnarr lab is primarily interested in the unique mechanisms associated with microbial generation of polyketides, a huge class of natural products from which a number of clinically useful drugs are derived. Their hope is that increased understanding of how microorganisms produce these valuable compounds will open doors to engineering improved drug candidates for treatment of bacterial and viral infections as well as certain types of cancer. This works nicely complements the current strengths in the department regarding chemical basis for disease and will bring additional perspective related to how highly-evolved enzymes carry out very specialized processes. This spring, Carrie Dulaney, Jon Amoroso, and Lawrence Borketey joined the Schnarr lab and are in the process of mastering modern techniques in Molecular Biology and Synthetic Chemistry. In addition, two undergraduates, Jacob Miller and Cornelius Taabazuing, joined the lab capping off a very successful year of recruiting.

Outside of research activities, Nate will be contributing to both graduate and undergraduate courses in Organic Chemistry. Last fall, he had the pleasure of teaching Advanced Organic Chemistry (CHEM 551) and will continue this assignment during Fall 2008 followed by Synthesis (CHEM 756) in the spring. In addition, Nate is currently serving as Chemistry Seminar Chair and will be coordinating the program for the 2008-2009 academic year.

**In the Stidham lab ...**
Let the world of Goessmann Gazette readers know that we have just had a paper entitled “Vibrational spectrum, ab initio calculations, conformational stabilities and assignment of fundamentals of the $C_i$ conformer of 1,4-dichlorobutane” accepted for publication in Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy.

This semester I am teaching a course in the fundamentals of spin resonance spectroscopy, CHEM 777. The course is primarily focussed on nuclear
magnetic resonance (NMR), but includes a little nuclear quadrupole resonance (NQR) and a nod to electron spin resonance (ESR).

In the Thayumanavan lab ...

The Thayumanavan group enjoyed another productive year in 2007. Please visit us at http://www.umass.edu/thaigroup/ for update on our news and achievements. We think it will be fun for you to learn about the people of our group.

Graduate students: The group welcomed Nagamani Chikkanagari early in 2007 and Reuben Chacko, Daniella Gonzalez, Bhooshan Popere, and Sompit Wanwong joined the group as graduate students early in 2008. Daniella had previously spent a summer in the group, when she was a student in the University of Puerto Rico. In January 2008, we also have a visiting student Kirsten Storch from Germany spending a semester in the group. Britto Sanandanaraj graduated with his PhD and took up the coveted Presidential Postdoctoral Fellowship with Novartis in Zurich, Switzerland. He is pursuing this postdoctoral fellowship in collaboration with Scripps Research Institute. Subhadeep Basu graduated a few weeks before Britto, but continued to stay in the group as his postdoctoral mentor, Prof. Fraser Stoddart, was on his move from UCLA to Northwestern University. He is now at Northwestern, starting January ’08.

Undergraduate students: Rob Demont graduated and became a graduate student in Chemistry at the Florida State University. He is pursuing his PhD with Professor Tyler McQuade. Dan Terk spent part of his 2007 in Australia and is back now. Sean Paradiso (UMass Amherst), Sarah Wardlaw (Smith College) and Jimmy Tran (UMass Amherst) spent summer of 2007 in the group as REU students. Sean was the MassNano REU student, while Sarah and Jimmy were part of the Collaborative Undergraduate Research in Energy (CURE-REU), which is the new REU program in the Chemistry department. Carolyn Sault, Kasey Mackay, Matt Sochat, Pardeep Thandi, David Waterman, Alicia Wood, and Yu Zhao all joined the group as undergraduate research students.

Postdoctoral associates: Ashootosh Ambade left the group to NYU to join Marcus Weck, while Suhrit Ghosh is spending a year in Germany as a Humboldt fellow before taking up his independent position at the Indian Association of Cultivation Sciences in Calcutta, India. Antara Dasgupta, Arisa Jaiyu, Jayaprakash Pagadala, Ja-Hyoung Ryu, Sunita Satav, and Punidha Sokkalingam joined as postdoctoral associates.

INVENTED AT UMASS AMHERST:
LOUIS CARPINO AND THE BOC GROUP

They were only short papers, but they signaled the beginning of Louis Carpino’s ground-breaking research on the amino protecting groups that are a vital part of protein and other organic synthesis today. In a 1956 ACS talk and a January 1957 paper in Journal of the American Chemical Society, Carpino’s interest in an easily removed amino protecting group, that gave only gaseous by-products on removal, was revealed. Others published later that year, but Carpino and his group were the chemists that developed the chemistry that made the tert-butoxycarbonyl or Boc group one of the foundation stones of modern protein synthesis. In 1964 Lou, his wife, Barbara, and graduate students, Paul Crowley, Chester Giza and Paul Terry, described preparation of t-butyl azidoformate, which became the reagent of choice for introduction of the Boc group in Organic Syntheses. Lou Carpino has gone on to invent other protecting groups that are vital to protein and other organic synthesis today. He holds the record for most patents by UMass Amherst faculty member receiving the Lifetime Award with over 20 issued patents.

Just what is a protecting group?

When we synthesize a large complex molecule from small less expensive pieces, we have many reactive groups to contend with. Typically, we want to transform one of these groups but to leave the others unchanged. Lacking the finesse of living cells with enzyme catalysts, our methods are crude and lack the selectivity we want. We use protecting groups to shield reactive groups from indiscriminate chemical reagents. Protecting groups are designed to be attached easily when they are needed and as easily removed when they are no longer necessary.
Krishnamoorthy was promoted to a Research Assistant Professor position. Zeynep Delen is a part of our research group, while she is working at Amherst College. She recently finished her PhD with Prof. Paul Lahti in our department.

In the Thompson lab ...
We welcomed two new graduate students and two undergraduates to the group this year. In October, Seena Koshi joined the group, bringing great experience and ideas. In February, Sheila Jones joined the group, fresh from undergraduate research with Myriam Cotten at Pacific Lutheran University. Both Seena and Sheila have joined senior students Dan Fowler and Fe Consolacion on the chemoreceptor project. Dan presented his work on site-directed NMR distance measurements characterizing the structure of chemoreceptor clusters at the Biophysical Society Meeting. Fe was supported by a CBI Traineeship to continue her work investigating the role of clustering in signaling activity. Professor Thompson was invited to present a talk on their work at a Gordon Conference on “Ligand Recognition and Molecular Gating” in Ventura, California in March. Two undergraduates, Ngoc Ho and Amid Hamidi, joined the group in September as a team working on our new ABC transporter project. Amid is an exchange student from South Carolina State University, and Ngoc is a junior biochemistry major/chemistry minor. She was awarded Academic Year HHMI internships supporting her project for both fall and spring semesters.

Alumni from the Thompson lab are thriving. Greg Gallagher moved from Massachusetts to Virginia where he is teaching at John Handley High School and reports that he is very pleased with his career change. Eleonora Del Federico, an Associate Professor at the Pratt Institute in Brooklyn, organized a symposium in September on “Magnetic Resonance and Art.” She does work with an NMR MOUSE (mobile NMR) to analyze degradation of pigments in paintings at the Metropolitan Museum of Art in New York City. In February, Profs. Thompson and Martin and family enjoyed a fascinating behind-the-scenes look at the work she and art conservators do at the Met. Another Thompson lab alumnus, Stacy Seeley, Associate Professor at Kettering University in Michigan, encouraged one of her students to apply to our graduate program and this student will be joining the department this fall.

In the Tyson lab ...
Many more undergraduate researchers have now contributed to the arsenic project. There were the usual 20-30 CHEM 122+312 students in the spring and a similar number of CHEM 121+315 students in the fall. We are also participants in the NSF-funded STEM program and this student will be joining the department.

In the Thompson lab ...

PROFESSOR PETER UDEN HONORED

The award was the 2007 ‘Eastern Analytical Symposium’ award for ‘Achievements in Separation Science.’ The citation reads ‘presented to Professor Peter Uden in Recognition of his Outstanding Contributions to the Field of Separation Science’ November 13, 2007.

The award was presented at an Honor Symposium organized at the Eastern Analytical Symposium held annually in Somerset, NJ. This is the second largest national gathering and exposition of Analytical Chemists in the United States. The award symposium was chaired by Prof. David Henderson (UMass Amherst PhD ’74), Trinity College. Participating speakers were Prof. Emeritus Ramon Barnes, UMass Amherst, Prof. Peter Carr, University of Minnesota, Prof. Joseph Caruso, University of Cincinnati, Prof. John Dorsey, Florida State University, and Dr. Steven Wise, National Institute of Standards and Technology.

Amongst other attendees at the symposium were more than 40 UMass Amherst alumni.

research academy for young scientists and have helped teachers in Franklin County run arsenic-related after-school programs. Interest in independent studies in the group continues to grow, reaching a new high of seven students (Shay Herschkowitz, Hagit Ben-Daat, Andrew Bell, Bart Smith, Berlinda Luong, Kathy Wong, and Ken Hutchinson) in the Fall of 2007. In the summer, we once again hosted three students from Lincoln University, Julia Greenfield, Lola Fatunmbi and Robert Jones, as part of the NE Alliance summer program of undergraduate research (SPUR). Hagit Ben-Daat, who was supported by a Bradspies Fellowship, and graduate student James Kearns, ably mentored the SPUR students. They will all present the results of their work at Pittcon 2008 in New Orleans. Prince Amoako successfully defended his dissertation and started at Monsanto in January 2008. Graduate student Maura Mahar spent the summer at Perkin Elmer Life and Analytical Sciences in Shelton, CT and came back with several projects. Graduate student Elena Dodova is enjoying some international interest in her work on compound-specific responses in plasmas, and, as a result, we are poised to enter some new collaborations with scientists in Israel, France and Austria. Professor
emeritus Peter Uden continues to be actively involved in the mentoring of students, and Prof. Edward Voigtman now makes valuable input to our group meetings. Professor Tyson was named a Discovery Corps Senior Fellow by the NSF, and will be broadening his knowledge of environmental and geochemistry issues by visiting experts in Thailand, Vietnam, Bangladesh and the UK.

In the Vachet lab ...

It was another busy and successful year for the Vachet lab. Professor Vachet organized a symposium and taught a two-day short course at the American Society for Mass Spectrometry meeting in June. He also co-organized a symposium on “Protein Misfolding and Disease” at UMass Amherst. One of the highlights of the year was to travel to Bucaramanga, Columbia to give a plenary lecture at the 10th Seminario Internacional de Medio Ambiente y Desarrollo Sostenible (International Conference on the Environment and Sustainable Development). While there he also spoke at the Universidad Industrial de Santander (UIS), where former graduate student and postdoc Yajaira Combariza (PhD ’04) is a chemistry faculty member. For his continuing collaborations with chemists there, Prof. Vachet was named a Visiting Professor in Chemistry at UIS.

In group news, Benjamin Vanderpuije and Ben Ditrolio received their MS and BS degrees, respectively. Ben V. is currently teaching at the Springfield High School of Science and Technology, and Ben D. is headed off to grad school in Chemical Oceanography. Also departing in 2007 was postdoc Yajaira Combariza. Yajaira is a chemistry faculty member at UIS, and she was also very recently named the Director of the Centro de Estudios e Investigaciones Ambientales (Center for Environmental Studies and Research) there. Current PhD student Vanessa Mendoza had a very good year. She received a CBI fellowship and also won awards at the Departmental Research Symposium and the CBI retreat for one of the top posters at these events. Finally, several new graduate students joined the group in 2007 including Adam Graichen, Nadnudda ‘Tan’ Rodthongkun, and Zhengjiang Zhu. Adam’s research focuses on understanding the molecular details of Cu(II)’s role in the amyloid formation of β-2-microglobulin. Tan is investigating new ways for amphiphilic polymers, synthesized by the Thayumanavan group, to be used with mass spectrometry to improve the analysis of complex protein mixtures. Zhengjiang, who is co-advised by Professor Rotello, is studying the interactions of gold nanoparticles with cells and is developing new approaches to distinguish cell types using nanoparticles and mass spectrometry.

Former Vachet group members also had very busy and productive years in 2007. On the personal front, Juma Bridgewater (PhD ’06) and his wife, Stacey, celebrated the birth of their daughter Gabrielle in February, and Kwasi Antwi (PhD ’07) and his wife, Dorcas, celebrated the birth of Emmanuela in the summer. Angela Fahey (PhD ’06), who works at Cytec Industries, was recently promoted to manager of the Analytical services group for Pressure Sensitive Adhesives (“the team that sticks together under pressure”). Amanda Chaparro (PhD ’04) was promoted to be the Vice Rector of Academics at the Universidad de Pamplona in Columbia, and Ji hyeon Lim (PhD ’04) joined the faculty in the Pathology Department at the Albert Einstein College of Medicine as a Research Professor.

In the Venkataraman lab ...

From the graduate student alumni side, Jason Field has become a senior advisor in the Ministry of Economic Development and Trade in Canada. In July, DV & family recently visited Jay, Lora and their daughter Rebecca. Derek Van Allen is a research Scientist at the US Naval Research Laboratory. Rattan Gujadhur has moved again and is now Manager of Chemical Manufacturing at Gilead Science in CA. Uche married Uche in September. He is still at Momentive Performance Materials. Craig Bates has moved back to Arqule. Craig, Gemma and their son, Isaac, visited us and DV had a chance to play with Isaac for few hours and show the lab that his father worked. Pranorm is still at Ubon Ratchathani University as faculty in the Department of Science. Travis Benanti graduated in Dec and is now a scientist at Solarity Inc. in PA. DV is still awaiting info from Margaret Trombley (MS ’04) and Arlicia Grant (MS ’04) about their whereabouts.

From the undergraduate alumni side, Claire Cohen Schmidt (BS ’01) continues to be at University of Toledo as research assistant professor. Karen Osman (BS ’00) is now an Account Manager at Kforce Scientific Staffing.
in Boston. Jeremy Kintigh (BS ’01) is in his final stages of his PhD with Prof. Glen Miller at University of New Hampshire. Tom Hill (BS ’02) is finishing up his PhD with Prof. Larry Scott at BC and will take a job in Springfield MA. DV visited BC in October to give a seminar and had a great time. Noah Tremblay (BS ’04) is also his final stages of his PhD with Prof. Collin Nuckolls at Columbia. Jaclyn Murphy (BS ’04) has moved to UIUC with her advisor Prof. John Hartwig. Jackie won an ACS Graduate Fellowship. She also won a Pine Fellowship from UIUC. Jackie is expect to finish her PhD this year and move to ETH for a postdoc. Jackie and Karen visited UMass Amherst one day apart to recruit our students. Mike Doherty (BS ’05) completed his MS degree from UNC and now works for Scynexis, Inc., in NC. Dan Burke (BS ’06) now works with Prof. Craig Hawker at UCSB. Dan squeezed in a visit to UMass Amherst in the fall and a visit to Bueno y Sano and Rao’s coffee. Jocelyn Scheintaub (BS ’06) finished her Fulbright fellowship and moved to UC Berkeley as a graduate student. She works with Prof. Angie Stacy on solid state materials. Gordon Smith (BS ’07) is now a graduate student at UCSB. Andy Kalaydjian (BS ’07) works for Silpro Corporation in Ayers, MA. DV is still awaiting details from Janice Chin (BS ’00), Kate Huber, and Ingrid Swenson (BS ’07) about their whereabouts.

The DV Group has a updated website at http://people.chem.umass.edu/dv/

In the Voigtman lab ...
Last year was a very eventful one for Ed Voigtman. Research started during the summer of 2006 was resumed with a vengeance during sabbatical leave in Spring 2007. By the end of August, three papers were submitted for publication and another two were submitted in October 2007. The first four are now published and the last one is in press. These five papers all deal with limits of detection and are arguably the deepest papers on the topic ever published. An invited talk on a small portion of the work was given at Pitcon in New Orleans on March 6, in the special session honoring the life and career of Prof. James D. Winefordner, Ed’s long-time postdoctoral mentor. Ed’s wife, Janiece, accompanied him and they greatly enjoyed re-uniting with long-time friends and colleagues. And the crawfish étouffee was fantastic!

Ed’s teaching load last fall was absurdly small (thanks, I used the time well), and this semester is the other extreme, but it all balances out. Students in CHEM 312 will be analyzing a 4.5 billion year old Fe-Ni meteorite (vide infra) and using fluorescence to determine riboflavin concentrations in beers, so what’s not to like?

In the Weis lab ...
Researchers in Professor Bob Weis’s lab have been quite busy. Over the past year, they published several notable papers regarding their work on chemotaxis, including an article in Methods in Enzymology, as well as a patent for reconstituting membrane-bound signaling proteins which formed the basis for a spin-off company.

fond FAREWELL

Physical organic chemist and undergraduate orgo-chem lecturer Dr. Gary Snyder will be leaving the department at the end of summer 2008. Gary got his PhD in 1988 at Caltech, working on physical chemistry of biradicals. He did postdoctoral work at University of Colorado Boulder on photoacoustic calorimetry, and went on to faculty/teaching positions that led him here in 2003. At the University of Chicago, he and his group published a remarkable account of a molecule that could have formed a structure with all electrons paired into bond, but which preferred to form a biradical state, which violates the Kekule rules of valence (McMasters, Wirz, Snyder, J. Am. Chem. Soc., 1997, 119, 8568). He continued related work with undergraduate researchers whom he mentored at UMass Amherst. In addition to encouraging undergraduate researchers, Gary has been one of the department’s most committed organic chemistry instructors from his arrival here, organizing and teaching both the large nonmajors organic chemistry courses and enriched majors organic sections with equal aplomb. His dedication to teaching his students how chemistry actually works has clearly been appreciated by his students—he has been nominated by them for the university Distinguished Teaching Award multiple times during his time here. His teaching excellence and focus on his students will be missed.
CHEMISTRY TO HOST NATIONAL FUEL CELL RESEARCH CENTER, LAUNCHED WITH NEW NSF GRANT

The University of Massachusetts Amherst will create a new research center focused on the cutting edge of hydrogen fuel cell science, the National Science Foundation (NSF) has announced, awarding a three-year, $1.5 million grant to the Fueling the Future Chemical Bonding Center. The center is one of only three in the nation funded through the NSF’s chemistry program that focuses on renewable energy, providing UMass Amherst a prominent role in the effort to reduce the country’s dependence on fossil fuels.

Professor Sankaran Thayumanavan leads a team of eight faculty from UMass Amherst and one faculty member from Yale University in the quest to better understand proton transfer, a critical component of fuel cells. Fuel cells offer a cleaner, more efficient alternative to fossil fuels; by capturing the power of hydrogen, they create a direct current of electricity without carbon dioxide emissions or particulate air pollution. Fuel cells will likely be used for powering portable devices such as computers and cell phones, means of transportation such as automobiles and boats, and perhaps buildings and homes.

The award to the UMass Amherst team also positions the campus to compete for $30 million in additional funding, according to the NSF. The initial $1.5 million award is for a three-year period; centers that demonstrate “high potential” then will be eligible for $15 million more in funding over five years, and another $15 million after that.

“The aim of these centers is to give scientists opportunities to tackle big challenges in chemistry, in an atmosphere that’s flexible and tolerant of risk,” says Katharine Covert, director of the Chemistry Centers Program at the NSF.

“We want to encourage very talented people to attack major challenges that also engage the public and have a long-term societal benefit.”

“This investment by the NSF recognizes UMass Amherst as a hub of leading clean energy research,” says Congressman John W. Olver, who recently helped secure $1.6 million in separate funding for UMass Amherst’s Center for Renewable Energy, Science and Technology (MassCREST). “The technologies that are likely to emerge from this important work will stimulate economic development and manufacturing opportunities in the state. This also provides a tremendous opportunity for the Commonwealth to train tomorrow’s workforce.”

The UMass Amherst center will focus on investigating the subatomic particles known as protons and the molecular conditions under which protons get transferred from one molecule to another. Proton transfer is widespread in the biological world, often happening when cells need to get something done. But understanding how proton transfer works and under what conditions also has immediate applications for fuel-cell efficiency. “A better understanding of proton transfer will allow us to address one of the greatest challenges to moving away from a fossil-fuel based economy,” says UMass Amherst Interim Chancellor Thomas W. Cole, who is also a chemist. “I’m thrilled that our outstanding team of researchers has been selected for this task.”

Fuel cells take advantage of breaking the chemical bonds of a molecule and using the released energy to generate electricity. On one side of a fuel cell, electrons are stripped from a gas such as hydrogen (H₂). The electrons travel through an external circuit, doing useful work. The protons (H⁺) also travel to the other side, but do so by passing through a special membrane that divides the cell and is only permeable to protons. Once on the other side of the membrane, the protons reunite with the electrons coming in from the circuit and combine with oxygen to form water, which drains from the cell. Since none of these involve carbon-based molecules, this is one of the cleanest forms of energy.

In theory, as long as there is hydrogen flowing in one end and oxygen in the other, a fuel cell will generate clean electricity. But scientists are still addressing the finer points of fuel-cell efficiency. One stumbling block has been how to best transport hydrogen’s positively charged protons—and only the protons—across the special membrane that divides the cell. Investigating this proton transfer is the charge of the new center.

“Nature has evolved systems for shuttling protons at really impressive rates—it’s happening in our cells all the time. But these molecules cannot be taken out of their native environments and installed onto a fuel cell,” says Thayumanavan. “Our objective is to discover the molecules and materials required to get really efficient proton transfer—which groups are best at donating protons, which are best at accepting them—and how can we optimize the handshake between the donor and the acceptor?”

Such questions don’t raise eyebrows at UMass Amherst—the new center builds on what is already an impressive body of chemical energy research at the campus. Under the umbrella of MassCREST, more than 25 scientists across five departments work on clean energy research, from designing solar cells to using engineering proteins to make fuel.

The center will also have extensive education and outreach at all levels, playing a key role in addressing the human resources needed for the rapidly growing area of renewable energy technology. Graduate and undergraduate students involved in the research will be at the leading edge of a dynamic field. The center will also have a Web-based interactive network that acts as a public portal where educators, students and the public can get accurate information on chemical energy topics. This National Chemical Energy Research Network will also provide an interface between researchers and centers involved in chemical energy research. –In the Loop
**P. A. TECH. LLC LAUNCHES ITS FIRST PRODUCT**

By the time Tony Shrout and Ed Esposito (PhD '05, Robert Weis and Craig Martin, resp.) graduated, their dream of starting a Biotech company had ‘taken shape’. Protein Attachment Technologies, LLC (P. A. Tech, http://www.patechllc.com) was founded February 2006 by Tony and Ed, with Weis and Tim Shront, to produce innovative high-throughput enzyme assays of kinase activity. Kinases are central figures in disease-related cell signal transduction pathways. As graduate students, Tony and his colleagues in the Weis lab had demonstrated that template-directed assembly (TDA) was an effective method to make membrane-associated enzymes function better—in a way that mimics cellular behavior. With an exclusive license from the University for the patent-pending TDA technology, Tony and Ed set out to create assays that identify promising drug leads more effectively.

Along the way, Tony and Ed have faced a many challenges, not the least is starting a biotech company in Amherst. Identifying a location, getting through the town and state permitting processes, designing the lab, overseeing its construction, as well as acquiring lab equipment, all had to be done while moving the technology toward commercialization. Just last December, P. A. Tech finalized a sales and distribution agreement with Millipore Inc., a world leader in life sciences products (www.millipore.com), to market the nanoparticle template material that forms the basis of TDA-enabled assays. Millipore’s marketing, distribution and sales prowess, screening services, and industry contacts will help to get the pharmaceutical industry to use new TDA-enabled assays, which is paramount to the fledging company. Because high-throughput screening is a multibillion dollar market, with billions of samples (wells) measured each year, a market acceptance of just a few percent translates into substantial revenue. P. A. Tech plans to make inroads with unique new valued-added assays. Scientific and business advice continues to be an essential part of this development. On the science side, the advisory board is comprised of Weis (chair), Prof. Dhandapani Venkataraman, Adj. Professor Tomi Sawyer (VP of Drug Discovery & Innovative Technologies at AILERON Therapeutics), and Dr. Tony Pawson (Samuel Lunenfeld Research Institute) a world-leader in signal transduction research. On the business side, advice is being sought from many sectors of the Biotech industry. As P. A. Tech progresses through the next stage of development—the introduction and adoption of new assays and biological reagents—both an infusion of capital and personnel are being sought—stay tuned for more exciting developments from this home-grown venture.

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**degrees AWARDED**

**BA/BS DEGREES**

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Professor John A. Chandler 1933-2007

By his own calculations, John estimated that he taught in excess of 20,000 students in general chemistry from 1959 to 2006. This single piece of data highlights the life and career of Prof. John Chandler. He was a teacher in all of its many incarnations. He advised, mentored, counseled, directed, and assisted many students pursuing their career and life dreams during his six-decade career. He once reflected that he had taught children and grandchildren of his former students. There had to be reasons they kept coming back. And those reasons were his competence, compassion, and excitement about teaching and learning.

John Allard Chandler was born on January 12, 1933 in Chillicothe, Ohio. He had a sister Julia, and grew up on his aunt and uncle’s farm. In high school one of his teachers convinced him there was no future in his favorite subject, math, and that he should major in something more practical. He chose chemistry. He graduated Phi Beta Kappa from Ohio University in Athens, Ohio in 1955 with minors in physics and math. At the University of Illinois at Urbana he earned the MS degree in 1958 and the PhD in inorganic chemistry in 1959. His PhD advisor was Russell Drago, a 1950 BS graduate of UMass Amherst. While a graduate student at Illinois he and his wife Joann visited Drago’s vacation camp on the Connecticut River so John knew of and about the Pioneer Valley.

In 1959 he responded to an advertisement in C&E News for a faculty position at UMass Amherst. He sent in letters of recommendation and was offered and accepted the position without interviews or visits. Quite a contrast to today’s hiring process! And so John, wife Joann, and sons Charlie and Jack set out for Amherst to begin his academic career. When John arrived in Amherst there were in place several situations that were to mold his future career. There was a paucity of graduate students, J. Harold Smith taught advanced inorganic chemistry and was reluctant to give it up, and, because the enrollment in general chemistry was exploding, that area needed direction and management. As a result, John taught general chemistry, functioned as a teaching assistant in the laboratory for the first few years he was here, and was recruited into the general chemistry leadership team. Because of these demands and the lack of graduate students, his research program suffered. He had three graduate students overall and produced a research paper working with Howard Stidham in 1968. By the early 1960s however, the die was cast; first year chemistry was to be his career - one crafted by circumstance, but embraced with vigor and caring. In 1966 his third child, daughter Michelle, was born.

When George Richason Jr. stepped down as director of general chemistry in the mid-1960s, George Oberlander took the reins for a year, after which John became Director of General Chemistry in about 1968. He held this post until Bill Vining arrived in 1996. During the last few years he was anxious to leave the post, but stayed on with Roberta Day acting a co-director. During his almost thirty years as Director of General Chemistry the department published several workbooks containing lecture notes and labs that all instructors used. All instructors also used the same exams. During his tenure the department moved from weekly quiz sections, to PLATO, to the beginnings of the OWL on-line homework system. The weekly two-hour lab was changed to a biweekly three hour lab.

Finally in 1996 John was happy to return to full time teaching, which he continued until his retirement in 2002. As Professor Emeritus he continued to teach part time until his vision and health no longer allowed it. During 2006 his health deteriorated, but he still came to his office in Goessmann Laboratory occasionally to see his friends and colleagues. He passed away on March 4, 2007 surrounded by his family. A memorial service was held on Monday, March 12. His family, wife Joann and children Charlie, Jack, and Michelle, created the John A. Chandler Memorial Scholarship in June 2007. This endowed scholarship is to support “scholarships for undergraduate students at the University of Massachusetts Amherst who have declared Chemistry as their major.” Preference for the Chandler Scholarship, true to the person for whom it is named, is given to students who plan on pursuing a career in teaching. The first recipient of the scholarship is Julia M. Kumpf, a member of the class of 2008. —David Adams

Roger Gordon Bates 1912-2007

Roger Gordon Bates, a Massachusetts State College (MSC) alumnus, class of 1934, died August 20, 2007 at 95 years of age. Roger was born on May 20, 1912 in the Western Massachusetts town of Cummington, twenty miles west of Northampton. After attending Cummington public schools for the first ten grades, he graduated in 1930 from Northampton High School. Although his family owned a diary farm, Roger has no inclination toward that career. He chose to enter college at Massachusetts Agricultural College (MAC), which became Massachusetts State College (MSC), in 1933. At MAC he majored in chemistry and pursued his life-long music interests as a member of the orchestra and chorus.

At MAC/MSC Roger lived in the North College building for a time and was a member of the Kappa Epsilon fraternity. He was also active in the chorus and orchestra, served as literary editor of the INDEX, and was pianist for the “State” chorus and orchestra, for which he won an academic medal in 1933. While at college he befriended...
many chemistry professors including Joseph “Shorty” Chamberlain, Charles Adams Peters, Richard “Doc” Fessenden, and Ernest Parrott. Roger once said that he regarded Prof. Chamberlain as a father figure because of his compassion, support, and interest. Roger did his senior honors thesis on the quantitative determination of zinc using organic reagents under the direction of “Doc” Fessenden.

Upon graduation from MSC, Roger applied to the University of Minnesota to continue his zinc analysis work under Prof. I.M. Kolthoff. Unfortunately he was unable to secure an assistantship to support this graduate work. Roger had other opportunities, however. He was offered the only teaching assistantship at MSC for the 1934-35 academic year, and had a similar offer from Duke University. He chose to go to Duke because of his interest in seeing other parts of the country. Roger received the MA in 1936 and PhD in 1937 at Duke working with Prof. Warren C. Vosburgh. After Duke Dr. Bates spent two postdoctoral years at Yale University on a Sterling Fellowship.

In 1939 Dr. Bates went to Washington as a physical chemist with the National Bureau of Standards (NBS). His career at the NBS spanned thirty years. While there, he literally “wrote the book” on the operational definition of pH. In his classic 1954 book “Electrometric pH Determinations” Bates detailed the confusion then surrounding pH determination and proposed the NBS pH standards now used throughout the world. After retirement from government service in 1969 he joined the faculty at the University of Florida at Gainesville. He taught there until 1979, when he retired as Emeritus Professor. From 1953 to 1983 he was very active in the IUPAC Commissions on Electrochemical Data, Electroanalytical Chemistry (chairman), and Physiochemical Symbols, Terminology, and Units. He was introduced to IUPAC work by I. M. Kolthoff, who years later told him that he wished Minnesota could have offered him an assistantship back in 1934 when Bates applied there.

During his government and teaching career Dr. Bates received many awards, including the ACS Washington Section Hillebrand Prize in 1955, the gold medal from the Department of Commerce in 1957, and special recognition from the Analytical Chemistry Division of the Royal Academy of Chemistry in 1995. During his career he published over 280 technical papers and authored three books.

In 2000, Prof. Bates funded the Roger G. Bates Chemistry Fund at UMass Amherst. The fund provides money for the enrichment and extension of programs within the department. Recently the fund has provided summer research opportunities for several undergraduate students.

Roger and his wife Jo lived in a retirement village in Florida. He was active in the village chorus, played the organ at church, gave community organ recitals for many years, and played tennis until three years ago. His wife Jo died in 2003; he is survived by his daughter May Daw.

--David Adams

WILLIAM E. McEWEN MEMORIAL SCHOLARSHIP FUND

When Professor William E. McEwen passed away in May of 2002, there was an outpouring of financial support by Chemistry alumni, family and friends. Since then, a yearly award has been made to support outstanding graduate students. That fund would have run out had it not been for two of Prof. McEwen’s former students. These two individuals, who wish to remain anonymous, have made two separate gift arrangements to endow the William E. McEwen Memorial Scholarship Fund.

One of the donors has pledged $10,000 over the next five years. However, because of the generous 3-1 matching gift policy of this donor’s company, the total gift will be $40,000. The second donor made a gift of $50,000. That gift will be matched by the Public Higher Education Endowment Incentive Program (the Commonwealth of Massachusetts program to encourage individuals to create endowments at the public colleges and university). All told, the scholarship will have more than $100,000 in new funding.

This scholarship will aid graduate Chemistry students and will be awarded as part of the ResearchFest tradition with the award given to the most outstanding graduate student. Professor McEwen virtually established the graduate program in the Department of Chemistry when he arrived in Amherst with an exceptional group of graduate students from the University of Kansas. It is only fitting that an award in his memory be awarded to the most exceptional graduate students.

To contribute to the William E. McEwen Memorial Scholarship Fund send your gifts to the Department of Chemistry, UMass Amherst, 710 North Pleasant Street, 701 Lederle Research Tower Room, Amherst, MA 01003.
RAY D’ALONZO AND DAVE MAZZO HONORED BY THE GRADUATE SCHOOL

The Graduate School celebrated its 100th anniversary on April 9, 2008 by hosting a series of talks and awards in a program entitled, “A Century of Scholarship, 1908-2008.” David J. Mazzo (PhD Chemistry, ’84) was chosen as one of the three representatives for the College of Natural Sciences and Mathematics. Mazzo, president and CEO of the global pharmaceutical company Aeterna Zentaris, Inc., discussed his professional development in his talk, “From Classroom to Boardroom: One Analytical Chemist’s Journey.”

Ray D’Alonzo (PhD Chemistry, ’77) and Dave Mazzo were recognized with the NSM Graduate Alumni Award at this centennial celebration. Receiving the award on behalf of Ray was his daughter. Congratulations, Ray and Dave!

new ADDITIONS

Jon Belanger has a new little sister, Cecelia Grace Zhifan Belanger. Her birthday is Feb 17, 2006 she was born in the Jiangxi province in China. She was adopted on December 2, 2007, and became a US citizen on December 12, 2007.

Finnley Grace Chambers was born at 3:45 AM on 3/1/08 and was 22 inches, 8 pounds, 9 ounces. She is quiet (so far) and is a happy camper. Her big sister, Noa Jane, is very proud, and so are her parents, Prof. Jim Chambers and his wife, Bekki.

Beckett Hardy Baird was born on September 16, 2007 and was 9 lbs 4 oz, 22 inches long. He kept mom, Prof. Jeanne Hardy, and dad, Bruce Baird (Languages, Literatures, and Cultures) waiting an additional eight days to meet him.

staff CHANGES

Susan Pixley, our Seminar/Alumni coordinator, was offered a job in her former field that she couldn’t pass up. She now works for the state as a Youth Program Coordinator for the National Guard. Her new position melds together her experience as a coordinator and social worker, as well as her education in sociology. Susan has a gift with people and children so her new job is a perfect match. We miss her smiling face and wish her well.

Carrie Morrison Penland joined our Chemistry team this spring as our new Alumni/Seminar Coordinator. It was a smooth transition into the main office because she was already familiar with the staff and most of the faculty as staff assistant to the CBI Program. We are excited to have Carrie on board. Her kind spirit and positive personality are a welcome addition to our department. She has done a wonderful job so far and she’s looking forward meeting many of you at the Alumni Reunion.
2007 SEMINAR SERIES

The 2007 seminar series provided a wealth of extraordinary speakers and diverse topics spanning all areas of the chemical sciences. From start to finish, we were continuously awarded with enlightening subject matter and informative interactions.

The annual *Five College Seminar* was graced with a visit by Professor Frances Arnold from the California Institute of Technology. As the certain leader in the area of molecular evolution, Dr. Arnold cleverly combines chemical and biological principles ideally suited for our broadly-based academic community. Her lecture entitled, “Lesson from Synthetic Protein Families,” revealed the enormous potential in utilizing both rational and evolutionary mechanisms to improve enzyme characteristics through the process of what she terms directed evolution.

On October 11, Professor Lewis Kay from the University of Toronto visited the department for the annual *Proctor & Gamble Honorary Seminar in Chemistry*. His lecture, “Seeing the Invisible by Solution NMR Spectroscopy,” beautifully illustrated the concept that nothing, at the atomic level, is as simple as it may seem. Using state of the art spectroscopic methods, the Kay lab is able to measure chemical species whose incredibly short lifetimes render them functionally invisible. This work continues to test and rewrite many of the historical paradigms involving how proteins fold.

The 2007 *Richard Stein-Bayer Corporation Honorary Seminar in Polymer Chemistry*, held November 1, brought a true pioneer of modern scientific thought. Professor George Whitesides from Harvard University delivered a provocative lecture entitled, “Reinventing Chemistry,” which asked difficult questions about the future of chemical research and education. The seminar garnered unprecedented interest and a second room, televising the talk, was needed for overflow. Professor Whitesides strongly encouraged next generation scientists to be daring and strive for the seemingly impossible.

Capping the 2007 seminar series, the *William E. Mahoney Annual Lecture* featured Nobel Laureate scientist and acclaimed writer, Professor Roald Hoffmann of Columbia University. Prior to his visit, chemistry department faculty and students participated in a staged reading of his award-winning play “Oxygen.” The premise of Oxygen is the awarding of a retro-Noble prize for the discovery of oxygen. It is a play that left the audience and performers still debating the question! His talk entitled, “Chemistry’s Essential Tensions: A Different Look at a Science,” was presented before a diverse set of several hundred students and faculty on November 15. Professor Hoffmann painted an interesting picture of the history of chemistry along with numerous parallels linking natural science and art. As part of an overriding theme, audience members were asked to consider elements of beauty from fundamental arguments of symmetry and complexity, sparking many “water-cooler” discussions throughout the subsequent days and weeks.

The Chemistry Department Seminar Series continues to attract top-notch researchers with a variety of cross-disciplinary interests. Our special thanks go out to all of our alumni who make these events possible through their generous contributions. As always, we look forward to the next year with hopes of continued success and even further improvement to this very important component of our program.
The 17th Annual Research Symposium was held on August 28, 2007. Four students were selected by a committee to give oral presentations and were given the following awards (from left to right):

**Procter & Gamble Outstanding Chemistry Graduate Student:** Mrinmoy De (Rotello Lab) for “Engineering the Protein–Nanoparticle Interface”

**Rohm & Haas Outstanding Chemistry Graduate Student:** Elamprakash Savariar (Thayumanavan Lab) for “Self-Assembled Polymer Nanostructures: Design, Synthesis and Applications”

**Momentive Performance Materials, Inc. Outstanding Chemistry Graduate Student:** Travis Benanti (Venkataraman Lab) for “Fluorocarbons in the Design and Synthesis of Conjugated Materials”

**William E. McEwen Fellowship:** Meaghan Germain (Knapp Lab) for “Fluorescence Quenching Mechanism of Zn(salophen) by Nitroalkanes and Nitroaromatics”

There was a wonderful turnout for the two poster sessions, which contained over 40 posters. The judges had a hard time choosing just four outstanding posters because every student did a great job. In the end though, there were four awards given out as well as an honorable mention, and they were as follows:

**Peter C. Uden Outstanding Poster Award Sponsored by Procter & Gamble:** Michael Odoi (Barnes Lab) for “A Photon-by-Photon Study of the Fluorescence Dynamics of Single Quantum Dot/Conjugated Organic Composite Nanostructures (CdSe-OPV)”

**C. Peter Lillya Outstanding Poster Award Sponsored by Rohm & Haas:** Shiv Redhu (Martin Lab) for “Mismatch at the Edge of the Transcription Bubble Rescue Abortive Cycling in T7 RNA Polymerase”

**George R. Richason Outstanding Poster Award Sponsored by Rohm & Haas:** Vanessa Mendoza (Vachet Lab) for “Probing Surface Topology of Proteins Using Selective Covalent Modification Combined with Mass Spectrometry”

**Marvin Rausch Outstanding Poster Award Sponsored by Fisher Scientific:** Sravanti Vaidya (Hardy Lab) for “Elucidation of Mechanism of Activation and Development of Allosteric Trigger in Caspase-6”

**Honorable Mention:** Kristen Huber (Hardy Lab) for “Caspase-9 Inhibition and Activation by Dimerization Control”

We would like to extend a thank you to the many organizations involved in making this event possible. We thank the sponsors: UMass Amherst Department of Chemistry, Rohm & Haas, Procter & Gamble, Fisher Scientific, Bruker Biospin, Momentive Performance Materials, Inc., Cambridge Isotopes Labs, and the William E. McEwen Endowment Fund for their financial contributions.

The BBQ at the end of the day gave everyone an opportunity to relax and enjoy the beautiful weather. It was nice to see members of the chemistry community bring their families to socialize and conclude a great day of science. We look forward to seeing everyone next year for ResearchFest 2008.
At its ninth annual Senior and Awards Dinner, held in the Lincoln Campus Center on the UMass Amherst campus on Tuesday, May 15, 2007, the chemistry department recognized those undergraduates who have distinguished themselves in the pursuit of academic excellence. More than a hundred students, parents, faculty and staff attended the event that included a buffet dinner followed by the presentation of 35 awards to 27 deserving undergraduates. The students and guests were welcomed by Department Head Bret Jackson, and the 29 graduating seniors were introduced by Prof. David L. Adams, who also acted as master of ceremonies. Marie Whalen, Undergraduate Program Manager, organized the evening’s activities, and Lisa Korpiewski, departmental Graphics Designer, providing the creative talents, designed the program and made the certificates and favors given to individual students. Additional information about the undergraduate awards is available at the departmental web site at www.chem.umass.edu/Undergraduate/scholarshipAwards.htm.

The following students received awards:

Christine M. Oslowski
– Outstanding Senior Undergraduate Award

Michael J. Hernon
– Connecticut Valley Section of the American Chemical Society (CVS/ACS) Student Award

Daniella M. Pizzurro
– American Institute of Chemists Award

Luke A. Miller and Gordon M. Smith
– Richard W. Fessenden Award

Daniella M. Pizzurro and Gordon M. Smith
– Senior Class Award

Antranig Kalaydjian and Brendan T. Keene
– Merck Index Award

Peter J. Kim
– Departmental Recognition Award

Michael J. Hernon, Antranig Kalaydjian and Ellen J. Swain
– Outstanding Undergraduate Researchers 2007

Michael J. Hernon
– Alumni Association Senior Leadership Award

Gordon M. Smith
– 21st Century Leaders Award (nominated)

Benjamin R. DiTrollo
– ACS Analytical Chemistry Award

Benjamin R. DiTrollo
– Jay A. Pirog Scholarship

Benjamin R. DiTrollo
– Bates Research Fellowship

Hagit Ben-Daat
– Bradspies Research Fellowship

Julia M. Kumpf and Karma Tsering
– Hach Fellowship

Jill Park, Shannon M. Brighenti and Jonathan T. Klaucke
– Robert Maxwell Williams Memorial Scholarships

Jennifer L. Fraser, Amanda M. Lincoln, Yin Wong, Brittany J. Chaney-Ryan and Arionela Jashari
– Edward Shapiro Scholarship

Sean D. Bickerton, Tamara L. Allen and Arjuna L. Baratham
– CRC Freshman Chemistry Award

Liam M. Casey, Elizabeth A. Otmaskin and Christopher M. Vercollone
– Honors General Chemistry Poster Award
Cell-death proteins with on/off switches. Cell death can be a good thing, as this allows for tissues to develop into organs. But if the proteins controlling cell death misbehave, then tissues may grow uncontrollably which can lead to diseases such as cancer. Cell death, as with many other biochemical processes, involves the concerted action of many proteins. The challenge to researchers then becomes one of identifying the best target for therapy.

Researchers in Jeanne Hardy’s lab are building tools for discovering which protein is the best drug target for treating a specific disease. To date, there is no systematic way to answer this question. They are developing “designed allosteric switches” in the proteins involved in apoptosis, programmed cell death. Apoptosis is involved in over 50% of the diseases for which there is presently no suitable treatment.

“To make these switches we design a cavity in a protein surface so that it can bind to an already well known drug. When the protein binds to the drug, the protein is inactivated,” says Prof. Jeanne Hardy. Using this technique they can determine the exact cellular role of proteins even when they are members of closely related families, which usually makes determining unique roles very difficult.

Protein teams at the membrane interface. Transmembrane signaling processes are the initial steps in many cellular events, including differentiation and cell death. As many diseases, notably cancer, are attributable to improperly regulated pathways, targeting these pathways is a major thrust in the pharmaceutical industry. The challenge is that transmembrane proteins are notoriously difficult to study, which makes structural and reactivity studies challenging.

Research conducted in Bob Weis’ and Lynmarie Thompson’s labs seek to understand the chemotaxis signaling system in E. coli, as a model signaling pathway. The information and tools that result from these model studies have pointed the way to better structural data as well as better screening tools. One important finding is that teams of proteins are needed for proper function of the signaling proteins. A new general method called ‘template-directed assembly’ developed in the Weis lab recreates these teams more easily, and it has been found to work well with signaling pathways that are the focus of drug development efforts. As a result, this technology has spun off from the University as a startup company to create more accurate and rapid tests of signaling protein activity. (See accompanying article “P. A. Tech. LLC Launches Its First Product,” pg. 15).

Another notorious challenge in studies of membrane proteins is the difficulty in getting high-resolution structural information. Such information is of practical importance for rational drug design for the large fraction of potential drug targets that are membrane proteins. Solid-state NMR approaches being implemented by the Thompson lab in this project are likely to prove useful for such efforts in the future.

Neuroscience and chemistry. It is strange to think of memory as a changing voltage signal. But that is exactly how workers in Jim Chambers’ lab define memory at the level of single neurons. By developing new tools to understand the chemical basis for learning and memory formation in single neurons, they will contribute to our understanding of how the brain works.

Researchers in the Chambers’ lab are designing new drugs that respond to a light pulse, to selectively turn-on or turn-off the receptors mediating memory formation. This will allow them to study the intricate circuitry that goes into memory formation. In a related project they are designing molecules that respond to light by changing shape reversibly. These molecules can be used to turn brain cells on and off, depending on which wavelength of light the researcher uses. “The goal of this work is to dissect the intricate network of brain cells involved in learning and memory,” says Prof. Jim Chambers.
Molecules and Pathways
While the biomolecules involved in many cellular pathways are known, it remains difficult to relate changes in these molecules to diseases. Understanding how cells communicate and regulate gene expression in response to environmental signals is an enormous challenge with the potential for pointing the way to improved therapies for diseases ranging from asthma to cancer.

Molecular machines and nucleic acids. Although proteins are traditionally recognized as the workhorses of the cell, they are encoded from genes through an intermediate called RNA (RNA is increasingly recognized as also performing many of the roles of proteins!). Many steps in gene regulation are controlled at the level of RNA, which has led to an explosive growth of RNA research in the biomedical community. This is reflected in the award of the 2006 Nobel Prize in Medicine to Craig Mello from the University of Massachusetts Medical School.

Researchers in Prof. Craig Martin’s lab focus on understanding the enzyme RNA polymerase. We now know that this protein nanomachine undergoes dramatic rearrangements in transitioning from a complex optimized for the initiation of RNA synthesis to one optimized for the stable addition of thousands of nucleotides onto the growing RNA. Studies in the Martin lab are testing and refining specific structural and mechanistic models for this dramatic transition.

From catalytic RNAs to riboswitch sensors, the role of RNA in biology is becoming much richer than the central, but simple “DNA makes RNA makes protein” paradigm. How synthesis (by proteins) of that RNA is controlled is key to understanding and exploiting the richness of the “RNA world.”

Structural heterogeneity in the ECM. The space between cells is often the most active for controlling how tissues grow. Normal growth requires complex signaling between nearby cells, but signaling molecules must first cross a chemically rich environment called the ECM (extra-cellular matrix). The challenge is to define the molecular components of the ECM at a chemical level, as they play an active role in storing, protecting and releasing these signaling molecules.

Researchers working with Profs. Paul Dubin and Igor Kaltashov are trying to understand the relationship between structure and biological activity of the most complex and versatile ECM components. These molecules, called glycosaminoglycans, not only modulate the many stages of cell growth, including proliferation and angiogenesis, but also affect other events such as adhesion between cancer cells and normal cells. “In terms of understanding of structure-property relations, complex polysaccharides like glycosaminoglycans are at the same stage as proteins 60 years ago” said Prof. Paul Dubin.

Oxygen sensing and angiogenesis. While blood is the aqua vitae, oxygen is the gas of life. The quantity of red blood cells, where blood vessels grow, and the use of iron to make hemoglobin, all are regulated to provide our cells with enough oxygen. Although how our cells respond to oxygen is central to lung development, cancer, and heart disease, the proteins that sense oxygen remain poorly understood.

Researchers within Mike Knapp’s lab are hard at work to understand the chemistry of oxygen sensing. They are combining the tools of enzyme kinetics and spectroscopy to understand the human oxygen sensors. These sensors require iron, and sense oxygen through their action on the transcription factor called the hypoxia inducible factor (HIF). “These enzymes are huge targets for the pharmaceutical industry, and can teach us much about O₂-activation chemistry,” said Prof. Mike Knapp. The long-range goal of this work is to discover how the oxygen sensors are regulated, and understand the chemistry involved in O₂-activation.
ligand and a single receptor. Sensory processes such as taste and smell, however, use “differential” binding in which multiple receptors bind to many different ligands with varied affinities, and the resulting binding pattern leads to molecular recognition.

Inspired by this approach to molecular recognition, Goessmann Professor of Chemistry Vince Rotello and his group are developing differential sensor arrays based on functionalized nanoparticles. In a recent study, a sensor array containing six gold nanoparticle-fluorescent polymer assemblies was created to identify and quantify protein targets. In this system protein analytes displace the nanoparticle-bound polymers, causing the fluorescence of these polymers to no longer be quenched by the gold nanoparticles providing fluorescence patterns that can distinguish and quantify individual proteins at physiological concentrations. Their sensor arrays have also been extended to identify bacteria with high accuracy. “Rapid and efficient sensing of this sort could revolutionize fields ranging from environmental monitoring to personal medicine” said Prof. Vincent Rotello.

Mass spectrometry-based methods to study protein amyloid formation. Amyloid fibrils are insoluble protein aggregates that are associated with many pressing diseases such as Alzheimer’s, Parkinson’s, and Lou Gehrig’s disease. Early diagnosis of these diseases is currently very difficult, but Prof. Richard Vachet and his research group are developing analytical methods to understand the early stages of protein amyloid formation. Molecular-level insight into this process could lead to methods that allow precursors of these diseases causing amyloids to be detected before they cause damage.

Workers in Vachet’s lab are studying the amyloid fibril formation of the protein β-2-microglobulin (β2m), which forms amyloid fibrils in the joints of patients undergoing long-term dialysis as a result of kidney disease. β2m is a convenient model system for studying amyloid formation and for developing new analytical methods to investigate the early stages of this process. The new methods that are being developed by the Vachet group are based on mass spectrometry, and they provide unprecedented molecular-level information about the early stages of oligomerization and protofibril formation.

The Future of Treatment
Improving therapies for infections is often a matter of outsmarting the pathogen. This can sometimes be accomplished by finding a unique nutritional requirement for the microorganism or by targeting some unique biochemistry of the pathogen.

Smart drug delivery. Development of therapeutics is an expensive process that can take 12 to 15 years from conception to market with costs often exceeding $500 million. Even so, for most drug formulations only a fraction of the active drug reaches the desired physiological location because much is lost in metabolism and excretion. Moreover, to be effective drug levels must remain at therapeutic concentrations, above which the drug is toxic and below which it is useless. Conventional drug administration results in frequent cycling between the toxic and ineffective levels depending on the frequency with which the drug is administered.

An attractive solution for maintaining therapeutic drug concentrations is a controlled release system, where a drug molecule is slowly released over time, thereby minimizing dosage fluctuations. The Thayumanavan lab designs polymers that act as smart delivery vehicles
which not only exhibit the desired controlled release properties, but also inherently respond to therapeutic need or toxicity biomarkers. “We have some promising candidates for a specific target that concerns pain-killers. The interesting thing is not only that we have some promising vehicles, but also that these vehicles exhibit no toxicity so far. We are very excited about the prospects,” said Prof. ‘Thai’ Thayumanavan.

*Engineering new bio-pharmaceuticals.* Antibiotic-resistant infections result from the rapid evolution of pathogens and form a growing threat to our health. Medical research has failed to keep ahead of the pathogens with a notable example being the increased prevalence of antibiotic-resistant staph infections nationwide. Where will chemists find the next generation of antibiotics?

**Professor Nate Schnarr** and his research lab are rising to the occasion. They are engineering bacteria for improved production of polyketides, which are a rich source of natural pharmaceuticals. The problem is that polyketides are produced from slow-growing fungi, making discovery of new polyketide drugs time-consuming. In addition to engineering bacteria to produce polyketides, Schnarr’s lab is striving to understand polyketide biosynthesis in order to generate libraries of these compounds for screening, or they hope to identify promising natural products for the next generation of antibiotics.

The Schnarr lab is exploiting the inherent flexibility of complex biosynthetic factories responsible for polyketide generation to access new small-molecule therapeutics based on promising natural molecular scaffolds. Successful demonstration of these methods will result in environmentally-benign construction of drug analogs exhibiting biological activities ranging from antibiotic to antitumor. Aside from the obvious pharmaceutical utility associated with this type of drug-discovery, mechanistic interrogation of these novel compounds in living tissue will provide substantial insight into how pathogens develop into drug resistant strains.

**Infections and nickel metabolism.** Transition metal ion concentrations are under tight control in our bodies. When these concentrations tip out of balance, health problems can emerge. Also, upon infection, certain pathogens compete for this same pool of metal ions, and limited access to these metal ions can reduce the growth rates of certain pathogens. A better understanding of the biochemical control of transition metal ions could then lead to new ways to address metal deficiencies or excesses and to control infection.

Researchers in Prof. Mike Maroney’s lab are hard at work to understand how bacteria acquire and utilize nickel. In addition to understanding the basic biochemistry of nickel metabolism, detailed insight into the molecular mechanisms involved should lead to a better general understanding of how life controls metal ion concentrations. This research could lead to new therapies for controlling metal ion concentrations, but another potentially exciting outcome is that ideas about new antibiotic strategies might arise. The metalloenzymes used by bacteria to control nickel have no known human versions, so these enzymes could be targets for the next generation of antibiotics.

**Protein structures by mass spectrometry.** Recombinant proteins are the fastest growing segment of bio-pharmaceuticals because of the specificity that proteins provide for the treatment of infections. Their market share is expected to outpace the traditional small-molecule medicines in the not-to-distant future. Since the biological activity of all proteins is intimately related to their higher order structure, the challenge is to retain native protein structure from production through delivery.

Professor Igor Kaltashov’s lab is developing novel mass spectrometry-based methods to sensitively detect changes in how a protein is folded. The much higher sensitivity, accuracy, and site specific spatial resolution of the information generated by these techniques when compared to other more classical biophysical techniques should enable it to find much more significant use in the monitoring of the activity of protein pharmaceuticals.
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ALL ALUMNI ARE CORDIALLY INVITED TO THE
CHEMISTRY ALUMNI REUNION 2008
Featuring Professors Jeanne Hardy and Richard Vachet talking about
“HEALTH & DISEASES: Discoveries and Treatments”

YOU are cordially invited to the next Chemistry Reunion on Saturday, June 7, 2008. The Department of Chemistry will feature lectures on issues related to HEALTH & DISEASES, by two of our faculty members: Profs. Jeanne Hardy and Richard Vachet. Please mark this date on your calendar. We hope to see you for Reunion 2008, an occasion to learn about disease issues that impact us all, and about research here in Chemistry at UMass Amherst that we hope will address these issues.

We plan the following schedule of events, open to all students, faculty, staff, alumni and friends:

Saturday, June 7, 2008

2:00-3:00 p.m. Reception
3:00-3:30 p.m. Prof. Jeanne Hardy
3:30-4:00 p.m. Prof. Richard Vachet
4:00-5:00 p.m. Social Hour

Please RSVP to Ms. Carrie Morrison Penland by phone at 413-545-2585, by email at carriemp@chem.umass.edu. For more information about the reunion weekend including lodging information, call Ms. Penland or visit our department website at http://www.chem.umass.edu.

The Reunion will take place in Lederle Tower room 1634. Lederle Tower is just north of Goessmann Laboratory; room 1634 is on the 16th floor. We hope to see you all there in June 2008!