

# Chemistry at Hamilton

A newsletter produced by the Department of Chemistry at Hamilton College

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December 2004



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# Hamilton

## INTRODUCTION

As I write this it is another beautiful fall day in central New York. The past year has been as eventful as the previous five, and it is a pleasure to bring our alumni and friends up to date. We graduated 16 chemistry, biochemistry, and chemical physics majors this past May. You can read about some of their activities inside these pages. We currently have 21 majors in the class of 2005, a record. In May we moved into the first phase of the new science building, a lovely space that brings smiles to everyone's faces whenever they enter the building. We worked with 36 students on research projects this past summer. Eighteen of our students made presentations of our joint research at national meetings, and five Hamilton college students published four papers with their faculty mentors this past year.

Perhaps the most significant event for the department was the development of a new Five-Year Plan, which will guide our efforts in the near future. We wrote this plan in response to an invitation from Research Corporation to be considered for a departmental development award. Both the physics and chemistry departments are under consideration for this prestigious award. Representatives from Research Corporation visited us twice last year, a team of consultants came and evaluated our program in the spring, Research Corporation gave us \$20,000 to travel to other institutions over the summer, and we submitted our new Five-Year Plans to Research Corporation at the beginning of October. The visits that the department made to four other colleges were very instructive, and showed us that

we are on the right path in terms of achieving an extraordinary balance of teaching and research excellence. These discussions affirmed what we had already come to believe – the timing couldn't be better for capitalizing on our hard-earned momentum. Every one of our permanent faculty members maintain active research programs supported by external funding. We enjoy a critical mass of talented and enthusiastic students. We have moved into a new, integrated science building with state-of-the-art facilities. We have the great support of the College administration, which has an explicit goal of advancing the sciences at Hamilton.

The two main goals of our new Five-Year Plan are: (1) to sustain significant primary research agendas for each faculty member, and (2) to provide first-rate research experiences for all of our students. We feel that all other successful outcomes will flow from successful attainment of these two goals. In writing this plan we are building on our recent success, as we have worked together to create a culture of quality undergraduate research, and we are committed to sustaining and nurturing that culture. Significant results from the past five years include: (1) The department grew to six full-time faculty members and four support staff positions. (2) For the four classes of 2003-06, the number of chemistry graduates has increased to an average of 18 per year (12.5 chemistry, 4.5 biochemistry, 1 chemical physics). (3) We worked with an average of 31.5 research students each summer, and published 4 papers each year. (4) Our five tenured faculty members have

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**Our five tenured faculty members have received nine grants totaling \$1,963,486 over the past five years to support research.**

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received nine grants totaling \$1,963,486 over the past five years to support research. On average, the chemistry faculty has secured \$392,697 in grant funds per year. Three NSF-MRI grants have significantly augmented our research infrastructure (Supercomputer; 500 MHz NMR; Raman Microscope) and have enabled us to add a computer staff position.

We learned from our visits this past summer that any plan for improvement must take into account the success that will inevitably result. Our plan anticipates an increase in general chemistry enrollments by 25 percent. Half of our general chemistry courses currently are comprised of first-year students (enrollments have averaged 94 students over the past five years). An increase of 25 percent will add 24 first-year students to the general chemistry courses. Based on recent figures (47 first-years yields 20 majors), this increase in enrollment will translate into 30 majors per class. The small sections of general and organic chemistry have been our hallmark; they are what have made chemistry attractive to Hamilton students. We don't have any other programs that require students to take chemistry as first-year students. To maintain excellence in undergraduate research, we need to continue to introduce research experiences early in the educational process. We encourage our first-year students to start research projects as soon as possible, again allowing us to capture student interest early in their educational careers. To accommodate the projected increased enrollments and also remain true to our teaching philosophy will require eight FTE faculty members in the chemistry department. As such, the addition of two new tenure-track positions is the centerpiece of our proposal to Research Corporation.

No plan is complete without meaningful assessment. We will assess individual research programs by the usual measures of research productivity: number of publications, establishing and maintaining federally funded research programs, and participation in professional meetings. We will assess the research experiences we provide to our students by the number of students who do research, by the number presenting posters at professional meetings, and by the number of papers

that undergraduates publish with the faculty. We will assess the success of the department by the degree to which we work together to ensure that we've reached our goals. Our primary aim as a department is to cultivate a culture that will extend the research activity we have built over the past 6 years, and allow us to sustain it over the next 20 years. Complete departmental success will only be evident far into the future, when the current faculty has retired. If we have accomplished our goal, future generations of chemistry faculty and students will have the opportunity to build upon and extend our successes.

Speaking of assessment, Professor Dan Chambliss of the Sociology Department has been overseeing an assessment project funded by a grant from the Mellon foundation. One of his first tasks was to assess advising, and he has reported to me that the Chemistry Department is off the top of the charts when it comes to advising. As measured by senior exit surveys, our students feel like we pay attention to their needs, and help them choose the best courses and extracurricular opportunities to help them succeed.

We have some changes in staff to report. Karl Kirschner, a former undergraduate researcher of mine from Lake Forest College, is teaching the physical chemistry courses this year. Jenn Sturm left the college this summer to relocate in the Washington D.C. area, and we've hired Steve Young as our new System Administrator and Research Support Specialist. We invite you all to come and visit us in our new teaching and research space.

### George C. Shields

Winslow Professor and Chair of Chemistry

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## FACULTY UPDATE

### Karen Brewer

Associate Professor of Chemistry  
Karen Brewer recently published two papers with her collaborators, including Professor of Physics Ann Silversmith, in the *Journal of Luminescence*. The complete citations are:

"Fluorescence enhancement by chelation of  $\text{Eu}^{3+}$  and  $\text{Tb}^{3+}$  ions in sol-gels" Magyar, A.P.; Silversmith, A.J.; Brewer, K.S.; Boye, D.M. *Journal of Luminescence* 108 (2004) 49-53.

"Transient and persistent spectral hole burning in  $\text{Eu}^{3+}$ -doped sol-gel produced  $\text{SiO}_2$  glass" Boye, D.M.; Valdes, T.S.; Nolen, J.H.; Silversmith, A.J.; Brewer, K.S.; Anderson, R.E.; Meltzer, R.S. *Journal of Luminescence* 108 (2004) 43-47.

Eight students spent their summer working on an interdisciplinary long-term research project that investigated the optical properties of rare earth-based solid materials under the supervision of Professors Karen Brewer and Ann Silversmith. Kate Schirmer '05, Peter Burke '06, Helena Grabo '06, Greg Armstrong '06 and Brendan Sullivan '07 each conducted specific parts of this interdisciplinary study, and current first-year students Tessa Olson '08, Katie Donahue '08 and John-Henry Forster '08 contributed to the work as well. The students synthesized compounds containing rare earth ions, and then incorporated the compounds into a sol-gel, which is a solution that gels to form a solid. Such materials have potential applications such as plasma television screens, solid state lasers and fluorescent lights.

## Tim Elgren

At the 2003 annual meeting of the Council on Undergraduate Research (CUR), Associate Professor of Chemistry Tim Elgren was elected to serve as the organization's president for a one-year term, which began in June 2004. With this election, Elgren began service on the CUR executive committee for a three-year term as president-elect in 2003. He will complete his term as recent past president during the 2005-06 academic year. The CUR national



Tim Elgren

office in Washington reports directly to the president. Elgren has been a member of CUR since taking his first faculty appointment and has been elected to serve as a CUR chemistry councilor for three consecutive three-year terms.

Elgren presented three talks at CUR's national conference in La Crosse, Wis., in June. The talks were titled "So You Have Tenure, Now What?," "Report on the NSF Summit on Undergraduate Research" and "International Programs with Research Opportunities."

Elgren was awarded two grants this past year. The Research Corporation has funded a proposal titled "Characterization of sol-gel encapsulated amine oxidase and chloroperoxidase" to support Elgren's continuing work to characterize the mechanism of action associated with these two metallo-enzymes. The award supports upgrading

existing equipment, supplies, and summer stipends for undergraduate collaborators. The Petroleum Research Fund of the American Chemical Society has funded a proposal titled "Characterization of Intermediates in the Catalytic Cycle of Amine Oxidases" to support half of Elgren's sabbatical leave in 2004-05. The research will be conducted at Montana State University in Bozeman.

Elgren published a paper on "Catecholase Activity Associated with Copper-S100B" in *Biochemistry*. This is a project funded originally by the Institute of Neurological Disorder and Stroke of the National Institutes of Health, a Cottrell Award from the Research Corporation and the Petroleum Research Fund of the American Chemical Society. Three undergraduate co-authors contributed to this project with summer research, senior thesis projects and a senior Fellowship project completed by Kim Kelly '96.

Elgren describes the research: "We have characterized the reactivity of the copper-bound form of S100-B, a ubiquitous protein found in mammalian brain. We have shown that this form of the protein is capable of catalyzing the oxidation of catecholamines, such as adrenaline and noradrenaline, to form insoluble dopaminergic melanins. This particular reactivity may have implications in the oxidative damage associated with Parkinson's disease in which high levels of copper and the presence of insoluble dopaminergic melanins have been tied to progression of the disease."

Elgren published a paper, "Mechanistic Implications for the Formation of the Diiron Cluster in Ribonucleotide Reductase Provided by Quantitative EPR Spectroscopy," in the *Journal of the American Chemical Society* (JACS, 125, 8748-8759) with co-authors from Carnegie Mellon University. This paper reports a novel physical probe of dinuclear metal cluster formation in metalloproteins. Ribonucleotide reductase remains the focus of intense investigation because it is the only biosynthetic pathway to the formation of deoxy-ribonucleotides, the build-

ing blocks of DNA. These metal clusters must fully form before the enzyme becomes active. This paper conveys new insight into how they form.

Assistant Professor of Biology Mike McCormick and Associate Professor of Chemistry Tim Elgren have received a grant from the National Science Foundation's Major Research Instrumentation (MRI) program to support the acquisition of a Raman Microscope. This instrument will be used to support the geo-microbiology research activities in McCormick's lab and bio-inorganic studies in Elgren's lab. The instrument will also be incorporated into chemistry, biology and geology laboratory courses. This is the third MRI grant received by the Department in the past four years.

Elgren also recently participated in a "Models in Academic Leadership" conference organized by the Research Corporation in Tucson, Arizona. Research Corporation gathered 40 individuals associated with highly effective programs to discuss the role that leadership played in establishing the success of these programs. The conference also considered means to cultivate future leaders.

## Robin Kinnel

Robin Kinnel, the Silas D. Childs Professor of Chemistry, received a \$9,000 grant from the 2003 Pittsburgh Conference, Memorial National College Grants Program, for "A Spectrofluorimeter for Research and Teaching." He also was the PI on an NSF MRI grant for a new NMR spectrometer. See the story on page 6.

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Robin Kinnel and his 2004 Summer Research Group

# FACULTY UPDATE

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## Ian Rosenstein

Professor Ian Rosenstein continues to pursue research projects on stereoselective radical addition reactions of electrophilic radicals and on the mechanism of the cyclopropylcarbinyl radical ring opening reaction. In addition, a collaborative project begun recently with Prof. Herm Lehman of Biology on the neurochemistry of the insect neurotransmitter octopamine continues to provide interesting research directions. This past summer Prof. Rosenstein had six students in his laboratory. Lou Vaickus '05 and Sarah Stewart '05 both worked on the radical addition project. Onica LeGendre '05, Becca Levinn '07 and Elizabeth Carnie '08 worked on the cyclopropane project and Becca Parkhurst '07 worked on the octopamine project. Henry Chicaiza '04 presented the results of his thesis work in a poster at the National Meeting of the American Chemical Society in Anaheim, CA in March. There are six senior thesis students working in Prof. Rosenstein's lab this academic year.

## George Shields

George Shields, Winslow Professor of Chemistry and Chair, gave an invited lecture at the 35th American Chemical Society Central Regional Meeting in Pittsburgh. His talk was titled "Formation of MERCURY to Enhance Undergraduate Computational Chemistry: Accurate  $pK_a$  Calculations in Aqueous Solution,

Progress and Challenges." MERCURY provides access to high performance computing resources or supercomputers for chemistry students and researchers at seven liberal arts institutions in the Northeast.

Shields has been awarded a Cottrell College Science Award for his research project, "Quantum Chemical Investigation of the Mechanism of Action of the Eneidyne Natural Products." The goal of Shields' research, as outlined in his own proposal, is to "use advanced computational methods to gain a thorough understanding of the mechanism of DNA cleavage by the enediyne family of natural products."

Shields recently served as a panel reviewer for the National Science Foundation (NSF). Shields attended the NSF Science, Technology, Engineering, and Mathematics Talent Expansion Program panel review meeting on April 26 and 27. He reviewed the proposals for the STEP Division of Undergraduate Education at the NSF.

The panel reviewed 160 proposals written by community colleges, four-year colleges, comprehensive universities and research universities. All proposals were aimed at expanding the number of students choosing to major in math, science and engineering. Roughly 10 percent of the submitted proposals were funded.

Shields published an article in the *Journal of Physical Chemistry*, titled "Accurate Experimental Values for the Free Energies of Hydration of  $H^+$ ,  $OH^-$ , and  $H_3O^+$ ." The paper, co-authored by Matthew Palascak '07, was published in April and is based on Palascak's research from summer 2003 and the fall 2003 semester.

## SIX STUDENTS PRESENT AT CONFERENCE

Two professors and six students from Hamilton traveled to Anaheim, Calif. from March 28 -April 1 to attend the American Chemical Society National Meeting and present papers and posters on their research. The students, Christopher Butts, Jessica Callahan, Henry Chicaiza, Brent Matteson, Jakub Sroubek and Andrew Vermilyea, are all members of the Class of 2004, and were accompanied by Chemistry Professors Karen Brewer and Stephen Waratuke.

The students presented their results under the auspices of the professional divisions of the American Chemical Society including the Divisions of Inorganic Chemistry, Organic Chemistry, Colloid and Surface Chemistry and Environmental Chemistry.

Jessica Callahan and Professor Brewer presented their research on sol-gel glasses with physics professor Ann Silversmith. At the meeting, in the Division of Inorganic Chemistry, they presented two posters, "Fluorescence of rare earth ions in binary zirconia-silica sol-gel glasses," and "Energy transfer from chelated ligands to rare earth cations in a sol-gel matrix."

Andrew Vermilyea presented a paper in the Division of Environmental Chemistry titled "Role of dichlorocarbene reduction during carbon tetrachloride transformation on the surface of magnetite." He co-authored the paper with biology professor Michael McCormick.

Jakub Sroubek presented his paper, "Stereochemical investigation of bromoallenic acetogenin synthesis," co-authored with chemistry professor Robin Kinnel, in the Division of Organic Chemistry.

Henry Chicaiza presented a paper he co-authored with chemistry professor Ian Rosenstein titled "Synthesis

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George Shields, Karl Kirschner and their 2004 Summer Research Group.

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## NEW FACULTY & STAFF MEMBERS

### Karl Kirschner

Last spring, Karl Kirschner was hired as a Visiting Assistant Professor of Chemistry. Kirschner earned a Ph.D. from the University of Georgia and bachelor's degree from Lake Forest College. Before coming to Hamilton, Kirschner held a post-doctoral assistantship at the University of Georgia's Complex Carbohydrate Research Center. He has published research in the *Journal of Computational Chemistry*, *Journal of Molecular Structure*, *Journal of Physical Chemistry*, and *Chemical Physics Letters*. A computational chemist, Kirschner is an expert in force field development for molecular mechanics and molecular dynamics simulations. He is teaching physical chemistry this year and advising students working on computational chemistry research projects.



Karl Kirschner



Steven Young

### Steven Young

Steven Young, system administrator and research support specialist in chemistry, received an AAS in electrical engineering technology from SUNY Canton and a bachelor's degree in computer science from SUNY Oswego. Steve was previously employed at Navisite (formerly Applied Theory) where he was a systems engineer, managing Web servers for customers like Johns Hopkins University, the Denver Broncos, America's Job Bank and the Guggenheim Museum. Steve has two children, a daughter, 7, and a son, 4. He enjoys hunting, fishing, camping, hiking and snowmobiling. A specialist in Unix operating systems, Steve manages all the computers in the chemistry department and for the MERCURY consortium.

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## FOUR STUDENTS & SHIELDS ATTEND THE 44TH SANIBEL SYMPOSIUM ON ATOMIC, MOLECULAR, BIOPHYSICAL AND CONDENSED MATTER THEORY

Professor and Chair of Chemistry George C. Shields attended the 44th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, March 1 - March 6, in St. Augustine, Fla. He chaired the plenary session on Metals in Biology and conducted a workshop for graduate students and undergraduates on combined Quantum Mechanical/Molecular Mechanical (QM/MM) hybrid methods.

In addition, four Hamilton College students presented their fundamental research focused on anti-cancer drug design, based on their previous summer work. Frank Pickard '05 presented his poster, "The Eneidyne Anticancer Antibiotics: A Study of the Bergman Cyclization Energy Barriers of Esperamicin A1 Using ONIOM DFT/MM Methods." Becky Shepherd '06 discussed her research, "Abstraction of Hydrogen after Bergman Cyclization of Benzannulated Eneidyne with Ortho Substituents."

Abby Markeson '04 presented her poster, "Anti-Breast Cancer Drug Design." Meghan Dunn, who has worked in the Shields group the past two summers, presented her atmospheric chemistry work that was published in the March 3, 2004 issue of the *Journal of the American Chemical Society*. Her poster was titled "Thermodynamics of forming water clusters at various temperatures and pressures using G2, G3, CBS-QB3, & CBS-APNO model chemistries; Implications for Atmospheric Chemistry."

Each student gave a brief talk before an international audience of more than 100 scientists, and then discussed his or her work with interested scientists during the poster session. Pickard won the award for top undergraduate student poster at the conference. All four of these students have spent multiple summers pursuing their research through the chemistry summer research program at Hamilton College.

## NATIONAL SCIENCE FOUNDATION AWARDS HAMILTON COLLEGE PROFESSORS \$238,356 GRANT FOR A NUCLEAR MAGNETIC RESONANCE PURCHASE



*Robin Kinnel and Lou Vaickus hugging the new NMR.*

The Chemistry Department, under the leadership of Robin Kinnel, the Silas D. Childs professor of chemistry, and with the assistance of Herman Lehman, associate professor of biology, Ian Rosenstein, associate professor of chemistry, and George Shields, professor of chemistry, has been awarded a \$238,356 grant from the National Science Foundation's Major Research Instrumentation (MRI) program. The award supported the purchase of a new 500 MHz nuclear magnetic resonance (NMR) spectrometer.

This is the fourth NMR that the College has acquired, and the third that has been procured with the assistance of grant funds from the National Science Foundation. The new instrument will provide improved sensitivity and resolution, which will enhance the research productivity of the faculty members involved in NMR projects. It will also provide easy access to two-dimensional experiments, which will permit undergraduate researchers to better appreciate the power of NMR at an earlier stage in their education.

The award was the result of over two and half years of planning, writing, and proposing from the group. Kinnel began by crafting a proposal for the Course, Curriculum, Laboratory, and Instrumentation program, a program designed to support the acquisition of equipment for usage in teaching settings. Although reviewers thought the proposal was strong, in that it would clearly enhance laboratory experiments at all levels including research, they noted that the proposal fell short in justifying the high field for the educational aspects of the proposal. Kinnel and his collaborators then submitted

a proposal to the MRI program in January of 2002. The MRI program is primarily focused on the research of faculty and, as such, the proposal highlighted the active research program of the department. The proposal was reviewed very favorably, but was not recommended at the highest level and an award was not granted. The reviewers indicated that several details needed clarification and that the field strength again needed to be better justified.

The group was encouraged by the positive feedback, and decided to rewrite the proposal and resubmit it to the MRI program. Kinnel felt that NSF was sympathetic and that with some minor revisions, they could be successful. "We didn't rewrite the entire proposal. We kept what worked and restructured the proposal to directly answer the reviewer's comments and concerns." The revised proposal was submitted in January of 2003. In early July, the group was notified that an award letter had been issued and the grant had been approved.

"The award was particularly gratifying because it not only allowed us to move forward with the acquisition of the new NMR, but it also was an endorsement of our research projects. It was energizing," Kinnel said. Moreover, the group felt a sense of satisfaction; they were able to help equip the new science facility without having to rely entirely on institutional funding. "Clearly, this award would not have been possible without institutional support," Kinnel said, noting that the award will be matched with nearly \$300,000 from an endowed fund designed to assist the College replace outdated equipment, "But we earned this and that is very satisfying for the group involved in the development of the proposal as well as for the department."

The new NMR, a Bruker Avance 500 MHz instrument, has been installed in the new Science Center. Already students from Organic Chemistry II, as well as research students and those in Superlab have been using the instrument. The Major Research Instrumentation Program of NSF is designed to improve the scientific and engineering

equipment for research and research training in academic institutions. This program seeks to improve the quality and expand the scope of research and research training in science and engineering, and to foster the integration of research and education by providing instrumentation for research-intensive learning environments.

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of radical precursors for the study of the cyclopropylcarbinyl radical ring opening reaction."

Christopher Butts presented his paper, "A Thermodynamic Characterization of Ca(II) Binding to Tetracyclines," co-authored with chemistry professor Tim Elgren in the Division of Inorganic Chemistry.

Brent Matteson presented "Antigen binding efficiency of micro-contact printed antibody nanostructures," which he co-authored with Margo Rockwell '05 and Daniel Roston '06. His presentation was in the Division of Colloid and Surface Chemistry.



*Superlab in the new Science Building.*

## STUDENT RESEARCH

This past summer, Kate Schirmer '05, Peter Burke '06, Helena Grabo '06, Katie Donahue '08 and John-Henry Forster '08 worked in Karen Brewer's laboratory. Michelle Skornicki '06 and Hilary Gamble '07 worked with Tim Elgren. Andy Glossner '06, Hiroki Ogawa '07 and Tenma Otsuka '05 worked in Stephen Waratuke's laboratory. Mary Beth Day '07, Meghan Dunn '06, Tim Evans '05, Sarah Felder '07, Matroner George '07, Amber Gillis '06, Dan Griffith '07, Philip Hanoian (who attends Wesleyan), Greg Hartt '08, Chenyan Huang '07, Kat Lexa '05, Heather Michael '07, Philip Holdredge '08, Daniel Tomb '08, and Frank Pickard '05 worked with Karl Kirschner and George Shields. Elizabeth Carney '08, Onica LeGendre '05, Rebecca Levinn '07, Rebecca Parkhurst '07, Sarah Stewart '06 and Louis Vaickus '05 worked in Ian Rosenstein's laboratory. Cindy Liang

'08, Danielle Masee '07, Eric Reile '08, Dan Roston '06 and Dan Seeger '06 worked with Robin Kinnel.

Tim Evans '05 worked on expanding a 20-year-old chemistry theory that deals with the formation of acid rain. While working under the advisement of Professor Shields, Tim found "examples in which clusters of gaseous water catalyze atmospheric sulfur reactions" other than in the reaction between sulfur trioxide and water in his project, "Effect of water clusters on the biogeochemical sulfur cycle." Evans hoped that his computational work would "reduce discrepancies between theory and experiment." Specifically, Tim investigated stable structures of carbon disulfide (OCS) bound with different-sized water clusters. He also modeled the atmospheric reaction between OCS and an oxygen atom to see if this reaction can be catalyzed with

water clusters. Tim, who is interested in teaching chemistry in the future, supervised three incoming Hamilton College students on different aspects of his overall research. Greg Hartt, Phil Holdredge, and Dan Tomb, all members of the class of 2008, made great progress working with Tim.

In July Shayna McHugh, '05, traveled to Phoenix, AZ, to present her poster "Exploration of Aqueous Extracts of *Stylotella aurantium* from Guam" at a meeting of the American Society of Pharmacognosy, held jointly with three European societies at the 2004 International Congress on Natural Products Research. The poster detailed work that Shayna had done during the summer of 2003 for which she had been awarded a highly competitive ASP research stipend.

## STUDENT AWARDS

This year on Class and Charter Day many biochemistry and chemistry students received awards for their academic achievements.

Jakub Sroubek, a chemistry major, received the Norton Prize, the Mary McMaster Hallock Prize in Science, the Kirkland Prize, the Underwood Prize in Chemistry and Phi Beta Kappa honors. Gabrielle Markeson received the Underwood Prize in Chemistry, the Norton Prize and Phi Beta Kappa Honors. Emma Timmins-Schiffman '06 received the Dr. Philip I. Bowman Prize Scholarship. Kathryn Dorsey '05 received the Lawrence K. Yourtee Prize Scholarship. Andrew Vermilyea won the Donald J. Denny Prize in Physical Chemistry and Phi Beta Kappa honors. John Fischer '05 received the Tarbell Book Prize in Organic Chemistry. Matthew Child received the Senior Prize in Biochemistry/Molecular Biology. Brent Matteson received the Donald J. Denney Prize in Physical Chemistry. Robert Parker received the Bristol Fellowship. Andreu Viader Valls '05 received the Willard Bostwick Marsh Prize Scholarship. Dan Seeger '06 received the ACS prize in Organic Chemistry. Emin Hodzic received the James Bennett Prize. Grant McSurdy '06 and Seeger received the CRC Press First Year Prize in Chemistry. McSurdy also received the Phi Beta Kappa book prize.

**Commencement Honors:** *Summa Cum*

*Laude:* Jakub Sroubek; *Magna Cum Laude:* Gabrielle Markeson and Andrew Vermilyea; *Cum Laude:* Matthew Child.

**Sigma Xi:** Students elected to Sigma Xi, the National Scientific Honor Society, were Christopher Butts, Henry Chicaiza, Gabrielle Markeson, Brent Matteson, Jakub Sroubek and Andrew Vermilyea. Chemistry minor Emma Pokon also graduated as a member of Sigma Xi.

In addition, Matthew Child received the Glass Fellowship and graduated with honors in biochemistry/molecular biology. Henry Chicaiza, Gabrielle Markeson, Jakub Sroubek and Andrew Vermilyea received honors from the chemistry department. Sam Baker and Brent Matteson graduated with honors in chemical physics. Lorena Hernández ('03), Brent Matteson, Jakub Sroubek and Andrew Vermilyea received Elihu Root Fellowships toward their graduate studies.

Congratulations to all graduates in chemistry, chemical physics, and biochemistry from the class of 2004: Anna Arnold, Sam Baker, Christopher Butts, Jessica Callahan, Henry Chicaiza, Matthew Child, Brian Clark, Emin Hodzic, Josh Kunkel, Daniel Leonard, Abby Markeson, Brent Matteson, Sinan Misirli, Robert Parker, Jakub Sroubek and Andrew Vermilyea.

## RUBINO '05 RECOGNIZED

Hamilton College student Jeffrey Rubino '05 is one of four undergraduate students to be recognized for using spectroscopy in the arts and sciences. The award is administered by the New York Section of the Society for Applied Spectroscopy (NYSAS). Rubino, advised by Associate Professor of Chemistry Tim Elgren, used spectroscopy to study enzyme reactions. NYSAS is a nonprofit organization dedicated to the dissemination of information related to spectroscopy. The other students recognized are from Union College, New York University and Cornell University. The announcement of the winners of the 2004 New York Section of the Society for Applied Spectroscopy Student Awards stated "the award winners were chosen from an extremely strong group of graduate and undergraduate nominations."



Jeffrey Rubino '05



Participants at the 2004 MERCURY Conference, hosted by Hamilton College.

## 3rd MERCURY CONFERENCE



Hamilton College hosted the 3rd MERCURY Conference in Computational Chemistry (<http://mars.chem.hamilton.edu/conference>) July 29-31. This national conference featured seven talks by invited speakers and 40 poster presentations by undergraduates, and was organized by George Shields. Each undergraduate had two minutes to advertise his or her work in front of the entire audience of 70 attendees, followed by a two-hour period where they explained their work in detail at the poster session. Shields and Visiting Assistant Professor of Chemistry Karl Kirschner had 15 summer research students present the results of their collaborative research projects at the conference:

“The Eneidyne Anticancer Antibiotics: A Study of the Bergman Cyclization Energy Barriers of Esperamicin A1 Using ONIOM DFT/MM Methods.” Frank C. Pickard & Chantelle Rein.

“Global Search for Minimum Energy  $(\text{H}_2\text{O})_n$  Clusters,  $n=3-5$ ” Mary Beth Day.

“Thermodynamics of forming water clusters at various temperatures and pressures using G2, G3, CBS-QB3, & CBS-APNO model chemistries; Implications for Atmospheric Chemistry” Meghan E. Dunn & Emma K. Pokon.

“Structures of Carbonyl Sulfide(OCS)-Water Cluster Complexes and Water Cluster Catalysis of Atmospheric OCS Reactions” Timothy M. Evans.

“Obtaining Experimental Results from Computer-Designed Anti-Breast Cancer Drugs” Sarah E. Felder, Gabrielle Markeson, Sarah A. Taylor & Professor of Biology Stephen M. Festin.

“CAP-DNA Complex Binding Energies” Matroner M. George.

“Inhibition of biological compounds directed at drug design” Amber Gillis.

“Determination of  $pK_a$  Values with PBE1PBE Density Functional Theory” Daniel Griffith & Matthew D. Liptak.

“Computational Study of Carbon Disulfide Oxidation with the Hydroxyl

Radical and Water Monomer” Gregory M. Hartt & Timothy M. Evans.

“Mutagenesis of Cocaine Catalytic Antibody 15A10 for Improved Binding to Cocaine Transition State Analog” Philip J. Hanoian.

“Structural Analysis of Dimethyl Sulfide and  $(\text{H}_2\text{O})_n$  for  $n=1-4$ ” Philip T. Holdredge & Timothy M. Evans.

“The Free Energy of Solvation for Ions Calculated by Thermodynamic Cycles” Chenyan Huang.

“Finding Energy Minima for a Breast Cancer Inhibiting Peptide derived from AFP” Katrina Lexa, Meghan E. Dunn, Heather Michael & Damien J. Ellens.

“Conformational Analysis of an AFP-derived Cyclic Peptide: cEQ” Heather Michael, Meghan Dunn, & Katrina Lexa.

“A Computational Study of the Thermodynamic and Kinetic Effects of Water Clusters on Hydrogen Sulfide in the Atmosphere” Daniel B. Tomb & Timothy M. Evans.