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# Program

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## COLLEGE OF THE HOLY CROSS

### Sixteenth Annual Undergraduate Summer Research Symposium



September 11, 2009

Hogan Ballroom

*Dear Members of the Holy Cross Community,*

*Welcome to the 2009 Undergraduate Summer Research Symposium. Now in its sixteenth year, the symposium is a college-wide event that brings together faculty and students from all disciplines at Holy Cross and provides an opportunity to celebrate their accomplishments over the summer of 2009. It also provides an opportunity for students to witness the breadth of research possibilities both on and off campus and to open a dialogue with a faculty member about conducting research during the upcoming year and summer. We hope you enjoy the impressive collection of research on display today.*

*Professor Sara Mitchell, Department of Biology  
Professor Brian Linton, Department of Chemistry  
2009 USRS Organizing Committee*

*In recognition of those whose financial contributions have made this research possible:*

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Chemistry, Biology, Psychology, Sociology, and Economics.

## Posters

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1. **Analysis of Glutamine-Based Dipeptides Using Infrared Spectroscopy**, M. Bauer and S. Petty, Department of Chemistry, College of the Holy Cross
2. **X-ray Analysis of Neutron Star X0921-630 and Black Hole J1550-564**, Joseph Palmieri, Robert Nazarian and Tom Narita, Department of Physics, College of the Holy Cross.
3. **Construction and Optimization of a Q-Switched Nd:YAG Laser**, Fallon M. Laliberte, Professor John Collins, Department of Physics, Wheaton College.
4. **Determining the Size of the Hydration Sphere Surrounding Myoglobin**, L. Tonge and S. Petty, Department of Chemistry, College of the Holy Cross.
5. **Investigation of murine model immunological protection after intranasal colonization by Streptococcus pneumoniae**, Aaron Goodwin (College of the Holy Cross), Nang Maung (UMass Graduate School of Biomedical Sciences), John Leong MD PhD (UMass Graduate School of Biomedical Sciences).
6. **Characteristics of Face-to-Face and Electronic Conversations**, Kerry Kareta, Jenna Sattar, Elizabeth Campbell, and Patricia Kramer, Department of Psychology, College of the Holy Cross.
7. **Three Dimensional Surface Model Based Investigation Of Avian Mandible Morphology**, Stephanie John, Megan Cooper, Michael Dmytriw, and Rachael Martinez, Advisors: Dr. Leon Claessens and Dr. Abby Drake, Department of Biology, College of the Holy Cross.
8. **Mechanism of protein splicing of the *Pyrococcus abyssi* lon protease intein**, Kevin O'Brien, Adam C. Nadelson, Daniel J. York, Lauren R. Duffee, Julie N. Reitter and Kenneth V. Mills, Department of Chemistry, College of the Holy Cross.

9. **Rhenium Chemistry: The Use of Various Metal Centers to Check for Optimal Coordination with Various Tripod Ligands**, Harun Rafi and Richard S. Herrick, Department of Chemistry, College of the Holy Cross.
10. **Grain size characteristics & potential mobility of road traction sand in Worcester, Massachusetts**, Renee Harkins & Sara Gran Mitchell, Environmental Studies and Department of Biology, College of the Holy Cross.
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12. **Hydrogen Bonding in Model Systems and the Synthesis of a Transition State Mimic**, Kevin Halloran, Brian R. Linton, Department of Chemistry, College of the Holy Cross.
13. **Acute Administration of Fluoxetine Increases Prepulse Inhibition of Acoustic Startle Response: Examining the Roles of the 5-HT<sub>1A</sub> and 5-HT<sub>1B</sub> Inhibitory Autoreceptor Subtypes**, Maryann Manatt, Brittany Fritz, Brenden Myers, and Daniel Bitran, Department of Psychology, College of the Holy Cross.
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19. **The Effect of Separations on Crime**, R. Baumann, B. Engelhardt, T. Ciavarra, Department of Economics, College of the Holy Cross.
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22. **Beta-sheet Mimetics**, J. Hillner and Brian R. Linton, Department of Chemistry, College of the Holy Cross.
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24. **Skeletal Muscle Function and Regeneration Following Acute Limb Ischemia Reperfusion**, C. Abularrage, S. Meng, R. Paranal, H. Yoo, A. Robaldo, B. Nguyen, G. LaMuraglia, M. Watkins, H. Albadawi, Vascular Research Lab, Massachusetts General Hospital.
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27. **Packaging of human protein APOBEC3G into HIV virions**, Emily Cartwright, Natasha Tobarran, Melissa A. Farrow, Ann M. Sheehy, Department of Biology, College of the Holy Cross.

28. **Development of protein purification strategies using the *Pyrococcus abyssi* PolII intein**, Adam C. Nadelson, Daniel J. York, Katherine T. Lewandowski, Deirdre M. Dorval, Katherine R. Connor, Julie N. Reitter and Kenneth V. Mills, Department of Chemistry, College of the Holy Cross, Worcester, MA, USA.
29. **Shutter Design in Laser Ion Mobility Spectrometry**, C. Corbett and J. Kelley, Department of Chemistry, College of the Holy Cross.
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34. **Uterine Artery Embolization Preoperative to Hysterectomy**, Emily Samartino and Michael Hallisey M.D., Department of Interventional Radiology, Hartford Hospital.
35. **Design and Testing of an Ion Mobility Spectrometer With the Use of SIMION Modeling Software**, J. DeLisio and J. Kelley, Department of Chemistry, College of the Holy Cross.
36. **Identifying APOBEC3G Domains as Targets for Therapeutic Intervention**, P. Cheney and A. Sheehy, Department of Biology, College of the Holy Cross.
37. **Investigating Excess Endowments at Private Liberal Arts Colleges**, Karen Teitel, Assistant Professor, Robert Baumann, Assistant Professor and Andra J. Belland, Department of Economics, College of the Holy Cross.
38. **When good is bad: The negative consequences of positive memories**, Kathryn O'Connor and Professor DiGirolamo, Department of Psychology, College of the Holy Cross.
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43. **Semi-Quantitative Laser-Induced Breakdown Spectroscopy: In Search of Metal Contaminants in Blackstone River Sediment**, B. O'Leary and J. Kelley, Department of Chemistry, College of the Holy Cross.
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45. **Analyzing Neural Responses to Optic Flow Patterns**, E. McCourt and C. Royden, Department of Math and Computer Science, College of the Holy Cross.

46. **Collaborative Paleontological Fieldwork in Arizona, New Mexico and Utah**, E. Blumhagen and Z. Lavender, Faculty Advisor: L. Claessens, Department of Biology, College of the Holy Cross.
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48. **Children's Mapping of Number Words onto Nonsymbolic Numerosities**, Caitlin O'Gallagher<sup>1</sup>, Heena Lakhani<sup>2</sup> and Susan Carey<sup>2</sup>, <sup>1</sup>College of the Holy Cross, <sup>2</sup>Harvard University.
49. **Temperature Dependence of splicing activity of the Pyrococcus abyssi PolIII Intein**, Daniel York and Prof. Ken Mills, Department of Mathematics, College of the Holy Cross.
50. **Exploring the Olefin Cross Metathesis Reaction**, Greg Faxon and Prof. Bianca Sculimbrene, Department of Chemistry, College of the Holy Cross.
51. **Assessing Actigraph Reliability Using the iRobot<sup>®</sup>**, R. Prendergast<sup>1</sup>, E. Soares<sup>1</sup>, and A. Wolfson<sup>2</sup>, <sup>1</sup>Department of Mathematics and Computer Science, <sup>2</sup>Department of Psychology, College of the Holy Cross.
52. **Computer simulation of the action potential from a geometric compartmental model of the human auditory nerve fiber**, M. Piltin and J. Watrous, Department of Biology, Saint Joseph's University.
53. **Launch of Aves 3D: A Digital Database of Avian Skeletal Elements**, M. Cooper, R. Martinez, S. John, M. Dmytriw, Advisors: L. Claessens, A. Drake, Department of Biology, College of the Holy Cross.
54. **Religious Motivation and the Religious Life among Worcester's Older Adults**, E. Farrington and M. Frongillo, Professor Andrew Futterman, Department of Psychology, College of the Holy Cross.
55. **Rhenium Chemistry: Bidentate complexes with Biologically Relevant Ligands**, Americo N. Gambella and Richard S. Herrick, Department of Chemistry, College of the Holy Cross.
56. **Simulating a Quantum Computer to Approximate the Jones Value of 4-Stranded Braids**, Matthew Brady and Prof. David Damiano, Department of Mathematics and Computer Sciences, College of the Holy Cross.
57. **A Preliminary Geometric Morphometric Analysis Of The Ecomorphology Of The Avian Sternum**, R. Martinez, M. Cooper, S. John, and M. Dmytriw, Advisors: L. Claessens, and A. Drake, Department of Biology, College of the Holy Cross.
58. **Tribolium castaneum Embryo Fate Mapping**, M. Gallant and K. Ober, Department of Biology, College of the Holy Cross.
59. **Frequency Control Elements for a Laser**, Chelsea Dalphond and Prof. Timothy Roach, Department of Physics, College of the Holy Cross.
60. **Atom Optics Research: Laser Intensity Control**, T. Roach, M. Vornle von Haagenfels, J. Ryor, C. Dalphond, Department of Physics, College of the Holy Cross.
61. **Investigating the Divergent Evolution of Scaphinotus Petersi**, M. Pratt and K. Ober, Department of Biology, College of the Holy Cross.
62. **Using NIR and Other Spectroscopic Methods for Rapid Assessment of Product Quality Attributes**, A. Buga and N. Melnikaitis, Analytical Sciences and Technology, Pfizer.
63. **Improving Control via Drugs: A mouse pilot study**, Kathryn O'Connor, Neha Patel, Maryann Manatt, Brittany Fritz, Brenden Myers, Professor Bitran and Professor DiGirolamo, Department of Psychology, College of the Holy Cross.

64. **3-D Organization of ParB-DNA Assembly in Human Pathogens: *M. tuberculosis* and *V. cholerae***, *Kelly Lyons* and Dr. Barnali Chaudhuri, Hauptman Woodward Biomedical Research Institute.
65. **Asymmetric Gold-Catalyzed [4+2] Cycloadditions of Allene-Dienes**, *Owen S. Fenton*<sup>1</sup>, *Ana Z. Gonzalez*<sup>2</sup> and *F. Dean Toste*<sup>2</sup>, Department of Chemistry, College of the Holy Cross<sup>1</sup>, Department of Chemistry, University of California, Berkeley<sup>2</sup>.
66. **An Analysis of Hydrogen Bonding Patterns in Small Peptides and Using Hydrogen Bonding to Catalyze Reactions of Nitro Compounds**, *Anthony J. Metrano* and *Brian R. Linton*, Department of Chemistry, College of the Holy Cross.
67. **Using Peptide Isosteres to Investigate Antibiotic Resistance**, *Ryan Quinn* and Prof. Bianca Sculimbrene, Department of Chemistry, College of the Holy Cross.
68. **Male Breast Cancer: “You gotta be kidding me!”**, *Alexandra Leichthammer*, and Edward Thompson, Department of Sociology and Anthropology, College of the Holy Cross.
69. **The Number of Points on a Family of Calabi-Yau Threefolds**, *Jonathan Root*, Department of Mathematics, College of the Holy Cross.
70. **Multiple Laser Excitation of Lithium for Atomic Spectroscopy**, *Pat Collins* and Prof. Paul Oxley, Department of Physics, College of the Holy Cross.
71. **The Effect of Ionic Strength on the Aggregation of Human- $\gamma$ C-Crystallin**, *J. Trubiano* and Dr. S. Petty, Department of Chemistry, College of the Holy Cross.
72. **Rapid Prediction of Pfizer and Competitor Product Stability Using ASAP Modeling**, *Anna Larkin*, Pfizer Global Manufacturing Division, in the Analytical Science & Technology Department, Department of Physics, College of the Holy Cross.

## Poster 1

### Analysis of Glutamine-Based Dipeptides Using Infrared Spectroscopy

*M. Bauer* and *S. Petty*  
Department of Chemistry, College of the Holy Cross

Huntington’s disease is caused by an extension of the glutamine chain at the N-terminus of the Huntingtin protein. The subsequent aggregation of this protein can be monitored through the use of infrared spectroscopy by studying the frequency of the carbonyl stretching vibration. In addition to the backbone carbonyl present in all amino acids, the side chain of glutamine also contains a carbonyl, complicating the spectra and limiting the use of infrared spectroscopy for structural studies of these proteins. Therefore, in order to develop an understanding of the infrared spectra in this region, the side chain and backbone signals must be differentiated.

Dipeptides containing glutamine, alanine, and asparagine were synthesized in order to mimic the presence of glutamine in proteins without allowing for the adoption of stable elements of secondary structures. The side chain:side chain and side chain: backbone interactions were monitored by studying the temperature dependence of each of these dipeptides at pH 5 and pH 7 at various concentrations. The data collected is fit primarily with two bands.

Future work will involve synthesizing longer peptides and inserting glutamine into peptide sequences with known secondary structure. These steps will allow for the interpretation of the spectra we have of pathogenic and nonpathogenic strands of polyglutamine.

The authors thank the Becton-Dickinson Foundation for funding this project

## Poster 2

### **X-ray Analysis of Neutron Star X0921-630 and Black Hole J1550-564**

*Joseph Palmieri, Robert Nazarian and Tom Narita  
Department of Physics, College of the Holy Cross*

Using the Rossi X-ray Timing Explorer (RXTE) and International Gamma-Ray Astrophysics Laboratory (INTEGRAL) satellites, we seek to discover the mechanism by which x-rays are produced in neutron stars and black holes

We studied the photon emission from X0921 through two observations in the x-ray energy band, but were unable to confirm the 9 day orbital period. No suborbital periods were able to be discovered because of a periodicity in the background. The RXTE spectrum is best modeled by power law and black body components in the 2 keV to 20 keV range. The power law models the emission from the disk and corona while the black body models emission from the neutron star. We were unable to study gamma ray emission because the source was too weak to detect using INTEGRAL's IBIS instrument which has a range of 15 keV to 10 MeV.

Additionally, we explored the correlation between the iron line and power law spectral components in transient black holes. Iron lines are spectral features which are produced when x-rays from the neutron star heat up iron atoms in the gaseous accretion disk. Preliminary data from black hole J1550-564 suggests an increased iron line as the power law flux increases during bursts.

We thank the Massachusetts Space Grant Consortium for financial support.

## Poster 3

### **Construction and Optimization of a Q-Switched Nd:YAG Laser**

*Fallon M. Laliberte, Professor John Collins  
Department of Physics, Wheaton College*

The purpose of this project was to construct a Q-switched Nd:YAG laser and to model the behavior of the laser by solving two coupled differential equations via MATLAB.

The construction of the laser took place in two stages. The first stage was to build a simple non Q-switched laser. The laser cavity consisted of a 99.9% reflective rear mirror, a 60% reflective output coupler, and a 6 mm x 15 cm Nd:YAG laser rod. The rod was pumped by a flashlamp having a pulse width of about 50 msec. The width of the laser pulse was roughly equal to that of the flashlamp. The second stage was a Q-switched laser, which was achieved by adding a Pockel's cell,  $\frac{1}{4}$  wave plate, and polarizer between the rear mirror and the laser rod. In this arrangement, the output of the laser was a single pulse with a width of approximately 20 nsec. This pulse was then used to generate green light by passing it through a potassium titanyl phosphate (KTP) frequency doubling crystal.

Modeling of the laser was done by numerically solving two coupled differential equations with MATLAB. These equations demonstrated the population inversion and number of photons in the laser cavity over time for the laser setup.

The non Q-switched laser showed a threshold of 5.2 Joules and a slope efficiency of 2.5%. The Q-switched laser showed a threshold of 12.4 Joules and a slope efficiency of -21.1%.

We thank Wheaton College for their financial support.

## Poster 4

### Determining the Size of the Hydration Sphere Surrounding Myoglobin

*L. Tonge and S. Petty*

*Department of Chemistry, College of the Holy Cross*

A protein dissolves when water molecules surround the protein forming a “hydration sphere” that overcomes the protein’s intramolecular interactions. Interactions between the protein and water help determine the protein’s native structure. Hence, an understanding of the hydration sphere contributes to the overall understanding of proteins in their native aqueous environment.

Using Infrared Spectroscopy, we strove to determine the size of the hydration sphere surrounding Myoglobin, a small, compact and well characterized model protein. We measured the size of the H<sub>2</sub>O association band at differing concentrations of Myoglobin. After correcting the area for cell pathlength and spectrometer energy, we discovered an inverse linear relationship between the area of the association band and the concentration of Myoglobin at low concentrations (less than 10 mg/ml). At concentrations greater than 10 mg/ml, this trend ends and the areas of the association band no longer vary with Myoglobin concentration indicating that the hydration spheres are overlapping. Our resulting calculations indicate that the hydration sphere surrounding a single molecule of Myoglobin is approximately 20-25 Å thick.

In the future, we hope to use this method to model the size of the hydration spheres of other, more complex proteins.

The authors gratefully acknowledge the Sherman-Fairchild Foundation for funding their project.

## Poster 5

### Investigation of murine model immunological protection after intranasal colonization by *Streptococcus pneumoniae*

*Aaron Goodwin (College of the Holy Cross), Nang Maung (UMass Graduate School of Biomedical Sciences), John Leong MD PhD (UMass Graduate School of Biomedical Sciences)*

*Streptococcus pneumoniae* naturally colonizes the upper respiratory tract of roughly 40% of the human population asymptotically. It is also responsible for approximately one million deaths every year, mostly children in developing countries. Our investigations have previously shown that intranasal colonization can protect mice from bacteria placed directly into the blood or lung. To better understand the lymphocytes involved in protection conferred from colonization, we compared the immune responses of mice at various time points after colonization. Immunological protection was generated by mice against lung infection at both 5 and 10 weeks after the last inoculation. This protection is thought to be independent of T-cells; therefore completely immunodeficient mice were given B-1 cells and intranasally colonized to verify the role of these cells. Although better able to survive intranasal colonization than non-colonized mice, these recipient convalescent mice were not well protected against lung infection. We performed tests to examine possible antigens capable of protecting against several pneumococcal strains but were unable to generate strain independent immunity most likely due to differences in the polysaccharide capsules. Several strains of knockout mice lacking specific lymphocyte subsets were colonized as well and their protection was observed after lung infection.

Funding provided by the American Recovery and Reinvestment Act

## Poster 6

### Characteristics of Face-to-Face and Electronic Conversations

*Kerry Kareta, Jenna Sattar, Elizabeth Campbell, and Patricia Kramer*  
*Department of Psychology, College of the Holy Cross*

The style and characteristics of conversations vary with the underlying purpose of the conversation and the mode of communication under which that conversation took place (e.g., Anderson, 2006; Baron, 2004; Doherty-Sneddon et al., 1997). The current work is part of a larger project in which 202 college students (with minimal or no acquaintance) worked in pairs on two activities (task-oriented, socially-oriented) in one of four modes of communication (face-to-face, video-conferencing, audio-conferencing, or instant-messaging). The task-oriented activity was a Map Task (Anderson et al., 1991) and the socially-oriented activity was a five-minute conversation. Measurements included completion time, accuracy, and frustration on the map task, perceived level of social presence, perceived quality of overall interaction, and ratings of personality (self and partner).

For this part of the project, we examined the content of the conversations (all of which were electronically recorded) that occurred for the task-oriented and socially-oriented activities. We transcribed and coded the conversations. The coding scheme included 44 different characteristics, most of which were adapted from prior research (Boyle & Anderson, 1994; Carletta et al., 1996, 1997; Doherty-Sneddon, et al., 1997; Joinson, 2001; Punyanunt-Cater, 2006). We present our coding scheme and initial analyses of the majority of the 101 conversations. We assess the degree to which the conversations' characteristics depended upon communication mode, task, and gender and relate to the efficiency of the task completion.

We thank the Richard Fisher Fellowship for financial support.

## Poster 7

### Three Dimensional Surface Model Based Investigation Of Avian Mandible Morphology

*Stephanie John, Megan Cooper, Michael Dmytriw, and Rachael Martinez*  
*Advisors: Dr. Leon Claessens and Dr. Abby Drake*  
*Department of Biology, College of the Holy Cross*

The great diversity in the shape and size of the beak of Darwin's finches and other birds are among the best known examples of adaptive evolution. Beak morphology is closely correlated with diet and species ecology. Long and pointed beaks such as those found in hummingbirds allow the probing of flowers for nectar. Flat and wide beaks as found in the spoonbills are used to sift through mud looking for insects or crustaceans. Curved, sharp, and powerful beaks are used by parrots for cracking open food like seeds and nuts, and hawks, for example, have pointed beaks that enable them to tear open their prey.

Utilizing the Holy Cross based National Science Foundation funded Aves 3D database ([www.aves3D.org](http://www.aves3D.org)), we have initiated a study of mandible (jawbone) shape variation in birds. Currently, we have approximately 15 jawbones from 9 orders to assist this new project on ecomorphological diversification of bird mandibles. We will use geometric morphometrics to study the patterns of phenotypic variation of mandible shape in birds.

Geometric morphometrics holistically captures shape information from organismal structures. Three-dimensional coordinates are captured for a series of homologous landmarks on each mandible. Then a generalized Procrustes superimposition is applied to all landmark configurations. Procrustes superimposition extracts shape information by translating, rotating and scaling each landmark configuration. Principal components analysis is then applied to the shape coordinates to expose the major axes of shape variation. Anovas are used to test for significant differences in shape (using the principal component scores) amongst the different functional groups of birds. All analyses will also test for phylogenetic convergence.

We thank the National Science Foundation for financial support.

## Poster 8

### Mechanism of protein splicing of the *Pyrococcus abyssi* lon protease intein

*Kevin O'Brien, Adam C. Nadelson, Daniel J. York, Lauren R. Duffee,  
Julie N. Reitter and Kenneth V. Mills  
Department of Chemistry, College of the Holy Cross*

Protein splicing is a process in which an intervening polypeptide, the intein, directs its own excision and the concurrent ligation of the two neighboring exteins. The intein from the *Pyrococcus abyssi* lon protease can be purified and expressed with non-native exteins. This intein lacks the normally conserved penultimate histidine residue, which aids in the third step of protein splicing, asparagine cyclization. This particular intein replaces the histidine residue with a lysine. The intein has another unusual feature: a stretch of glycine residues flanking its C terminus. We transferred the intein to a new *E. coli* expression vector to aid in the identification of protein bands appearing on SDS-PAGE through the use of Western blot analysis. The new expression vector has a glutathione-S-transferase tag at its C extein, allowing for detection through Western blot. We plan to test the flexibility of the penultimate residue through site directed mutagenesis to see what effect different residues have on the intein's activity. We also will observe the influence of the glycine residues on the activity of the intein.

This material is based upon work supported by the National Science Foundation under grant number 0447647

## Poster 9

### Rhenium Chemistry: The Use of Various Metal Centers to Check for Optimal Coordination with Various Tripod Ligands

*Harun Rafi and Richard S. Herrick  
Department of Chemistry, College of the Holy Cross*

Technetium Chemistry has been studied by inorganic chemists because it is the most commonly used element in diagnostic imaging scans. In our lab, Rhenium chemistry has been studied because the two elements are in the same group and the lanthanide contraction means that rhenium can be studied in place of the radioactive technetium. Recently,  $\beta^-$ -emitting nuclides of rhenium are becoming readily available and have suitable properties that enable the possible development of compounds to be used for tumor radiative therapy.

The chemistry of rhenium compounds attached to tripod ether ligands was explored because ether is absorbed by heart tissue. The major advantage of using a tripod ligand is that it coordinates with the metal center at 3 different sites, which promotes a smaller chance of decomposition when injected into the human body. The problem with these ligands is their structure does not produce a perfect octahedral structure, which consists of all 90-degree angles, meaning that each bond can be easily broken. Our goal is to find the proper tripod ligand or metal center to create a stable complex.

The tripod ligands were attached to  $\text{Re}(\text{CO})_3(\text{H}_2\text{O})_3^+$  and other metal centers such as Manganese, Magnesium, and Barium by dissolving each compound in water and heating the solution at reflux for 4 hours. By slightly varying the atomic radii, different metal centers were chosen. The various tripod ligands that were tested were tris-imidazole methyl ether, tris imidazole PEG ether, tris pyridine methyl ether, and tris pyridine PEG ether. Future work in this area will consist of attaching our tripod ligands to even more metal centers to discover the optimal atomic radius that coordinates with the tripod ligands. Solving crystals by using an x-ray crystallography diffractometer will produce bond angles that can be evaluated and compared to the angles needed for a perfect octahedral structure.

We thank the Richard Fisher Foundation for financial support.

## Poster 10

### Grain size characteristics & potential mobility of road traction sand in Worcester, Massachusetts

*Renee Harkins & Sara Gran Mitchell*  
*Environmental Studies and Department of Biology,*  
*College of the Holy Cross*

We hypothesized that stormwater runoff may transport traction sand into Worcester streams, thereby increasing sediment loads with negative environmental effects. We compiled municipal records of road sand application and removal, monitored precipitation events, calculated stream discharge, and determined suspended sediment concentrations for the 13.4 km<sup>2</sup>, urban Beaver Brook Watershed in Worcester, MA. The City of Worcester deposits  $\sim 1.9 \times 10^4$  Kg of sand on city roads annually,  $\sim 2.6 \times 10^3$  Kg of which is applied in the Beaver Brook watershed. Grain size analysis of sand samples show that road sand applied during the winter months may have a narrower grain size distribution than road sand collected in the spring, suggesting that road sand breaks down after abrasive wear and the silt and clay fraction is washed into streams. Because summer suspended sediment values in Beaver Brook range between 2.1 mg/L to 50.1 mg/L, we believe that the contribution of  $5.44 \pm 2.44$  mg/L from road sand downstream in the Blackstone River is probably not a significant environmental concern. The majority of coarse sand applied during the winter is likely to be recovered from storm drain catch basins and in the city street sweeping program. Sand tracer experiments show a flow of 0.031 cms (0.141 cfs) is sufficient to entrain and remove sand in the 4 mm fraction. Entrainment of 4 mm sand occurs approximately once a week. Therefore, coarse sand that does reach the channel is rapidly flushed from our study reaches. While the City of Worcester applies  $\sim 19,000$  Kg of sand to local roads each year, it appears that the city does a sufficient job removing road sand to minimize negative environmental consequences.

We thank the Fisher Summer Research Fellowship for financial support.

## Poster 11

### Modeling the Immunological and Virological Response to HIV-1 after HAART

*Maria S. Cavicchi and David B. Damiano*  
*Department of Mathematics, College of the Holy Cross*

Patients in the chronic phase of HIV infection typically show heightened activation and lowered counts of CD4+ (helper) T cells (the primary target of HIV) and heightened activation and heightened counts of CD8+ (killer) T cells. For many patients, upon initiation of highly active anti-retroviral therapy (HAART), these activation levels and counts return to normal.

As part of an ongoing retrospective study of data from the HIV clinic at the University of Massachusetts Medical School, we have found that for a large cohort of patients, the return to normal is accompanied by a linear rise in CD4:CD8 ratios. This is regardless of whether the patients are virological responders (HIV counts drop to undetectable levels), immunological responders (CD4+ levels increase to near normal levels), or both. This is of potential clinical significance because it is counter to current clinical guidelines which suggest that tracking CD4:CD8 ratios is not relevant.

Though still in a preliminary stage, we hope to develop a mathematical model utilizing CD4+ T-cell counts, CD8+ T cell counts, and viral loads which explains the linear rise in the CD4:CD8 ratio.,

This is a joint endeavor with Dr. Richard Ellison, Dr. Jennifer Daly, Dr. Thomas Greenough, and Regan Savas from UMass Medical Center. The first author would like to thank the Sherman Fairchild Grant for summer financial support

## Poster 12

### Hydrogen Bonding in Model Systems and the Synthesis of a Transition State Mimic

*Kevin Halloran, Brian R. Linton*  
*Department of Chemistry, College of the Holy Cross*

Hydrogen bonding is a common molecular force that involves hydrogens that are covalently bonded to electrophilic atoms interacting with other electrophilic atoms. The strength of hydrogen bonds are difficult to quantify and it is generally accepted that they can range from 1kcal/mol- 5 kcal/mol. However, through the use of hydrogen-deuterium exchange, we believe it is possible to determine the strength of the hydrogen bond. By finding the rate of exchange using of  $^1\text{H}$  NMR, we will be able to determine the equilibrium constant which then can be related to Gibbs free energy. In doing so, the strengths of the hydrogen bonds are determined.

Our lab has also developed small beta-turn peptides that are used to catalyze the 1, 4 conjugate addition of nitroalkanes stereoselectively. In order to understand the source of the stereoselectivity, we must look at the reaction mechanism. The transition state of the mechanism will prove crucial in our understanding of the mechanism for providing stereoselectivity. Since transition states contain partial bonds and cannot be isolated, a transition state mimic can be a useful stand-in to investigate how a reaction occurs. Mimics are designed in a manner to have the same shapes and electron densities as the actual transition states but in a molecule that can be isolated and manipulated. The mimic will be investigated with the peptide to determine binding interactions through use of two-dimensional  $^1\text{H}$  NMR.

Acknowledgment is made to the donors of the American Chemical Society Petroleum Research Fund for support of this research. This material is based upon work supported by the National Science Foundation under CHE-0852232.

## Poster 13

### Acute Administration of Fluoxetine Increases Prepulse Inhibition of Acoustic Startle Response: Examining the Roles of the 5-HT<sub>1A</sub> and 5-HT<sub>1B</sub> Inhibitory Autoreceptor Subtypes

*Maryann Manatt, Brittany Fritz, Brenden Myers, and Daniel Bitran*  
*Department of Psychology, College of the Holy Cross*

Drugs that alter the brain's serotonin (5-HT) neurotransmitter system affect sensorimotor gating, a phenomenon involved in selective attention, which is measured by prepulse inhibition (PPI), a decrease in startle reactivity to a pulse when preceded by a prepulse of a low intensity. A deficit in PPI has been implicated in several psychiatric disorders including obsessive compulsive disorder and schizophrenia. Serotonergic regulation of PPI appears to depend on a number of receptor subtypes. Our lab previously found that acute administration of fluoxetine, a selective 5-HT reuptake inhibitor, increased PPI. Mechanisms by which fluoxetine elicits its effects on PPI, more specifically, the roles of the 5-HT<sub>1A</sub> and 5-HT<sub>1B</sub> inhibitory autoreceptors, were examined in this study. In a two by four repeated measure design, we tested the effect of fluoxetine in animals pretreated with WAY 100635, a 5-HT<sub>1A</sub> antagonist, or GR 127935, a 5-HT<sub>1B</sub> antagonist. Overall, fluoxetine treatment increased PPI as we had previously found. Low doses of WAY and all doses of GR blocked the effects of fluoxetine. Thus the increase in PPI observed in fluoxetine-treated animals is in part mediated by enhanced activity of 5-HT<sub>1A</sub> somatodendritic autoreceptors and 5-HT<sub>1B</sub> terminal autoreceptors. Stimulation of 5-HT<sub>1A</sub> autoreceptors decreases the rate of activity of serotonergic neurons, whereas stimulation of 5-HT<sub>1B</sub> terminal autoreceptors decreases serotonin release per action potential. These data suggest that *decreased* serotonergic tone is associated with an increase in prepulse inhibition, and suggests further that psychiatric disturbances in PPI reflect an overactive serotonergic system, which would be desensitized over repeated antipsychotic drug administration.

This research was made possible by the Richard Fisher Summer Research Fellowship and we thank the Sherman Fairchild Foundation for their financial support.

## Poster 14

### **The Antiviral and Mutagenic Activity of Apobec3G, an Anti-HIV Protein**

*Emily Kinn and Ann Sheehy  
Department of Biology, College of the Holy Cross*

Apobec3G (A3G) is a human protein that has been shown to inhibit HIV reverse transcription, an essential process in the HIV life cycle, that when hindered suppresses the virus. However, the molecular basis of this interference is somewhat controversial. While it has been definitively shown that A3G mutates the viral DNA during reverse transcription, some described mutations in A3G eliminate its enzymatic activity while the protein seems to still retain antiviral activity. In this project, ninety-two mutants of the A3G protein that have retained their antiviral function are examined for their mutagenic activity in a bacterial assay. Further characterization of these mutants may give some insight as to specific regions of the A3G protein important for the mutagenic activity and address whether a suppressive function, independent of its enzymatic activity, of A3G may exist.

We thank the Arnold and Mabel Beckman Foundation for financial support

## Poster 15

### **Can Tamarins Learn an Artificial Grammar Implicitly?**

*Meaghan Collins and Maura Conway  
Department of Psychology, College of the Holy Cross  
Sponsor: Dr. Charles Locurto*

Based on a pilot study conducted in the spring of 2009, we investigated cotton top tamarins' knowledge of an artificial grammar using a serial reaction time task. Elements were presented in a list on a touchscreen following a pattern specified by an artificial grammar. The list contained one instance of each grammatically-acceptable transition between elements. The list was arranged to provide a continuous loop of grammatical transitions. In this grammar each element can be followed by two different possibilities for a total of 163 possible transitions. The list was presented continuously, without an intertrial interval, and was interrupted only for the delivery of reinforcement, scheduled at  $p = .17/\text{element}$ . Following acquisition training, three separate tests were used to determine whether subjects had acquired knowledge of the artificial grammar, or whether they had simply memorized the list. The first test entailed a number of pair-wise choices between a grammatical and a non-grammatical element. The second test presented a choice between a "next" element and a non-grammatical element. The third test gave the tamarins a choice between a grammatical and a next element in the grammar. Results indicated that the two tamarins had learned something about the grammatical list.

We thank the Richard Fisher Summer Research Fellowship for financial support and the New England Primate Research Center for allowing us to use their facility.

## Poster 16

### Understanding Laser Diode Output with 6.8GHz Sidebands

*J. Ryor and T. Roach*

*Department of Physics, College of the Holy Cross*

We have seen experimentally that it is possible to produce light at three frequencies using an extended cavity laser diode with both a direct and alternating (or modulation) source of current into this diode. However, it was our goal to better understand how the intensity of these two sideband frequencies depends on the optical and electrical set-up of the diode, and how it can be altered by both types of current inputs into the diode.

We found that the difference between the diode impedance and cable impedance, along with other electrical elements, creates feedback in our electrical system which disturbs the output. This was observed for both a 6.8 GHz and 3 GHz alternating source. We also explored the relationship between the extended cavity grating alignment and sideband intensity as well as that between the cavity length and output. We discovered that the sideband intensity was maximized when the resonant frequency of the cavity matched the modulation frequency, in agreement with theoretical expectations..

We also explored how changing the DC laser current affected light output and sideband intensity. At certain current ranges we see a surprisingly large range of sideband intensities within one stable optical mode. This result is matched by detailed laser power-current curves which make jumps at these same current ranges.

We thank the American Chemical Society Petroleum Research Fund for financial support.

## Poster 17

### Rotational Spin Decay Rate of an MLB Baseball

*K. Sullo, T. Booth and Professor M. Koss*

*Department of Physics, College of the Holy Cross*

Many forces act on a baseball in flight but the details how these forces affect the ball still contain some mysteries. One of the main concerns of the Physics of Baseball Team this summer was to measure how quickly the spin of the ball diminishes free of any velocity vectors (due to gravity or any other outside forces). To do this, our team conducted experiments on a “zero gravity” flight which provided an apparent weightlessness environment. We used a high speed camera to capture the relative position of a ball at known time intervals. We used those position measurements to calculate the angular velocity of the baseball as it was suspended in this weightless environment. We then compared the angular velocity values as a function of time to determine a characteristic rotation decay time,  $\tau$ , for each specific test. We also conducted two additional experiments on campus: one to record the rotation of a ball during flight at two times and another using a drop experiment that kept the high speed camera within a moving reference frame close to that of the a ball as it fell. We found the results of all of these experiments to be consistent with each other given the experimental uncertainties.

We would like to thank the Fischer Fund, Massachusetts Space Grant Consortium, the Department of Physics, Dean Austin, Father McFarland, and CISS for financial support

## Poster 18

### Sleep Deprivation Impairs Conscious Control But Improves Unconscious Control

*K. Chiong & Ryan Prendergast,*

*Department of Psychology, College of the Holy Cross*

Two types of control determine human behavior: Conscious control (active and effortfully and exerted with awareness of the stimuli) and unconscious control (automatic, unaware acquisition of the parameters that determine successful performance). The factors that determine the breakdown of control are one of the most important topics in the field of cognitive neuroscience. This study asked a simple but important question: Does sleep deprivation affect equally how an individual exerts conscious and/or unconscious control.

In this task, sequential arrows (>> >> or << >>) are presented and participants are asked to respond to the direction of the 2<sup>nd</sup> set of arrows. Participants are slower at responding and more likely to make an error if the 1<sup>st</sup> arrows point in the opposite direction. When the 1<sup>st</sup> and 2<sup>nd</sup> arrows frequently disagree, participants are capable of exerting control to reduce the interference caused by the 1<sup>st</sup> arrows. The ability to control the interference is true whether the 1<sup>st</sup> arrows are consciously perceived (conscious control) or covered so that they cannot be perceived (unconscious control).

Young adult participants performed significantly worse on the conscious control task after 24 hr sleep deprivation compared to a night of good sleep. Remarkably, participants performed significantly better on the unconscious control task while they were sleep deprived compared to when they were not. These findings demonstrate two important results: First, sleep deprivation is destructive to conscious effortful behavior; and second, automatic cognitive processes can be enhanced when released from the interfering effects of consciousness.

We thank the Sherman Fairchild Fellowship Foundation for the financial support. Profs. Gregg DiGirolamo & Amy Wolfson were the faculty sponsors.

## Poster 19

### The Effect of Separations on Crime

*R. Baumann, B. Engelhardt, T. Ciavarra (Class of 2010)*

*Department of Economics, College of the Holy Cross*

Prior research has shown that an increase in unemployment causes an increase in crime. Unemployment alone, however, is too broad to predict crime. Unemployment is a function of job separations, and an increase in separations exposes more people to unemployment, a period during which one can acquire crime specific human capital. We isolate the effect of changes in the job separations rate on property crime. Our preliminary results show a percentage point increase in unemployment results in 496,000 additional property crimes, and a percentage point increase in separations results in 1.7 million additional property crimes. These marginal effects are substantial given the regional average of property crimes is 2.5 million.

We thank the May and Stanley Smith Charitable Trust for financial support.

## Poster 20

### Estimating the Social Benefits of NFL Franchises

*Katherine Kiel, Associate Professor,  
Victor Matheson, Associate Professor,  
Christopher Sullivan (Class of 2009),  
and Kevin Golembiewski (Class of 2010)  
Department of Economics, College of the Holy Cross*

NFL franchises are often given public subsidies by city and state governments. Whether these subsidies are an efficient use of tax-payer dollars has been debated by economists for several years. While several economists have asserted that NFL franchises have negligible effects on cities, Carlino and Coulson (2003) claim that the presence of an NFL team provides enough social benefits to a city to justify public subsidies.

Carlino and Coulson (2003) use rents to measure the impact of an NFL team on a city. They conclude that NFL teams provide social benefits to cities because their study suggests that people are willing to pay more for rent in NFL cities. In our study, we sought to replicate Carlino and Coulson's results using housing values instead of rents as a measure of the social benefits associated with NFL franchises.

We have found that NFL franchises do not significantly affect housing values. A possible explanation of why our results differ from Carlino and Coulson's is based on the effect of public subsidies on taxes. Homeowners feel more of a burden when taxes are increased than renters, and this tax burden leads to a decrease in perceived home value. When we include a variable controlling for the amount of public subsidies given to NFL franchises in our regression, the variable is significant and negatively correlated with home values.

In sum, our results will be important to the above mentioned debate as they indicate that the public subsidization of NFL teams is an inefficient use of tax-payer dollars.

We thank the May and Stanley Smith Charitable Trust for their support.

## Poster 21

### The Influence of Sleep on the Relationship between Externalizing Behavior and Academic Performance in Young Adolescents

*Jordan Burko, Elizabeth Spellman, and Dr. Amy Wolfson  
Department of Psychology, College of the Holy Cross*

Sleep is an important biological process that affects daily functioning. It can alter many aspects of functioning such as mood, cognitive performance, and behavior (Curcio et al., 2006). This study examined the influence of actigraphically estimated sleep on the relationship between externalizing behaviors and academic performance in young adolescents. 7<sup>th</sup> graders (N=143) from two urban middle schools completed a series of questionnaires including the Achenbach Youth Self Report, Center for Epidemiologic Studies Depression Scale (CESD), and the School Sleep Habits Questionnaire. In addition the students were required to wear a wrist actigraph and to complete a daily sleep-wake diary for a period of seven days to gather data on sleep patterns and daytime functioning. Academic performance and behavior information were obtained through school reported student transcripts.

Using Barron and Kenny's mediator model the study examined four sets of relationships: (a) Between externalizing behavior and academic performance, (b) between externalizing behavior and the mediator (actigraphically-estimated sleep patterns), (c) between the mediator and academic performance, (d) and between externalizing behavior and academic performance, while controlling for sleep pattern variables. It was found that higher levels of externalizing behaviors were associated with poorer academic performance. Moreover, increased externalizing behaviors were correlated with poorer weekday sleep onset, mid-sleep and duration, as well as weekend onset, offset and mid-sleep. In addition, later weekday sleep onset and weekend sleep offset and mid-sleep were related to poor academic performance. Overall, using this approach, actigraphically estimated sleep pattern variables mediated the relationship between externalizing behaviors and academic performance in young adolescents.

Funding for this study came from the National Institute of Child Health and Human Development (PI: Amy Wolfson).

## Poster 22

### Beta-sheet Mimetics

*J. Hillner and Brian R. Linton*

*Department of Chemistry, College of the Holy Cross*

Beta-sheets are a secondary protein structure characterized by two parallel protein strands joined together by hydrogen bonds. Their prevalence in nature as well as their tendency to aggregate in various diseases makes them of interest for study. Our syntheses aim to create beta-sheet mimics that join synthetic proteins together with a disulfide tether. We have synthesized beta-sheet precursors which elongate distance between beta-sheet strands and introduce steric hindrance. The modified beta-sheets resulting from these syntheses can be used to determine optimal beta-sheet structure. Other syntheses have created beta-sheet precursors that replace hydrogen bond donors with acceptors. These modifications seek to inhibit beta-sheet aggregation that is characteristic of diseases such as Huntington's and Alzheimer's disease.

In synthesizing peptides, we utilize the additive HOBt. When this additive is used in conjunction with the coupling reagent EDC, it gives rise to multiple products. We are currently exploring whether or not these mixtures limit the success of syntheses.

We are focusing on completing beta-sheet syntheses to study these molecules as well as further exploring the phenomenon of HOBt's multiple products.

We thank the National Science Foundation for its support.

## Poster 23

### The 1960 Evacuation of Inis Airc

*C. Tynan*

*Department of History, College of the Holy Cross*

The study of Irish history is filled with narratives of evacuation, eviction and emigration. In the 20<sup>th</sup> century, many of the small islands off Ireland's rugged coast were evacuated and the inhabitants were relocated to the mainland. Previous studies have focused on the narratives and stories of the people who were evacuated from islands like the Great Blaskets; which were predominately Gaelic speaking.

The Cultural Landscapes of the Irish Coast Project has conducted in depth research into the process of evacuation on Inis Airc which lies off the Connemara Coastline in County Galway. The island was evacuated in 1960 after several drowning incidents at sea and medical emergencies on the island. The community was then relocated to the mainland where they could be close to the sea. In addition to this the project also studied the daily life and culture of the island's inhabitants in the 19<sup>th</sup> and 20<sup>th</sup> centuries. By studying school records and daily reports we were able to extract some knowledge as to the daily routine of children. This also provided a glimpse into the use of Irish Gaelic and English on the island as well as other important subject matter that was being taught in the classroom. This is the first comprehensive study of the island life and culture of its inhabitants.

I thank the University of Notre Dame Irish Studies Department for their support.

## Poster 24

### Skeletal Muscle Function and Regeneration Following Acute Limb Ischemia Reperfusion

C. Abularrage, S. Meng, R. Paranal, H. Yoo, A. Robaldo, B. Nguyen,  
G. LaMuraglia, M. Watkins, H. Albadawi  
*Vascular Research Lab, Massachusetts General Hospital*

**Introduction:** Acute therapy for skeletal muscle ischemia reperfusion injury (IR) is rarely feasible. These experiments were designed to define the temporal, histological and functional aspects of skeletal muscle regeneration after acute IR.

**Methods:** Six groups of C57BLKS mice underwent unilateral hind limb IR for 1.5hr (MIR) or 3hr (SIR) ischemia followed by 1, 7 and 14 days reperfusion (DR). At each time point, mice were evaluated for functional limb recovery, histological evidence of acute injury, regenerating fibers, tissue levels of ATP, and molecular markers of regeneration (MyoD, Myogenin).

**Results:** At 1DR, SIR resulted in a 5 fold greater number of injured fibers than MIR. At 1 and 7DR, SIR resulted less ATP than MIR; by 14DR, levels were equivalent, but less than the contralateral. No difference occurred in functional recovery at 1DR, but by 7 and 14DR, MIR mice recovered to normal function, but the SIR mice sustained ongoing deficits. SIR had greater numbers of immature (centrally nucleated) myofibers at 7 and 14DR. MyoD and Myogenin expression were greater in the MIR group at 7DR, but were equivalent by 14DR and all higher than at 1DR and contralateral.

**Conclusions:** IR caused depletion in ATP in skeletal muscle. Functional recovery after MIR associated with greater expression of MyoD, Myogenin and fewer immature fibers at 7DR. In the time interval leading up to 7DR, there may be a therapeutic window where pharmacologic interventions might facilitate functional and metabolic recovery.

We thank the Vascular Department fund at MGH and the National Institute of Health for financial support.

## Poster 25

### Making Sense of Economic News in the Press

Nicolas Sanchez, Professor and Katherine Tedesco (Class of 2011)  
*Department of Economics, College of the Holy Cross*

Basing decisions on misinformation is not likely to be successful in the long run, which is unfortunate because misinformation is extremely common in the media. In this case, misinformation can be broken down into two categories: wrong information and lack of information. Generally, the information reported in the press is raw data, which means the values are taken out of context and cannot be compared to other values or across time periods. In order to correctly make these comparisons, values must be expressed in real, rather than nominal, terms. In addition, the media tends to not provide complete information about topics that are reported, such as local labor market conditions. It is near impossible to completely understand something without having all of the facts.

We used the *Worcester Telegram & Gazette* as an example of providing misinformation in the media. Hopefully this will serve as a guide to inform the general public what to look for while reading a newspaper.

We thank the May and Stanley Smith Charitable Trust for financial support.

## Poster 26

### **Global Autism Public Health Initiative Background Report: India, Chile, and South Africa**

*A. Simcoe-Matthews*

*Autism Speaks Etiology Department Intern  
Department of Psychology, College of the Holy Cross*

Autism is a complex neurodevelopmental disorder characterized by impaired communication and social interaction, and restricted, repetitive, or stereotyped behaviors. In the U.S. it's estimated that the odds of a child having autism are 1 in 150, which is an increase from past figures. This apparent rise in prevalence has sparked interest in autism prevention and treatment throughout the world. However, little is known about the current state of services, awareness, and research infrastructure in international territories.

Using internet searches, information was collected regarding public and professional awareness of autism, research capabilities, and service provision in India, Chile, and South Africa with the goal of identifying potential challenges and specific areas of needed improvement in each country. It was found that while each country is lacking in all three areas, they each face unique challenges. India struggles most with the incredible diversity of its peoples which creates difficulties when unifying support systems and awareness campaigns across multiple languages and cultures. Chile, on the other hand, has to combat the prevailing attitudes that Thimerosal-containing vaccines are the cause of autism and detoxification can cure the disease in some children. In South Africa, the greatest challenge is shared by all three countries: resources are limited and often inaccessible because of the area's physical size.

To overcome these challenges and others, researchers, service providers, parents, and awareness groups must work together to bring about key changes to aid the autism community.

I thank the Holy Cross Leadership Council of New York for financial support.

## Poster 27

### **Packaging of human protein APOBEC3G into HIV virions**

*Emily Cartwright, Natasha Tobarran, Melissa A. Farrow, Ann M. Sheehy  
Department of Biology, College of the Holy Cross*

APOBEC3G (hA3G) is a human protein found expressed in T-cells and macrophages, that has been found to have powerful anti-HIV capabilities. This viral suppressive function is attributed to its enzymatic ability as a cytidine deaminase. hA3G is packaged into assembling virions. When these virions infect the next round of target cells, hA3G interferes with the essential viral process of reverse transcription of the HIV genome. With the short-circuiting of this process, the viral life cycle comes to a halt. In a counter-response to hA3G activity, HIV expresses the viral protein Vif (Viral infectivity factor), which degrades hA3G and prevents it from being packaged into the virion.

In order to further characterize regions of hA3G that play a role in this critical packaging step, an alanine mutagenesis scan was performed on the 384 amino acid protein producing 135 mutants. Of these 135 mutants, ~10 had were unable access the virion and thereby did not exert an anti-viral effect. To determine whether this ability to be packaged is the sole defect of these 10 mutants, fusion constructs were made in which a delineated packaging signal was fused to the N-terminus of each of the 10 mutants. Experiments are underway to test both the ability of these fusion proteins package into virions and subsequent exertion of the anti-viral effect. We thank the Sherman Fairchild Foundation for funding this project. We thank the Sherman Fairchild Foundation for funding this project.

## Poster 28

### Development of protein purification strategies using the *Pyrococcus abyssi* PolIII intein

*Adam C. Nadelson, Daniel J. York, Katherine T. Lewandowski, Deirdre M. Dorval, Katherine R. Connor, Julie N. Reitter and Kenneth V. Mills*  
*Department of Chemistry, College of the Holy Cross, Worcester, MA, USA*

The intein that interrupts the DNA polymerase II DP2 subunit in *Pyrococcus abyssi* is unusual in that it can be isolated following expression in bacteria as an unspliced precursor and induced to splice *in vitro* by incubation at temperatures greater than 37°C. We have taken advantage of this activity to develop a method to isolate highly purified protein. We have modified the intein sequence by mutation to promote *in vitro* cleavage between the N-terminal extein and intein. A separate modification of the expression vector results in an intein that can direct *in vitro* cleavage between the intein and the C-extein. We have used these two expression vectors to create two protein purification schemes. In each scheme, one extein binds the fusion protein to an affinity resin. Followed by thorough washing, controlled intein cleavage releases the other extein.

We thank the National Science Foundation for their financial support

## Poster 29

### Shutter Design in Laser Ion Mobility Spectrometry

*C. Corbett and J. Kelley*  
*Department of Chemistry, College of the Holy Cross*

Laser ion mobility spectroscopy uses an ionization source that has many potential advantages over traditional radioactive ionization sources. Because a laser sends out a pulse at a single wavelength it can be used to ionize specific molecules. Laser ionization does not have the problems of disposal and exposure associated with radioactive ionization sources.

Laser ionization creates a coulomb explosion, a three dimensional cloud of ions that expands in all directions. This expansion leads to a broad temporal signal in the IMS. To fix this problem an ion shutter was designed and used to flatten out the cloud into two dimensions. The ion cloud hits the shutter, flattens out and is then quickly released. In this scenario the ions expand in a plane parallel to the detector so that temporal broadening due to ion-ion interactions is minimized. Also, multiple pulses of ions can be captured by the shutter to increase signal intensity and hence the sensitivity of the instrument. The research focused on the shutter's design, construction, controlling electronics, and timing optimization.

We would like to thank the Richard Fisher Fellowship for financial support.

### Poster 30

#### **Influence of conserved residues on individual steps of protein splicing of the non-canonical *Pyrococcus abyssi* PolII intein**

*Lauren R. Duffee, Adam C. Nadelson, Daniel J. York, Deirdre M. Dorval, Julie N. Reitter and Kenneth V. Mills*  
*Department of Chemistry, College of the Holy Cross*

Protein splicing is directed by an intein, an intervening polypeptide flanked by exteins. The intein directs its own excision and the ligation of the exteins. The intein from *Pyrococcus abyssi* that interrupts the DNA polymerase II DP2 subunit can be purified as a precursor fusion protein flanked by non-native exteins. Splicing can be induced *in vitro*, allowing for detailed kinetic analysis of the individual steps of protein splicing. We have created mutant intein fusion proteins to study the molecular steps of protein splicing separately, and are interested in the influence of conserved residues on each of these steps. The first step of splicing is influenced by the residue immediately upstream of the intein. This step is significantly slowed by substitution of the native Asn to Phe or Leu, and the rate is increased by substitution to Ala or Asp. Significant alteration of this rate results in splicing side reactions instead of splicing. Substitutions at conserved Thr and His residues in the intein B-block reduce the rate of the first step of splicing, and also result in intein side reactions instead of efficient splicing. Mutation of conserved His residues in the final two conserved domains of the intein affect the third step of splicing and the efficiency of the overall splicing reaction.

This material is based upon work supported by the National Science Foundation under Grant No. 0320824 and CAREER grant No. 0447647.

### Poster 31

#### **Identification of Novel Oncogenes associated with MMTV-induced Breast Cancer**

*J. Trautwein, P. van den Heuvel, S. Ross*  
*Department of Microbiology, University of Pennsylvania*

Mouse mammary tumor virus (MMTV) induces breast cancer in mice by insertional activation of oncogenes. A screen of integration sites in MMTV-induced tumors was performed to identify novel oncogenes. Among the identified candidates were TCF7L2 and BAI3. TCF7L2 is involved in the Wnt signaling pathway and has been implicated in tumorigenesis. BAI3 may play a role in brain tumor progression. To validate these genes as oncogenes, cell-based assays were performed. Cells over-expressing TCF7L2 were grown in low serum conditions to test for abnormal proliferation. Initial results indicate that TCF7L2 can override low serum-induced growth arrest. Effects on apoptosis will be examined using DNA laddering assays. Similar assays will be performed with BAI3 once the vectors have been cloned and the appropriate cell lines have been made. We hope our discoveries will lead to new target genes in human breast cancer.

Funded by an ARRA supplement to PHS R01 CA114273.

### Poster 32

#### A Spectral Analysis of Black Hole Candidate 4U1630-472

*R. Nazarian and T. Narita*

*Department of Physics, College of the Holy Cross*

Using the Chandra X-Ray Observatory, we seek to find traces of absorption lines from highly ionized iron in the 6-7 keV range in black hole candidate (BHC) 4U1630-472 during its outburst state in 2004. Subsequently, the photon emission dips will provide evidence for possible warping within the BHC's accretion disk (AD). This theory of gaseous warping will be proven by quantitative traces of stronger and weaker emission lines as a function of time, which varies from time-independent functions seen in non-warping ADs.

We studied the photon emission from BHC 4U1630-472 during a 50180 second continuous-clock mode observation in the X-ray band. A spectral analysis of the data suggests the BHC to be modeled by various components including absorption from interstellar gases, blackbody radiation from a hot gaseous disk surrounding the BHC, and atomic absorption from iron. We see signs of one absorption line at approximately 6.98 keV. The width of this absorption line and the suspected AD warping have not yet been confirmed.

We thank the Massachusetts Space Grant Consortium, a subgroup of NASA and the National Space Grant Project, for their financial support.

### Poster 33

#### Anomalies in Tournament Design: The Madness of March Madness

*R. Baumann, V. Matheson, C. Howe*

*Department of Economics, College of the Holy Cross*

Tournament design is of crucial importance in competitive sports. The primary goal of effective tournament design is to provide incentives for the participants to maximize their performance both during the tournament and in the time period leading up to the tournament. In spectator sports, a secondary goal of tournament design is to also promote interesting match ups that generate fan interest. Seeded tournaments, in general, promote both goals. Teams or individuals with strong performances leading up to a tournament receive higher seeds which increase their chances of progressing further in the tournament. Furthermore, seeding ensures that the strongest teams or players are most likely to meet in the final rounds of the tournament during which time fan interest is at its peak. Under some distributions of team or player skill, however, a seeding system can introduce anomalies that could affect incentives.

Our analysis of the NCAA men's basketball tournament uncovers such an anomaly. The seeding system in this tournament gives teams with better success in the regular season more favorable first round match ups, but the tournament is not reseeded as the games progress. Therefore, while higher seeds progress to the 2nd round of the tournament at uniformly higher rates than lower seeds, this relationship breaks down in later rounds. We find that 10th and 11th seeds average more wins and typically progress farther in the tournament than 8th and 9th seeds. This finding violates the intended incentive structure of seeded tournaments.

We thank the May and Stanley Smith Charitable Trust for their financial support.

### Poster 34

#### Uterine Artery Embolization Preoperative to Hysterectomy

*Emily Samartino and Michael Hallisey M.D*  
*Department of Interventional Radiology, Hartford Hospital*

Uterine artery embolization is a technique that has been reported as an effective procedure for controlling life threatening hemorrhage following delivery, cervical biopsy, and pelvic trauma. A retrospective study of 20 women who underwent preoperative uterine artery embolization prior to hysterectomy was performed. The results were used to evaluate and assess the effectiveness of immediate preoperative uterine artery embolization in the reduction of intraoperative and perioperative blood loss of women undergoing hysterectomy with large fibroid uteri. The results of the data collected during the study were compared to standards reported in the literature. The results showed that preoperative uterine artery embolization reduces the intraoperative blood loss of patients who undergo a hysterectomy. The patients studied had approximately the same blood loss as patients who did not undergo the embolization; however, our patients had uteri that were almost ten times larger than the standard. Therefore, the uterine artery embolization preoperative to the hysterectomy should be considered as a viable treatment option for women with large fibroid uteri.

We thank the Hartford Hospital for financial support.

### Poster 35

#### Design and Testing of an Ion Mobility Spectrometer With the Use of SIMION Modeling Software

*J. DeLisio and J. Kelley*  
*Department of Chemistry, College of the Holy Cross*

Ion mobility spectrometry (IMS) is a fast and efficient way of trace chemical detection of explosives and narcotics. IMS differentiates molecules by the time it takes their ions to travel down a drift tube with an electric field gradient to a detector. A shutter is used to trap the ionized molecules, compress the ion packet, and release it into the drift tube in order to produce sharp peaks at the detector. This technique can be very effective in detecting and differentiating large organic molecules based on how long it takes them to travel down the drift tube.

SIMION ion optics software was used to design and test the drift tube and shutter grid. The SIMION program allowed for creation of IMS designs and simulation of how ions would respond to them. SIMION was programmed to create an identical environment to our IMS setup to give an idea of what settings should be used in the actual IMS. A program was also written to simulate the opening and closing of our shutter. This program also adjusted the voltages on the drift rings based on the voltage that is applied to the system.

The data collected through SIMION was used to design a more efficient drift tube and shutter. The virtual flight times of the ions were extremely valuable in determining real world time settings for the operation of the shutter system. The use of SIMION helped eliminate time that would be used for trial and error and SIMION automatically performed calculations to make the design process as efficient as possible.

We would like to thank the Sherman Fairchild Foundation for their support of our research

### Poster 36

#### Identifying APOBEC3G Domains as Targets for Therapeutic Intervention

*P. Cheney and A. Sheehy*

*Department of Biology, College of the Holy Cross*

It has been more than 28 years since the first reportings of the disease that was to become known as AIDS and, to date, therapies used to treat HIV-infected individuals are complex and require careful supervision. The relatively recent discovery of the innate anti-viral cellular protein Apobec3G (A3G), has offered a unique direction for research aimed at a better understanding of a natural viral defense that may be able to be successfully manipulated in the clinic. In the absence of Vif, a viral protein, A3G suppresses HIV replication; however in the presence of Vif, A3G activity is counteracted thereby enabling the virus to sustain a spreading infection. A comprehensive understanding of both the viral protein, Vif, and the cellular protein, A3G, will provide a better understanding of their interaction and this important Vif-A3G regulatory circuit. We have generated a library of 135 A3G mutants and a subset of these mutants will be surveyed as candidates that may be able to suppress viral infectivity in the presence of Vif. Identification of such A3G mutants would describe a relevant gain of function and would reveal domains within the A3G protein critical to its interaction with Vif. These domains may provide a successful therapeutic avenue by liberating A3G and harnessing its innate anti-viral power.

We thank the Richard and Susan Smith Family Foundation for financial support.

### Poster 37

#### Investigating Excess Endowments at Private Liberal Arts Colleges

*Karen Teitel, Assistant Professor, Robert Baumann, Assistant Professor and Andra J. Belland, Class of 2011*

*Department of Economics, College of the Holy Cross*

Endowments at colleges and universities have provoked interesting and controversial discussions in recent years. One of the chief responsibilities of college and university presidents is to grow or maintain their endowments. Incentives coupled with external pressures may result in excessively large endowments or endowment under spending at the expense of benefits for others within the college community. Excess endowments are positively correlated with managerial compensation and reduced program-to-expense ratios.

In our research we look at private, liberal arts colleges and universities collected from the 2000 Carnegie Classification of Institutions of Higher Education. Collecting information from the IRS Form 990 (filed by all non-profits) from 1997 to 2005, we test whether excess endowments exist due to program growth or agency problems. We control for state and year and we winsorize our data at the 1<sup>st</sup> and 99<sup>th</sup> percentile.

This research is important in determining whether the size of endowments at colleges and universities are justified given the amount of expenses allocated to program growth. Our preliminary results show that colleges and universities with endowments in the highest, most extreme quartile, pay their presidents higher wages and have lower program-to-expense ratios when compared to schools that do not have excess endowments.

We thank the May and Stanley Smith Charitable Trust for their support.

### Poster 38

#### When good is bad: The negative consequences of positive memories

*Kathryn O'Connor '10 and Professor DiGirolamo, Faculty Advisor  
Department of Psychology, College of the Holy Cross*

Numerous therapeutic approaches to major depression disorder (MDD) concentrate on focusing the patient on positive thinking. It is assumed that the symptoms of depression are alleviated by this positive focus. In agreement with this idea, when non-depressed people recall positive memories their positive affect increases, alleviating depressed mood. Remarkably, when patients suffering from MDD recall positive memories their affect drastically *decreases*, deepening their depressed state. The underlying mechanism for this counterintuitive mood depression following positive memory recall in MDD remains unidentified. We postulate that the act of recalling positive memories in MDD patients increases their stress level which, in turn, deepens their depression. To test this prediction, we will measure cortisol levels (a hormone that increases with increased stress) in the saliva of college students across a range of depression scores. As expected, control participants are able to self-regulate their mood. After either negative mood induction or no mood induction, positive memory recall increased positive affect and/or lowered negative affect based on the Positive and Negative Affective Scale.

We thank the Fisher Fellowship for financial support.

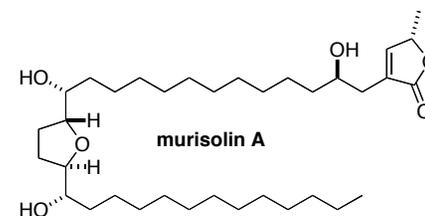
### Poster 39

#### Development of a Stereodivergent Approach to Tetrahydrofuran Natural Products

*Livio Islamaj, Kathleen E. Shanley and Kevin J. Quinn  
Department of Chemistry, College of the Holy Cross*

Tetrahydrofurans, five-membered rings containing four carbon atoms and one oxygen atom, are common structural motifs among biologically active natural products including the Annonaceous acetogenins. We have developed a stereodivergent approach to synthesis of mono(tetrahydrofuran) acetogenin cores which allows access to all possible diastereomeric permutations from a common hydroxy alkene precursor. Our strategy makes use of the reliable Sharpless asymmetric epoxidation and dihydroxylation reactions for the establishment of four stereocenters and complementary  $S_N2$  cyclizations for ring formation. The development of this strategy and our efforts toward its application in a convergent total synthesis of murisolin A, a potent cytotoxin that is currently being explored as an anti-cancer agent, will be discussed. Key to the total synthesis is the coupling of two suitably functionalized terminal alkenes by cross metathesis.

Financial support of this work by the National Science Foundation and the Sherman Fairchild Foundation is gratefully acknowledged.



## Poster 40

### Discounting by Law: Legal Factors Affecting Forensic Economic Appraisals in the States

*David Schap, Professor  
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Maria Salame, College of the Holy Cross (Class of 2011)*

States differ in their statutory and case law requirements affecting how practicing forensic economists compute appraisals in cases involving lost income over time. Ordinarily, a court awards damages in lump sum fashion. Forensic economists assist at trial by converting what otherwise would be a stream of dollar amounts into an equivalent present value total after giving due consideration to the time value of money. Our legal research found four key characteristics in state law governing the practice of discounting by forensic economists in cases involving personal injury or wrongful death: (1) dictates concerning the discounting procedure itself, including those in certain jurisdictions specifying a particular discount rate; (2) applicable rules related to pre- and post-judgment interest; (3) the presence or absence of directives covering treatment of income taxes; and (4) legal requirements addressing how future inflation is to be handled. Our results have been compiled in the form of fifty multi-page descriptions (one for each state) and distilled into a table summarizing and categorizing the applicable law in the various states.

We thank the May and Stanley Smith Charitable Trust for financial support.

## Poster 41

### Measuring Control Over Behavior in Opiate Addiction

*N. Patel  
G. J. DiGirolamo, Faculty Advisor  
Department of Psychology, College of the Holy Cross*

The 2007 National Survey on Drug Use & Health indicated a growing resurgence in opioid use with 2.1 million initiates to drugs beginning with the abuse of opioid pain relievers (a larger number than initiates of marijuana). Recent models of addiction suggest that drug abuse is a shift from voluntary, conscious processes to automatic, unconscious processes. This study measured cognitive abilities in control over behavior in people addicted to opiates.

When presented with sequential arrows (>> >> or << >>) and asked to respond to the direction of the 2<sup>nd</sup> set of arrows, people are slower at responding and more likely to make an error if the 1<sup>st</sup> arrows point in the opposite direction. When the 1<sup>st</sup> and 2<sup>nd</sup> arrows frequently disagree, control subjects are capable of exerting control to reduce the interference caused by the 1st arrows. The ability to control the interference is true whether the 1<sup>st</sup> arrows are consciously perceived (conscious control) or covered so that it cannot be perceived (unconscious control).

42 patients from the Detox Unit at Community HealthLink were tested on both a conscious and unconscious version of this task. Patients with opiate addictions were highly impaired in both conscious and unconscious control. The majority of the patients were unable to exert control either consciously or unconsciously, suggesting that opiate addiction impairs both voluntary processes as well as unconscious processes on control over behavior. Further studies will seek to determine if treatment medications for addiction improve conscious and/or unconscious control.

We thank the Stransky Research Fellowship for financial support.

## Poster 42

### Prevalence of Intimate Partner Violence in an Urban Emergency Department Population

*Ela Banerjee and João Delgado, M.D.  
Hartford Hospital, Division of Emergency Medicine*

Intimate partner violence (IPV) is a pattern of abusive, controlling, and coercive behavior that is used to gain power and control over an intimate partner. It can include physical assault or the threat of physical assault, sexual violation and psychological abuse. There are many indirect health impacts of domestic violence such as difficulty managing comorbid illnesses and increase in adverse health behaviors. The purpose of this study was to determine the prevalence of IPV in the Hartford area and to study if patients presenting to the Emergency Department (ED) after an intentional drug overdose are more likely to be involved in an abusive relationship than other emergency department patients. Female patients that came into the Hartford Hospital Emergency Department over a four-hour period were interviewed using the modified Partner Violence Screen (PVS) that assessed for current, recent and lifetime prevalence of IPV. There are 317 participants in this study to date, with a mean age of 46.5 years. Forty-five percent of this sample screened positive for IPV and 15.4% of this sample screened positive for high-risk or as undergoing current and/or recent IPV. Furthermore, no statistically significant correlation was seen between IPV and ethnicity. More participants need to be enrolled in the study in order to study a correlation between intentional drug overdose and IPV. In conclusion, IPV is a very common and serious problem with about 7,500 women presenting to the Hartford Hospital ED as a high-risk population.

This project was funded by Hartford Hospital and the Division of Emergency Medicine.

## Poster 43

### Semi-Quantitative Laser-Induced Breakdown Spectroscopy: In Search of Metal Contaminants in Blackstone River Sediment

*B. O'Leary and J. Kelley  
Department of Chemistry, College of the Holy Cross*

Laser-Induced Breakdown Spectroscopy (LIBS) is an exciting new field in which a high power focused beam is used to excite a sample to a plasma that then re-emits visible and ultraviolet light characteristic of the constituent atoms. This method of atomic emission spectroscopy is fast, requires little or no sample preparation, and can be used to identify solids, liquids and gases. However, shot-to-shot variations in the amount of ablated sample lead to large variations in absolute and relative peak intensities yielding difficulties in quantitative analysis.

In this work we have developed a method of making semi-quantitative measurements (accurate to at least the order of magnitude of the concentration) of metal contaminants in river sediment by averaging many spectra per sample to reduce shot-to-shot variations and to overcome variations due to the heterogeneity of sediment. We have applied this technique to search for Copper, Nickel, Lead, Chromium, and Zinc in Blackstone River Sediment using calibration functions and correlation methods.

A quantitative analysis of sediment taken from the Fisherville pond in Grafton, Massachusetts is underway and will aid in assessing LIBS as a feasible and reliable method for detection of metal contamination “hot spots” throughout the Blackstone River Watershed.

We thank the Becton Dickinson Foundation for financial support.

## Poster 44

### Testing affordable and portable three-dimensional laser surface scanning technology

*M. Dmytriw, M. Cooper, S. John and R. Martinez*

*Advisors: L. Claessens and A. Drake*

*Department of Biology, College of the Holy Cross*

One of our projects this summer focused on obtaining a more portable and cost-effective method of scanning objects using the DAVID-Laserscanner system. All that is needed is a commercial hand-held laser and a webcam in addition to a free 3-D scanning and editing software package developed by DAVID Vision Systems. The DAVID-Laserscanner, which is much more portable than our current scanners, the Konica Minolta Range7 and Roland Picza LPX-1200, is also much less expensive, costing only a few hundred dollars (compared to \$20,000 and \$78,000 for the Roland and Konica Minolta systems respectively). This would potentially enable us to maximize the number of objects scanned in our lab for only a fraction of the cost. One drawback to this more affordable and portable scanner is that the detail of the scans is inferior to that of our current scanners. We are currently experimenting with lasers of various power outputs and wavelengths in order to determine the maximum resolution possible using the DAVID-Laserscanner system. This resolution can be quantified and compared with the resolution of our current scanners using the program Rapidform XOV Verifier, and this comparison can be shared with other scientists.

The affordability of the DAVID-Laserscanner could potentially help spread the use of three-dimensional non-contact laser surface scanning to smaller institutions and parts of the world that have minimal financial resources. Widespread use of this scanning technology could lead to a greater amount of data collection and availability as well as catalyze biological shape analysis using geometric morphometrics.

We thank the National Science Foundation for financial support.

## Poster 45

### Analyzing Neural Responses to Optic Flow Patterns

*E. McCourt and C. Royden*

*Department of Math and Computer Science, College of the Holy Cross*

As an observer moves through the world, the images that the observer sees move across the retina, creating an optic flow pattern. A person moving in a straight line generates a radial pattern, the center of which coincides with the person's direction of motion, or heading. Some cells in the medial superior temporal (MST) area of the brain respond to radial patterns of motion, and are thought to process information about the observer's heading. A computer model based on these cells uses template cells with shifted centers of motion to compute heading (Royden, 1997).

However, some electrophysiological data suggests that some cells in MST are tuned to spiral patterns of motion, rather than radial patterns (Graziano, Andersen & Snowden, J. Neurosci, 1994). Data from the computer model show that these cells may only appear to be tuned to spiral motions, but are in fact tuned to radial patterns that have been shifted off the center of the receptive field of the cell. To further analyze this result, we created a mathematical model for the response of these cells by integrating the value of the velocity vectors in the optic flow pattern combined with the radial pattern preference of the cell over the entire receptive field of the cell. We tested a variety of parameters and structures for the model. Results showed that some cells that are tuned to shifted radial patterns also appear to be tuned to certain spiral motions.

Supported by NSF grant IOS-0818286.

## Poster 46

### Collaborative Paleontological Fieldwork in Arizona, New Mexico and Utah

*E. Blumhagen and Z. Lavender*

*Faculty Advisor: L. Claessens*

*Department of Biology, College of the Holy Cross*

In June and July of 2009 we prospected, quarried, prepared, and catalogued numerous vertebrate fossils from Early Permian through Late Cretaceous rock exposures at Petrified Forest National Park in Arizona, Ghost Ranch in New Mexico, and other localities throughout southern Utah, in collaboration with the Yale Peabody Museum of Natural History (YPM) and the Utah Museum of Natural History (UMNH).

Some of the most significant finds of this fieldwork season included several rare aetosaur specimens at two different localities. Aetosaurs are a poorly known extinct group of reptiles that are characterized by a pig snout nose with an armadillo looking body with numerous dermal armor plates. At Petrified Forest we helped excavate an articulated skeleton of a *Typhothorax* from Late Triassic Chinle Formation outcrops.

At Ghost Ranch in New Mexico, we worked with the UMNH excavating four quarries in a single Chinle Formation exposure. At one quarry site we excavated two intertwined articulated aetosaur skeletons. In a quarry 30 feet removed, we found numerous disassociated limb bones, teeth, skull fragments, vertebrae, and armor plates of aetosaurs and phytosaurs.

The remainder of our research was spent prospecting and collecting fossils from several localities throughout southern Utah, as part of a general survey of Early Permian through Late Cretaceous rock exposures for the UMNH. During this period, a complete labyrinthodont amphibian skull was recovered, as well as numerous disassociated skeletal remains from dinosaurs and related extinct archosaurian reptiles.

All of the collected bone specimens this summer will be prepared at the YPM and UMNH, respectively, and further research on these specimens will help to enhance our understanding of the terrestrial vertebrate faunas of the Triassic, and faunal turnover throughout the Mesozoic era. We would like to thank the Yale Peabody Museum of Natural History and Utah Museum of Natural History for this incredible opportunity and the Sherman Fairchild and Fisher Foundations for their financial support.

## Poster 47

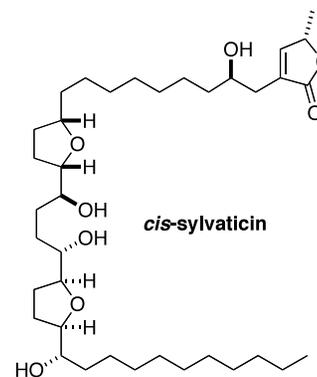
### Efforts Toward the Total Synthesis of *cis*-Sylvaticin

*Shalise M. Couvertier and Kevin J. Quinn*

*Department of Chemistry, College of the Holy Cross*

*cis*-Sylvaticin is an unusual member of the Annonaceae acetogenin class of natural products possessing a  $C_2$ -symmetric nonadjacent core of two tetrahydrofuran rings. Due to its low natural abundance and nanomolar cytotoxicity toward human tumor cells, *cis*-sylvaticin has been the target of numerous synthetic studies. We will describe a two-directional approach to the core of *cis*-sylvaticin that takes advantage of its symmetry to significantly shorten its synthesis. Key steps include silicon-tethered ring-closing metathesis, Sharpless asymmetric dihydroxylation and  $S_N2$  ring formation. Terminus differentiation of the  $C_2$ -symmetric core should provide a highly efficient synthesis of this complex natural product.

Financial support of this work by the National Science Foundation is gratefully acknowledged.



## Poster 48

### Children's Mapping of Number Words onto Nonsymbolic Numerosities

*Caitlin O'Gallagher<sup>1</sup>, Heena Lakhani<sup>2</sup> and Susan Carey<sup>2</sup>*  
<sup>1</sup>*College of the Holy Cross*  
<sup>2</sup>*Harvard University*

Previous studies have shown that children learn how to count before they understand the meanings of the number words like “five” or “ten.” In order to understand how kids grasp the meanings of number words, this study examines how children come to map number words to nonsymbolic numerosities (dot arrays). Specifically, we are interested in how the following factors affect children's mappings: 1) the presence of an anchor - small numbers such as 2, 4, and 7; 2) an explicit example of what ten dots looks like; 3) and knowledge of the numeral list.

In this study, four and five year olds were assessed in their counting abilities and completed a task in which they estimated the number of dots presented on a computer screen. Three important findings have been revealed from the data thus far: 1) presenting children with small numbers (an anchor) improves their mappings; 2) giving children who have not already been presented with small numbers an explicit example of what ten dots looks like aids them in their mappings; and 3) children who are able count up to 100 reliably are much better at their mappings than those who are unable to do so.

We thank the National Science Foundation REESE for financial support.

## Poster49

### Temperature Dependence of splicing activity of the *Pyrococcus abyssi* PolIII Intein

*Daniel York and Prof. Ken Mills*  
*Department of Mathematics, College of the Holy Cross*

Inteins are intervening polypeptides within a protein. They are able to direct their excision from the flanking polypeptides, called exteins, as well as facilitate the ligation of the exteins. This process, called protein splicing, produces the ligated, functional protein. We wish to determine the temperature dependence of the rates of each of the steps of protein splicing of the *Pyrococcus abyssi* PolIII intein. We over-expressed and purified this construct as an unspliced precursor for further study.

We have mutated amino acids within the intein through site directed mutagenesis. We designed each mutant to inhibit a certain step in the protein splicing mechanism, such that we can study each step of the reaction separately. Preliminary results confirm that the Wild Type intein, with a C-terminal Gln, splices with a first order rate constant of  $9.5 \times 10^{-6}$  at 60°C. When the C-terminus is replaced with an Asn, the rate constant is increased to roughly  $3.6 \times 10^{-5}$  at 60°C. The pseudo-first order rate constant of the first step is  $1.84 \times 10^{-4} \text{ s}^{-1}$  at 65°C and that for the first and second steps combined is similar at 65°C. To measure any possible correlation between these rate constants and temperature, the proteins were placed in Phosphate Buffer, pH 7.0. Results indicate that the first step depends somewhat on temperature; however the second step appears unaffected by variations in temperature.

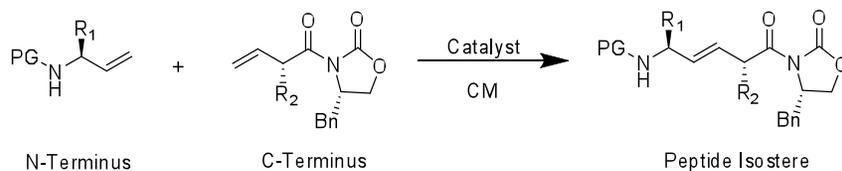
This material is based on work supported by the National Science Foundation.

## Poster 50

### Exploring the Olefin Cross Metathesis Reaction

*Greg Faxon and Prof. Bianca Sculimbrene*  
*Department of Chemistry, College of the Holy Cross*

Our research lab focuses on the synthesis of a class of molecules known as peptide isosteres. The key reaction for their synthesis is the Nobel-Prize winning olefin cross metathesis (CM) reaction. This reaction involves the coupling of two alkene termini, known as N & C termini, to form the desired peptide isostere. Our work this summer concentrated on making libraries of these termini. The termini synthesized in lab contain varying properties including their protecting groups (PG) and R groups. We can use these libraries of termini to gain more insight into the factors that control selectivity in CM. One particular area of interest is in the reactivity of the different termini. Our preliminary results have indicated that the N-terminus is more reactive in the CM if it contains an NH group. Future work will focus on fully understanding this versatile reaction for the synthesis of peptide isosteres.



We would like to thank the Becton-Dickinson Foundation and the Camille and Henry Dreyfus Foundation for financial support.

## Poster 51

### Assessing Actigraph Reliability Using the iRobot®

*R. Prendergast<sup>1</sup>, E. Soares<sup>1</sup>, and A. Wolfson<sup>2</sup>*  
<sup>1</sup>*Department of Mathematics and Computer Science*  
<sup>2</sup>*Department of Psychology, College of the Holy Cross*

We have developed a methodology by which actigraph reliability can be objectively assessed. An iRobot® was used to create frequency of movement (FOM) data, by programming the robot to traverse a motion pattern that would produce a square wave FOM profile. The data were measured for a period of 60 minutes with an epoch length of 30 seconds (120 data values for each actigraph). The sample mean and sample standard deviation FOM were then computed for each epoch individually. Based upon these measures, we could identify those actigraphs that produced FOM profiles that lay outside a two-sided 95% confidence region. We also computed an *F*-statistic for each actigraph. This would serve as a summary statistical measure over all epochs for each actigraph. The *F*-statistic is based on the sample mean vector and sample covariance matrix for the pool of actigraphs being tested. However, the feature space of each actigraph first was reduced by the principal components transformation, in order to obtain an invertible sample covariance matrix.

The results showed that some actigraphs under-estimated FOM relative to the sample mean FOM derived from the pool of actigraphs. These became possible candidates for outliers of our *F*-distribution. When examining the *F*-scores for these actigraphs relative to the pool, they indeed corresponded to outliers of the *F*-distribution as well. However, the computed *F*-scores were a function of the number of principal components retained. As this parameter was increased, these *F*-scores lost their significance as outliers. We are currently investigating the robustness of our methodology to determine if a true outlier can be identified from an arbitrary pool of actigraphs.

We thank the Sherman-Fairchild Foundation for financial support.

## Poster 52

### **Computer simulation of the action potential from a geometric compartmental model of the human auditory nerve fiber**

*M. Piltin and J. Watrous*

*Department of Biology, Saint Joseph's University*

Hearing loss and degeneracy of auditory function affects not only the elderly, but also a growing population of more youthful individuals. Through social movements such as portable music devices, auditory nerve fibers may be at risk for some level of degradation. Of the limited approaches available for solving hearing loss, cochlear implants rehabilitate profoundly deaf persons by electrically stimulating the fibers in the auditory canal. However, the information being transported to the brain is insufficient for producing meaningful translation of speech. In order to gain the ability to improve implants or other hearing devices, one must further understand the complexity and behavior of the fibers located in the inner ear.

Through the use of computer simulation, we are able to gain insight into the electrical activity and nature of a stimulated healthy auditory nerve fiber. In a paper published in the South African Journal of Science titled, "Predicting action potential characteristics of human auditory nerve fibers through modification of the Hodgkin-Huxley equations" by Smit *et al*, a figure depicting the geometric accuracies of a compartmental model of the fiber is presented. In our laboratory, we used the computer program SNNAP (Simulator for Neural Networks and Action Potentials). The program provided the ability to create and modify a compartmental model of a neuron. Also, we changed both the shape of each compartment as well as the dimensions, in order to understand the details of the electrical axonal propagation. The graphical results in SNNAP that we achieved illustrated standard action potential behavior throughout the entire fiber. Once this model has been perfected, degeneracy can be simulated by removing functionality of a portion of the fiber so that deafness may be investigated more accurately.

## Poster 53

### **Launch of Aves 3D: A Digital Database of Avian Skeletal Elements**

*M. Cooper, R. Martinez, S. John, M. Dmytriw*

*Advisors: L. Claessens, A. Drake*

*Department of Biology, College of the Holy Cross*

This summer saw the launch of the National Science foundation funded Aves 3D database, [www.Aves3D.org](http://www.Aves3D.org). This website provides 3D models of a wide diversity of avian skeletal elements, including the sternum, humerus, tarsometatarsus, mandible, furcula and cranium of a wide variety of bird species. The undergraduates in this lab contributed to database growth through specific research projects on avian sternal morphology, mandible shape, and new surface scanning systems, for instance. Visitors to the Aves 3D website can rotate and zoom the interactive three dimensional skeletal models, which allows them to examine all aspects of the bones. In addition, two-dimensional graphics are provided to further aid in ecomorphological, functional, and phylogenetic analyses. Digital models for the Aves 3D Database are generated through non-contact laser surface scanning, and we currently employ a Roland LPX 1200 and a Konica Minolta Range7, with a maximum resolution of 100 and 40 micrometers, respectively. Skeletal specimens are obtained from, amongst others, the Harvard Museum of Comparative Zoology and the Yale Peabody Museum of Natural History. The continuously expanding database can be used as a digital resource for studies using methods such as geometric morphometrics or finite element analysis, or as an archive for anatomical comparison of skeletal material and avian phylogenetic relationships. The convenience of having this on-line collection of 3D scans allows for rapid global dissemination of data on rare and fragile specimens.

We thank the National Science Foundation for financial support.

## Poster 54

### Religious Motivation and the Religious Life among Worcester's Older Adults

*E. Farrington and M. Frongillo*  
*Professor Andrew Futterman*

*Department of Psychology, College of the Holy Cross*

Using measures of religious orientation derived from Allport and Ross (1967) and Batson (1991), we describe a three-factor model of religious motivation in a random sample of 345 older adults living in Worcester, MA, and examine the convergent validity of the three religious motivation factors. Three religious factors in keeping with the religious orientations "religion as an end in itself" (Ends), "religion as a means to other ends" (Means), and "the search for purpose and meaning of life in a religious context" (Quest) emerged from exploratory factor analyses, and were confirmed in randomly selected halves of the sample. Means and Quest were associated ( $r > .25$ ), as were Ends and Means ( $r > .20$ ), but Quest and Means largely were largely independent of one another ( $r = .05$ ). Ends and Means religious orientations were differentially related to religious involvement, belief, experience, and knowledge; Quest religiousness was largely unrelated to religious measures with the exception of positive correlations with self reported religious experience. By contrast, Quest was predicted by background characteristics (e.g., married, higher levels of Quest), personality characteristics (e.g., Neuroticism, Extroversion, Openness on the NEO), by functional impairments (e.g., ADL's), and by other non-religious measures.

We thank the Richard Fisher Fellowship for financial support.

## Poster 55

### Rhenium Chemistry: Bidentate complexes with Biologically Relevant Ligands

*Americo N. Gambella and Richard S. Herrick*  
*Department of Chemistry, College of the Holy Cross*

Technetium, in the form of  $^{99m}\text{Tc}$ , is the most commonly used nuclide in diagnostic imaging. Recently,  $^{188}\text{Re}$  has shown potential for possible tumor radiation therapy as a  $\beta$ -emitter. Rhenium, whose chemical properties closely resemble those of technetium, can also be used as a cold analogue of technetium in the laboratory to test suitable biomolecules and ligand systems for their ability to chelate to the metal.

Biologically relevant ligands contain nitrogen and oxygen donor atoms. These nucleophilic atoms of the bifunctional ligands can bind easily to the metal Rhenium center in a bidentate complex. Once in the human body, they target specific locations. Target-specific agents can be used for imaging or as a radiopharmaceutical in different areas of the human body.

Different biologically relevant ligands were studied with different functional groups off the  $\alpha$ - carbon. Various derivatives of histidine were used due to their useful nucleophilic donor atoms, testing how the peptides bind to the rhenium complex. Ethylenediamine derivatives were also studied to test the possible insertion of these ligands on a carbon monoxide group bound to the starting material, while still binding to rhenium through a nitrogen atom. Different reaction conditions yielded different results.

Future work in this area includes continued testing of dicarboxylic acids and their ability to chelate to the metal center. These ligands play roles in various biochemical processes and form a bidentate complex to rhenium due to the two carboxyl oxygens, providing a more stable rhenium complex.

We thank the Becton Dickinson Corporation for financial support.

## Poster 56

### Simulating a Quantum Computer to Approximate the Jones Value of 4-Stranded Braids

*Matthew Brady and Prof. David Damiano  
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College of the Holy Cross*

Intuitively, a mathematical  $n$ -braid is a set of  $n$  strands that are collinear except for pairwise twists of adjacent strands. Developed by E. Artin in the 1930's, braids have been used as a tool in the study of topological knots. An important aspect of the study of braids and knots is the study of their algebraic invariants, in particular, the Jones polynomial. An open problem is whether two distinct knots must have distinct Jones polynomials, or equivalently, whether a non-trivial knot can have a trivial Jones polynomial. This is related to the question of whether a certain representation of 4-stranded braids is faithful. Complicating matters, it is computationally complex to compute the Jones polynomial.

In 2006, Vaughn Jones, Dorit Aharonov, and Zeph Landau built a "quantum" algorithm for approximating the value of the Jones polynomial at a root of unity of any  $n$ -stranded braid. In this project, we created a Matlab program which simulates their quantum algorithm providing approximations to Jones values for 4-stranded braids. We use our program to explore Jones values for large collections of randomly generated braids, By analyzing the statistics of these approximations we hope to provide insight into whether the Jones polynomial of a non-trivial knot can be trivial

The first author would like to thank the Fisher fund for financial support.

## Poster 57

### A Preliminary Geometric Morphometric Analysis Of The Ecomorphology Of The Avian Sternum

*R. Martinez, M. Cooper, S. John, and M. Dmytriw  
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Birds engage in a wide variety of locomotor behavior, including continuous flapping flight, soaring flight, swimming, diving, walking, and running. The ventral surface and keel provide an attachment site for the pectoral and supracoracoidal muscles associated with the flight stroke. Flying birds generally have a large sternal keel, whereas in birds that are flightless the sternal keel is highly reduced or absent. Our study aims to further explore the differences in avian sternal shape between different functional groups, especially with respect to keel curvature and shape of the apex of the sternal keel.

We quantified the diversity of keel shapes using geometric morphometric analyses with the software package MorphoJ. Landmarks were captured on the sternal body, rib facets and along the keel. Generalized least-squares Procrustes superimposition was used to extract the symmetric components of shape. Relative warps analysis was performed to determine the major axes of sternal shape variation across Aves, and Anovas were carried out on the relative warp scores to reveal significant shape differences among locomotor groups. Canonical variates analysis was employed to investigate differences between major functional groups.

We thank the National Science Foundation for financial support.

## Poster 58

### *Tribolium castaneum* Embryo Fate Mapping

*M. Gallant and K. Ober*

*Department of Biology, College of the Holy Cross*

Insect wings are a key innovation that has contributed to the spectacular success of the clade that they characterize. However, the developmental basis for the origin of this trait remains poorly understood and there are currently two competing hypotheses. The wing (a dorsal appendage) may be derived from a portion of the leg (a ventral appendage) of ancestral arthropods by dorsal migration of wing primordia around the circumference of the body. Alternatively, the feature may be a true novelty, a structure that arose *de novo* by lateral outgrowth of the dorsal thorax. By using DiI to label appendage primordia cells we will attempt to determine which cells in *Tribolium* give rise to legs and which cells give rise to dorsal thoracic structures.

We developed an effective and efficient procedure for DiI injections of *Tribolium* embryos. We were able to inject 70 embryos per collection with a survival rate of ~50% through incubation and vitellin membrane removal. Most embryos lost burst during injection. Although at this point we do not have enough evidence to support either of the hypotheses, the sheer number of embryos able to be injected at once will prove extremely beneficial once more accurate injections take place.

We thank the Sherman-Fairchild Fund for financial support.

## Poster 59

### Frequency Control Elements for a Laser

*Chelsea Dalphond '11 and Prof. Timothy Roach*

*Department of Physics, College of the Holy Cross*

We studied the behavior of various parts of our extended cavity diode laser in order to gain better control over the frequency of the laser. The laser is used for laser cooling of Rb atoms, and the absolute light frequency must be controlled with 1MHz accuracy.

A reflective grating sends light back to the diode chip, forming the extended optical cavity. By changing the position of the grating with a piezoelectric transducer, we are able to change the length of the cavity to precisely control the frequency of the laser light.

We sometimes need to adjust the cavity in a very short time period, so we measured the frequency response of several different piezos to understand their behavior. We used a lock-in amplifier with LabVIEW to monitor the piezo response as frequency changed. Some showed a sudden spike in amplitude and phase as frequency increased, meaning there were resonances within the piezo. These are undesirable because they make it difficult to actively control the grating position. Understanding the piezo behavior was crucial in finding the best piezo for our system.

The grating reflectivity also affects control of the frequency. The more light sent back, the more stable the system. We measured the polarization dependence of the grating reflectivity so we can choose the best orientation.

Finally, we improved the mechanical mounting of the laser and grating, so we can have a shorter extended cavity and can attach a mirror mounted parallel to the grating that redirects the laser light to the original direction of travel.

We would like to thank the Sherman Fairchild Foundation for its financial support.

## Poster 60

### Atom Optics Research: Laser Intensity Control

*T. Roach, M. Vornle von Haagenfels, J. Ryor, C. Dalphond*  
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Our research involves the interaction of laser light with very cold, slowly moving rubidium atoms (Rb). We need to be able to control the laser intensity very precisely in time during the experimental cycle.

I used an Acousto-Optic Modulator (AOM) which was able to deflect the light very quickly, using Bragg diffraction. I maximized the power by rotating the AOM until it diffracts most of the original beam. We turn off the light by shutting off the electrical signal to the AOM. The AOM shuts off the light very fast almost instantaneously, but some light can still get through about 0.03% of the original beam.

To completely turn off the laser I constructed an electro-mechanical shutter out of an 8 ohm speaker. The shutter is able to completely turn off the light but it is slower and takes about 2 milliseconds to completely block the light. So with the AOM and shutter combined we are able to shut off the laser very quickly and very completely.

We thank the American Chemical Society Petroleum Research Fund for financial support.

## Poster 61

### Investigating the Divergent Evolution of *Scaphinotus Petersi*

*M. Pratt and K. Ober*  
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*Scaphinotus petersi* is a flightless carabid beetle endemic to Arizona. Due to the arid climate, these beetles cannot survive outside the sky islands, which are forested mountain tops separated by a dry sea of sand and stone. There are six such islands with known populations of *S. petersi*, and the total isolation from other populations each island provides sets the stage for allopatric speciation.

We are investigating the degree to which these individual populations of *S. petersi* have drifted from one another by comparing sequence differences in the mitochondrial genes ND1 and CO1. DNA isolation proved to be a difficult process, as our specimens are all two to fifteen years old. Initially we homogenized a tissue sample and performed a phenol-chloroform extraction, however this consistently yielded inadequate DNA. Our solution is a DNA extraction buffer which digests the soft tissue of *S. petersi*. After digestion, the DNA can be isolated by the same phenol-chloroform procedure as before, but with drastically improved results according to nanodrop spectrophotometry. Once the gene has been selectively amplified, it is sequenced by dye-terminator sequencing.

Those genes which have been sequenced thus far are beginning to indicate a pattern of divergence which correlates with the mountains and rivers of Arizona. Upon completion of this project, we plan to have an evolutionary timetable for each subspecies of *S. petersi*.

We thank the Becton Dickinson Grant for funding our research.

## Poster 62

### Using NIR and Other Spectroscopic Methods for Rapid Assessment of Product Quality Attributes

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Spectroscopy allows for quick measurements, identification of products, and counterfeit testing with little or no sample preparation. Spectroscopy also provides information regarding the consistency and overall quality of the products. The resulting spectra provide a wealth of information pertaining to moisture content, potency level, and degradation. This information can be obtained much faster than conventional testing, speeding the decision making process for assessing the overall quality of Pfizer and competitor products. This project focused on utilizing FT-IR, NIR, and Raman spectroscopy to provide a more efficient way of identifying products, obtaining information about quality of products, and predicting product quality attributes under different conditions. FT-IR did not exhibit clear differences among tested products under different storage conditions. In contrast, both Raman and NIR spectroscopy showed efficient ways of obtaining information about the products. Raman showed clearer differences in the zero order between products in different storage conditions. Degradation at different temperatures and humidity conditions and product quality can be determined through NIR and Raman spectroscopy. If spectroscopic differences are detected performing additional work using conventional methods for assay, impurities, and dissolution can be justified. However, if no significant differences are detected, no further testing may be necessary depending on the purpose of the study.

I thank Pfizer for their financial support.

## Poster 63

### Improving Control via Drugs: A mouse pilot study

*Kathryn O'Connor '10, Neha Patel '10, Maryann Manatt '10, Brittany Fritz '10, Brenden Myers '10 and Professor DiGirolamo  
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Despite numerous treatments for addiction, successful treatment for opiate addiction remains elusive due to high relapse rates. One plausible explanation for high relapse rates is greater impulsivity and inability to inhibit behavior. In order to increase control among opiate addict, the noncompetitive NMDA antagonist, memantine, has been suggested. Memantine increases dopamine levels in the prefrontal cortex. The subsequent increase in dopamine may allow greater control over behavior and inhibiting impulsive responses. In order to test this idea, mice, first, learned to associate one of two odors with a reward (1+), while the other odor signaled no reward (2-). A trial was deemed successful if the mouse took the reward and made no movement toward "reward" on unrewarded side. After acquisition, the mice were randomly sorted into four groups: reversal-learning memantine, reversal-learning saline, new-learning memantine, and new-learning saline. The reversal-learning task consisted of inverting the rewarded and unrewarded scents (1-/2+), while the new learning task required the mouse to associate a reward with one of two novel scents (3+/4-). Both the reaction times and number of successful trials were used to measure learning and control. If memantine increases control as predicted, the reaction times and error rates for mice injected with memantine will be better than saline mice for the reversal task, while reaction times and errors for both the memantine and saline mice will be similar for both the acquisition and new-learning tasks.

We thank the Fisher & Stransky Fellowship for financial support.

## Poster 64

### 3-D Organization of ParB-DNA Assembly in Human Pathogens: *M. tuberculosis* and *V. cholerae*

*Kelly Lyons and Dr. Barnali Chaudhuri*  
*Hauptman Woodward Biomedical Research Institute*

The segregation mechanism of bacterial chromosomes remains both structurally and functionally a mystery compared to that of eukaryotic mitosis. One main system involved in chromosomal segregation is the parAB system. Composed of three components, parAB is hypothesized to drive segregation by forming a nucleoprotein complex and using a Walker ATPase. Furthermore, the parAB system plays an essential role in the division of *Myobacterium tuberculosis* (TB) and *Vibrio cholerae* (VC) chromosomes.

The goal of our research is to obtain the structures of each component of the parAB system for TB and VC chromosomes, most specifically focusing on the nucleoprotein complex formed by ParB-DNA. TB and VC ParB1 protein were expressed and purified using Fast Protein Liquid Chromatography (FPLC). Purification was confirmed by SDS/PAGE Electrophoresis. Construction of the nucleoprotein complexes was conducted using varying lengths of DNA from 14-meric DNA to 24-meric. Each complex was confirmed using an Electrophoretic Mobility Shift Assay (EMSA).

To obtain structural information, crystallization trials were run using a hanging drop method with three screens: SPAMAT, Natrix, and Hampton. Plates were set for both TB and VC ParB-DNA complexes. Further investigation was conducted using Small Angle X-Ray Scattering (SAXS). Radius of gyration values obtained for TB ParB-DNA constructs were analyzed and confirmed polymerization along the complex. Currently, Hydroxyl Radical Foot-Printing is being conducted to obtain more results.

The author would like to thank the Hauptman Woodward Research Institute for their financial support.

## Poster 65

### Asymmetric Gold-Catalyzed [4+2] Cycloadditions of Allene-Dienes

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*Department of Chemistry, University of California, Berkeley<sup>2</sup>*

An asymmetric gold(I)-catalyzed [4+2] cycloaddition of allene-dienes is described. Previous work from the Toste laboratory on an achiral variant of this transformation demonstrated that by varying the ancillary ligands on the gold(I) catalyst either the [4+2] or [4+3] cycloadduct could be formed selectively. From these studies we concluded that phosphitegold(I) complexes solely produce the formal [4+2] cycloaddition products. As a result, various chiral phosphite- as well as the electronically-similar phosphoramidite-gold(I) complexes were explored in hopes of developing an enantioselective reaction. Towards this end, a new class of C<sub>3</sub>-symmetric phosphitegold(I) catalysts was synthesized. From these, we found that 1-adamantylcarbonyl-H8-BINOL monoester-derived phosphitegold(I) complex promoted the cycloadditions of a variety of allene-dienes in good yields (50-94%) and good to excellent enantioselectivity (up to 91%). The said catalyst showed tolerance towards different functionalities and substitution patterns on the substrates studied. The full scope of these completed studies and the work in progress in the Toste laboratory will be discussed in due course.

The authors acknowledge funding from the National Institute of General Medical Services (GM073932), Merck Research Laboratories, Bristol-Myers Squibb, and Novartis. The authors would also like to gratefully acknowledge the Amgen Foundation for O.S.F.'s fellowship.

## Poster 66

### **An Analysis of Hydrogen Bonding Patterns in Small Peptides and Using Hydrogen Bonding to Catalyze Reactions of Nitro Compounds**

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Hydrogen bonds are particularly strong dipole-dipole interactions that are implicated in many chemical systems. Despite its importance, hydrogen bonding is poorly understood. By synthesizing and studying small peptide molecules, we hope to elucidate more information about the functionality of hydrogen bonds in larger, biologically important molecules.

A series of three small thioamide compounds were synthesized in order to examine the effect of the carbonyl sulfur on the hydrogen bonding patterns of the molecules. Hydrogen-Deuterium exchange analysis of the three synthesized compounds will demonstrate the hydrogen bonding abilities of thioamides. Also, two dipeptide molecules were synthesized to investigate the effect of amino acid side chain sterics on the backbone hydrogen bonding that allows for adoption of particular peptide structural conformations, in this case beta-turns.

The placement of hydrogen bond donor groups in receptor molecules allows for the stabilization of negatively charged groups on the substrate molecule. The increased stability of the substrate molecule allows the reaction to proceed at a faster rate. A molecular receptor for nitro compounds was synthesized in an effort to stabilize the reactive intermediate of the nitroaldol reaction, the nitronate anion. Stabilization of the nitronate anion should provide an alternate reaction pathway with a lower activation energy requirement, allowing for an increased rate of reaction. Nitroaldol catalysis has a wide variety of uses, especially in the pharmaceutical industry.

We would like to thank the American Chemical Society Petroleum Fund, The National Science Foundation (CHE-0852232), and the Sherman-Fairchild Foundation for financial support.

## Poster 67

### **Using Peptide Isosteres to Investigate Antibiotic Resistance**

*Ryan Quinn and Prof. Bianca Sculimbrene  
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Vancomycin is a last resort antibiotic used to treat serious bacterial infections such as MRSA. This drug functions by binding to a peptide sequence on the cell wall of bacteria via a network of hydrogen bonds. Our goal was to understand the importance of individual hydrogen bonds by synthesizing a mimic of the peptide (called a peptide isostere) that lacks the ability to form certain hydrogen bonds.

Once the peptide and the isostere were synthesized, their ability to bind to vancomycin was measured. Titrations monitored by the absorption of UV light were used to formulate binding curves and calculate binding constants. A binding constant measures the affinity of the vancomycin and peptide/isostere in solution. A smaller value for a binding constant denotes a "tighter" or better binding event. The peptide was found to bind approximately 40 times stronger to the vancomycin than the isostere, with preliminary binding constants of 2 $\mu$ M and 80 $\mu$ M respectively. This information will be used to guide in the development of new isosteres to further investigate how changes in the bacterial cell wall allow bacteria to become resistant to antibiotics like vancomycin.

We would like to thank the Sherman Fairchild Foundation and the Camille and Henry Dreyfus Foundation for financial support.

## Poster 68

### Male Breast Cancer: “You gotta be kidding me!”

*Alexandra Leichthammer, and Edward Thompson*

*Department of Sociology and Anthropology, College of the Holy Cross*

When one thinks of breast cancer, images of pink ribbons and the female body commonly come to mind. The notion of breast cancer as a ‘feminine disease’ is one that parallels the concept that testicular cancer is a ‘young man’s’ disease and that prostate cancer is an ‘old man’s’ disease. However, this gendered conception contributes to lack of awareness that breast cancer in men is possible, and leads directly to later detection and higher mortality rates among the 1,800 men annually diagnosed with male breast carcinoma. Much as media stories harp its rarity and present afflicted men as spectacles, but unworthy of the pink hero status granted to their female counterparts, the research literature has dwelled primarily on this medical oddity and its post-mastectomy treatment protocols. Neglected is a systematic study of the gendered nature of this disease and its management. The personal implications of breast cancer and treatment may challenge men’s sense of themselves as men and embodiment of masculinity.

To investigate the claims that male breast cancer diagnoses are coupled with emasculation and threatened masculinity, the challenges and experiences of 12 male breast cancer survivors were elicited through conversational interviews that ranged in length from 45 to 90 minutes. Findings disprove the initial hypothesis that men would sense emasculation. The men we spoke with commented “I never knew I had breasts” and thus viewed the word “breast” as simply an adjective locating the site of their cancer. Some men divulged initial feelings of the indignity of having breast cancer, however they also detailed how quickly they abandoned gender qualms to embody the cancer in a masculine way and fight hard. Most of the men in our study did the opposite of hide in shame; they publicized their experience as if a duty. All the men detailed feelings of being a medical, but not social oddity. They remain men embodying and performing masculinity, despite a mastectomy and the side effects of hormonal therapy. This has therefore been an enlightening project and we intend to continue interviewing into the fall.

We are grateful for the Richard & Sarah Greisch Research Fellowship for its financial support.

## Poster 69

### The Number of Points on a Family of Calabi-Yau Threefolds

*Jonathan Root, S. M. Frechette*

*Department of Mathematics, College of the Holy Cross*

In 1984, Greene introduced the notion of hypergeometric functions over finite fields. Special values of these functions are of arithmetic significance, as they have been shown to be related to the number of points on algebraic varieties over finite fields and to Fourier coefficients of modular forms.

Let  $p$  be an odd prime, and let  $F$  denote the finite field with  $p$  elements. We establish a formula for the number of points in  $F$  on the one-parameter family of Calabi-Yau threefolds given by

$$X_\lambda : P(x, \lambda) = \prod_{i=1}^n (x_i^2 + 1) - 2^n \lambda \prod_{i=1}^n x_i = 0$$

in terms of finite-field hypergeometric functions. The formula depends on the residue class of  $p$  modulo 4.

We would like to thank the Richard B. Fisher Summer research grant.

## Poster 70

### Multiple Laser Excitation of Lithium for Atomic Spectroscopy

*Pat Collins '12 and Prof. Paul Oxley  
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Atoms in which one electron is excited to a high energy state can be used to study some of the most fundamental aspects of atomic physics. Exciting an atomic electron to a high energy state can be done by using multiple frequency-stabilized lasers. However, each laser can negatively affect the frequency stability of the other lasers, which in turn would prevent the atomic electron from being efficiently excited. We have made a theoretical analysis to discover the optimum conditions for frequency stabilizing three lasers for efficient excitation of Lithium atoms.

Guided by this theoretical analysis we have efficiently excited Lithium atoms using three frequency-stabilized diode lasers, and used a fourth laser to make a spectroscopic measurement of the excited Lithium atomic structure. Specifically, we have measured the fine structure interval of the  $10p$  atomic state, which has never before been measured. We are currently in the process of determining the uncertainty in our measurement, but it is likely that it will be lower than any other previous measurement of the fine structure of excited  $p$  states.

In a related project we have built a sophisticated mount for an optical filter that is to be placed inside a dye laser cavity. This project will be important in the future as the dye laser has many applications in future multiple-laser experiments of excited Lithium atoms.

We are very grateful to the Sherman Fairchild Foundation for its financial support and to the Holy Cross Summer Research Program for making our work possible.

## Poster 71

### The Effect of Ionic Strength on the Aggregation of Human- $\gamma$ C-Crystallin

*J. Trubiano and Dr. S. Petty  
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Cataracts affect 50% of people over the age of 65 and are the leading cause of blindness worldwide. Cataracts form due to the aggregation of crystallins, which are structural, soluble proteins found in the lens of the eye.

Infrared (IR) spectroscopy was used to study the aggregation of Human- $\gamma$ C-Crystallin. Band shifts in the Amide I region of IR spectra are primarily due to the C=O stretching vibration, and thus reveal information about the secondary structure of the protein. The kinetics and thermodynamics of H $\gamma$ C-Crys aggregation were observed in different buffers and in various concentrations of Sodium chloride. Aggregation was monitored by the conversion from soluble, globular  $\beta$ -sheet (IR band at  $1636\text{cm}^{-1}$ ) to a fibrous, amyloidogenic cross  $\beta$ - structure (IR band at  $1616\text{cm}^{-1}$ ).

The difference between the kinetics of aggregation in Citrate and Malate buffers showed that the buffering anion present in solution affects the rate of H $\gamma$ C-Crys aggregation, as well as the amount of aggregate present at equilibrium. The aggregation proceeds more rapidly in Citrate than Malate, but goes further to completion in Malate. However, when Sodium chloride was added to the Malate buffer, increasing the ionic strength until it was comparable with that of the Citrate buffer, the rates of aggregation were approximately equal. Consequently, our experimentation showed that it is an increase in the ionic strength of the buffer that causes the increase in the rate of Human- $\gamma$ C-Crystallin aggregation in the Citrate buffer, not the size or charge distribution of the anions.

The author acknowledges financial support from the Sherman Fairchild Foundation.

## Poster 72

### **Rapid Prediction of Pfizer and Competitor Product Stability Using ASAP Modeling**

*Anna Larkin*

*Pfizer Global Manufacturing Division, in the Analytical Science & Technology Department, Department of Physics, College of the Holy Cross*

The Accelerated Stability Assessment Program (ASAP) can provide the data needed to assess the stability of products being introduced to regions of the world with extreme heat and humidity. The goal of this project was to develop a rapid, systematic approach for using ASAP to predict long term stability of marketed Pfizer products. This tool will help predict susceptibility of products to Zone IV climatic conditions. Additionally, it can help with competitor evaluation for potential quality issues.

A very important aspect of the stability assessment was the protocol design. Sample handling proved to be crucial to the outcome of the project because samples needed to be placed into ovens for a certain time period before NIR and HPLC testing was performed. After pulling samples from the ovens set at specific temperatures and humidities, a very elaborate method was required to prepare the samples for analysis. Non-destructive NIR testing was performed prior to HPLC analysis, and finally the assay and purity of each product was calculated. Finally, a specific software allowed me to input these impurity values to predict long-term shelf life at various ambient temperatures and humidities by using the moisture-corrected Arrhenius equation. From these data, I was able to compare which products proved to be more stable than others.

It was deduced that temperature and humidity both significantly affect samples and their degradation rate. ASAP is a tool that can obtain significantly more information about the stability profile of a product that is not obtained through classical stability testing. Rather than testing products for months or years to discover the shelf life of a drug, ASAP can generate enough knowledge in only a matter of days or weeks to predict the stability rate at various storage conditions.