

COLLEGE OF THE HOLY CROSS

Fourteenth Annual
**Undergraduate
Summer
Research
Symposium**

September 7, 2007
Reception to Hogan Ballroom
2:00 – 4:00 pm



Sponsored by
The Office of the Science Coordinator

Members of the Holy Cross Community,

Welcome to the 2007 Undergraduate Summer Research Symposium. Now in its fourteenth 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 2007. It also provides an opportunity for students to witness the breadth of research possibilities on 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 Sarah Petty
Professor Bianca Sculimbrene
2007 USRS Organizing Committee*

We would like to recognize those whose contributions have made this research and this day possible, including:

The Richard B. Fisher Summer Research Grant
The Simeon J. Fortin Foundation
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Departments of Biology, Chemistry, Economics, Mathematics
and Computer Science, Physics, and Psychology

Posters

1. **The Rotating Baseball**, *Christopher Amante, Michael Knierim, Dennis Wirth, John Singleton, Matthew Koss and Timothy Roach, Department of Physics, College of the Holy Cross.*
2. **The Hydrogen Bonding of pQ32 Aggregated Huntingtin Protein**, *Alexandria Andrew and Dr. Sarah Petty, Department of Chemistry, College of the Holy Cross.*
3. **The Effect of Length Dependency in Huntington's Disease through the Expression of pQ43**, *Kelly Lyons and Dr. Sarah Petty, Department of Chemistry, College of the Holy Cross.*
4. **Structure-Function Analysis of APOBEC3G**, *Michelle Arata, Justin Rucci, Melissa Farrow and Ann Sheehy, Department of Biology, College of the Holy Cross.*
5. **Carbon Monoxide Poisoning and Capture Recapture**, *Ela Banerjee, Hartford Hospital.*
6. **Synthesis of Non-Natural Amino Acids**, *J. Beaudoin, R. Herrick, and B. Sculimbrene, Department of Chemistry, College of the Holy Cross.*
7. **Investigation of Metallo-enzymes and Proteins**, *Brittany W. Bergeron and Joshua R. Farrell, Department of Chemistry, College of the Holy Cross.*
8. **Development of a Universal Surface Coating for Microfluidic Chips**, *Stephen Crowley and Professor Kimberly Frederick, Department of Chemistry, College of the Holy Cross.*

9. **Investigation of nucleophile-catalyzed phosphorylation of alcohols using modified dibenzylchlorophosphates**, *Patrick Brady and Bianca Sculimbrene, Department of Chemistry, College of the Holy Cross.*
10. **Developing Diagnostic Imaging agents**, *William Cupelo and Prof. Herrick, Department of Chemistry, College of the Holy Cross.*
11. **Timing Analysis of the Neutron Star MS 1603.6+2600**, *Joseph Palmieri, Erica Tow and Tom Narita, Department of Physics, College of the Holy Cross.*
12. **A Forensic Economist's Challenge: Assessing Personal Injury and Wrongful Death Damages in Rhode Island**, *Professor David Schap, RA: Caitlin Street, Department of Economics, College of the Holy Cross.*
13. **Efforts Toward the Total Synthesis of Annonaceous Acetogenins by Tandem Olefin Metathesis**, *Brendan L. Mackinson, Stacy A. Powell and Kevin J. Quinn, Department of Chemistry, College of the Holy Cross.*
14. **Simulation of a Polarized Photon Beam Detector**, *S. Kondak and T. Narita, Department of Physics, College of the Holy Cross.*
15. **Laser Excitation of Lithium Atoms**, *James Daly, and Professor Paul Oxley, Department of Physics, College of the Holy Cross.*
16. **Apparatus for Creation of Ion Beam**, *Suzy Flaherty and Professor Paul Oxley, Department of Physics, College of the Holy Cross.*
17. **Quantitative Analysis of Illicit Drugs Using Raman Spectroscopy and Chemometrics**, *O. Fenton, D. Damiano and K. Frederick, Departments of Chemistry and Mathematics, College of the Holy Cross.*
18. **Utilizing Olefin Cross Metathesis for the Synthesis of Peptide Isosteres**, *Amelia Cianci and Professor Bianca Sculimbrene, Department of Chemistry, College of the Holy Cross.*
19. **Overexpression of IGF-1 disrupts migration of primordial germ cells in zebrafish**, *Matthew Curran and Antony Wood, Vincent Center for Reproductive Biology, Vincent Obstetrics and Gynecology Service, Massachusetts General Hospital, Harvard Medical School, Harvard Stem Cell Institute.*
20. **The Aggregation of Human- γ -C Crystallin**, *Amy Trojanowski and Dr. Sarah Petty, Department of Chemistry, College of the Holy Cross.*
21. **Investigation of Aggregation Pathways of Human Lens Gamma-C Crystallin Protein**, *Daniel Goulet¹, Sarah Petty¹, Yongting Wang², and Jonathan King², ¹Department of Chemistry, College of the Holy Cross, ²Department of Biology, Massachusetts Institute of Technology.*
22. **Isothermal Dendritic Growth Experiment Archive**, *Marina Vornle von Haagenfels, Matthew Koss, Department of Physics, College of the Holy Cross.*
23. **Patterns and variability in recruitment densities of scleractinian coral spat on Caribbean reef flats**, *A.C. Dempsey and A. Dikou, Ph.D, Center for Marine Resource Management, School for Field Studies.*
24. **Understanding Mechanisms of Flow in Polyelectrolyte Coated Capillaries**, *K.Swords and K. Frederick,*

Department of Chemistry, College of the Holy Cross.

25. **Protein Splicing of Three Inteins in *Pyrococcus Abyssii***, Adam Kerrigan, Taryn Powers, Deirdre Dorval, and Prof. Ken Mills, Department of Chemistry, College of the Holy Cross.
26. **Synthetic Studies on (+)-Boronolide**, John M. Curto and Kevin J. Quinn, Department of Chemistry, College of Holy Cross.
27. **Quality Control with Principal Components Analysis of Actigraph Data**, Nischal S. Nadig¹, Edward J. Soares^{2,3}, Amy Wolfson¹, ¹Department of Psychology, College of the Holy Cross, Worcester, MA, ²Department of Mathematics & Computer Science, College of the Holy Cross, Worcester, MA, ³Department of Radiology, University of Massachusetts Medical School, Worcester, MA.
28. **Protein Splicing in Glutamine Transaminase**, A. Schufreider and K. Mills, Department of Chemistry, College of the Holy Cross.
29. **Spectral Analysis of the Neutron Star MS 1603**, E. Tow, J. Palmieri and T. Narita, Department of Physics, College of the Holy Cross.
30. **Implicit Learning in Cotton-top Tamarins**, Lindsey Driscoll, Lauren Nutile, Katie O'Gorman, and Dr. Charles Locurto, Department of Psychology, College of the Holy Cross.
31. **Fishing with Worms: Using Genetics and Molecular Biology to Identify Interactors**, K. O'Brien, J. Claycomb, C. Trzepacz, and C. Mello, Department of Molecular Medicine, UMass Medical School.
32. **Diagnostic Imaging and the possibilities of Rhenium**, Joseph Lopez and Prof. Richard Herrick, Department of Chemistry, College of the Holy Cross.
33. **Investigating gbb expression and function in the red flour beetle**, B. Hendrickson and K. Ober, Department of Biology, College of the Holy Cross.
34. **Magnetic Properties of Commercial Stainless Steels**, Jennifer Goodell, and Professor Paul Oxley, Department of Physics, College of the Holy Cross.
35. **The Physics of Baseball: The Importance of Weather in Baseball**, J. Singleton, M. B. Koss, T. Roach, C. Amante, M. Knierim, and D. Wirth, Department of Physics, College of the Holy Cross.
36. **Using Algebraic Geometry in the Circular, Restricted Four-Body Problem**, Julianne Kulevich, Christopher Smith, and Prof. Gareth Roberts, Department of Math/CS, College of the Holy Cross.
37. **Instruments and Experiments For Determining Effects of Spin on a Baseball**, D. Wirth, M. Koss, T. Roach, M. Knierim, C. Amante, and J. Singleton, Department of Physics, College of the Holy Cross.
38. **Applications of Computational Commutative Algebra in Statistics**, Jocelyn Baker¹, Cidmarie Odiott², Alexander Simao, Jr.³, Dr. John B. Little³, ¹University of Arizona, ²University of Puerto Rico, ³Department of Mathematics and Computer Science College of the Holy Cross.
39. **Solution of Laplace's Equation in an Atom-Ion Collision Chamber**, J. Golde and J. Shertzer, Department of Physics, College of the Holy Cross.

40. **BEZ235 – A New Step in Targeted Chemotherapy**, Dr. W. Tap, M. Eckardt, A. Desai, K. Clarke, Dr. D. Slamon, Department of Medicine, Division of Hematology Oncology, University of California, Los Angeles Medical Center.
41. **Insights Into the Mechanism of DNA Replication in Tumor Viruses and its Regulation**, Ankur Patel (1), Paul Phelan (2), Anu Kumar (2), Stephanie Monie (2), Dr. Peter Bullock (2), (1) College of the Holy Cross, (2) Tufts University School of Medicine, Dept. of Biochemistry.
42. **Cell Rearrangement: Mathematical Modeling of Branching Morphogenesis and other Biological Phenomena**, S. Mattis¹, G. Pauley², E. Reilly³, 1.University of Notre Dame, 2.University of South Carolina, 3.College of the Holy Cross.
43. **Abstract: Replacing the Fragmin[®] Kjeldahl Method with the Leco TruSpec Elemental Determinator**, C. Govern and W. Workman, Scientific Laboratory Services-Biopharma Operations, Pfizer Global Manufacturing, Pfizer Inc.
44. **A Selective Estrogen Receptor β Agonist Fails to Replicate the Effects of Estrogen in a Spatial Working Memory Task**, Michael J. Dean, Shmuel J. Bitran¹, and Daniel Bitran, Department of Psychology, College of the Holy Cross and ¹Mesivta Yesodei Yeshurun.
45. **Protein splicing and extein activity of the Pyrococcus abyssi lon protease intein**, Melissa A. McGill, Kathryn M. O'Brien and Kenneth V. Mills, Department of Chemistry, College of the Holy Cross.
46. **Exploiting Thermo-responsive Guanosine Gels for Sample Pre-Concentration in Capillary Electrophoresis**, Ann Kotze and Kimberly Frederick, Department of Chemistry, College of the Holy Cross.
47. **Ferrocene Chemistry: non-isotopic tracers and β -sheet mimetics**, Laura Rose Condon and Richard S. Herrick, Department of Chemistry, College of the Holy Cross.
48. **Localization of circadian gene expression in the brain of *Xenopus tropicalis***, A. Casserly and C. Constance, Department of Biology, College of the Holy Cross.
49. **Uncovering Molecular Signatures of Rapid Evolutionary Radiation in the Phylogenies of Carabid Beetles**, T. N. Heider and K. A. Ober, Department of Biology, College of the Holy Cross.
50. **Recruitment of Proteins to Syndecan-4 Mediated Focal Adhesions**, M. McKenna, E. Morse, S. Sreepathi, M. Frigault, R. Bellin, Department of Biology, College of the Holy Cross.
51. **Socioeconomic Status as a Potential Factor in Determining Sleep Patterns and Well-being**, Stephanie Apollon¹, Andrea C. Azuaje¹, Nischal S. Nadig¹, Michaela Sparling¹, Amy Wolfson¹, ¹Department of Psychology, College of the Holy Cross, Worcester, MA.
52. **Individual Differences in Regret and Maximization Moderate the Endowment Effect**, Tara Richards and Mark Hallahan, Department of Psychology, College of the Holy Cross.
53. **Exploration of the Triassic Chinle Formation of Southern Utah**, S. Moss and A. Moczula, Department of Biology, College of the Holy Cross.

54. **Sequential Mannich condensations to prepare ligands with oxygen, nitrogen donors with systematic variations in steric and electronic properties to model the active site of protocatechuate 3,4-dioxygenase, E. Yoon and Prof. J. Farrell, Department of Chemistry, College of the Holy Cross.**
55. **The Mathematics behind the Schroedinger Equation, S. Walsh and A. Hwang, Department of Mathematics, College of the Holy Cross.**
56. **The Influence of an Intein on the Activity of the Methanococcus jannaschii UDP-Glucose Dehydrogenase, Jennifer Winslow, Matthew Drago, and Kenneth Mills, Department of Chemistry, College of the Holy Cross.**
57. **Aldosterone Protects Kidney Cells from Ouabain Inhibition of Gap-junction Communication, W.T. Cavanaugh, T.D. D'Aquila, and M.R. Sallah, Department of Biology, College of the Holy Cross.**
58. **Novel Electrochemically Grown Materials, Gil Gomez and Josh Farrell, Department of Chemistry, College of the Holy Cross.**
59. **Interactions between Chemical Treatments in Yeast, G. Hoffmann and J. Tartaglione, Department of Biology, College of the Holy Cross.**

Poster 1

The Rotating Baseball

*Christopher Amante, Michael Knierim, Dennis Wirth,
John Singleton, Matthew Koss and Timothy Roach
Department of Physics, College of the Holy Cross*

The lift force that results from a rotating baseball in flight can be attributed to the Magnus Effect. Due to the rotation of the ball, the velocity is enhanced and the pressure is decreased on the side where its rotation is in the same direction as the wind stream in which it is traveling. On the opposite side of the ball traveling against the direction of the wind the velocity is slower and pressure is greater. It is this difference in velocity and pressure that causes the Magnus Effect and creates a lift force directed at right angles to the direction of the air velocity and the axis of rotation.

The rotation rate is critical in understanding the forces on the baseball in flight. An imperative question that we hope to answer in our research is if the rotation rate is a function of time. It is not well understood and many of the leading researchers in baseball aerodynamics widely disagree on the rotation rate decay over the flight of a hit baseball. We hope to collect enough raw data to determine how the rotation rate actually decays. In order to do this we developed a method of imparting spin on the baseball using an electric drill. Also, we have constructed a wind tunnel which will be able to simulate a baseball traveling through the air. More specifically, we will use a 200 frames per second camera to calculate the change of the rotation rate. By examining successive camera shots of the baseball in motion we can record the pixel position of a dot on the ball. From this we can determine the rotation rate in each frame and calculate the change over time.

We thank the Fisher Fellowship for financial support as well as Richard Miller, Jesse Anderson and Diane Jepson for their assistance with the apparatus.

Poster 2

The Hydrogen Bonding of pQ32 Aggregated Huntingtin Protein

*Alexandria Andrew and Dr. Sarah Petty
Department of Chemistry, College of the Holy Cross*

Huntington's disease (HD) is a neurodegenerative disorder that causes uncontrollable movements, loss of intellectual faculties, and emotional disturbance.¹ It is a familial disease, affecting 8 in 100,000 people. HD is caused by a trinucleotide repeat expansion in the Huntingtin gene, which results in an abnormally long stretch of glutamine residues at the N terminus of the protein. Aggregates of the Huntingtin protein, which are formed when the glutamine tract exceeds the pathogenic threshold, have been found in neuronal inclusions upon post-mortem examination of the brains of HD patients.

The side chain of glutamine contains an amide group and a carboxyl group, therefore hydrogen bonds which mimic those between backbone groups responsible for stabilization of protein secondary structure, can also occur between side chains. This additional hydrogen bonding potential is one theory as to the stability of the aggregates.² Using FT-IR Spectroscopy, aggregates containing 32 glutamine residues (pQ32) were analyzed to determine the hydrogen bonding potential of the pQ. In order to make accurate band assignments, individual glutamine and alanine amino acids in D₂O and dimethyl sulfoxide were also studied. Comparison of the peaks allows more thorough analysis of the spectra of the aggregates.

The author acknowledges financial support from the Becton Dickinson Summer Research Fellowship Fund.

¹Bates, Gillian P. *Nature* (2005), **6**: 766-773.

²Perutz, Max F *et al.* *Biochemistry* (1994). **91**: 5355-5358.

The Effect of Length Dependency in Huntington's Disease through the Expression of pQ43

Kelly Lyons and Dr. Sarah Petty

Department of Chemistry, College of the Holy Cross

Huntington's Disease is a hereditary neurodegenerative condition resulting in a loss of decisive abilities and abnormal physical movements. An expansion of polyglutamine (pQ) at the N-terminus of the Huntingtin protein and the subsequent aggregation of these repeats directly leads to onset of the disease. Previous research has shown the age of onset of symptoms correlates to the number of pQ repeats;¹ the typical pathogenic threshold length of pQ is 35 residues.

The goal of this research is to determine the relationship between protein structure and length of the pQ. A protein containing 43 glutamines (pQ43) fused to a small ubiquitin modifying protein (SUMO) was expressed in bacterial cells; the SUMO group improves expression and prevents pQ aggregation by mediating correct folding. The protein was then purified using a Ni-NTA column; the isolation of pure SUMO-pQ43 was confirmed using SDS/PAGE electrophoresis. Different protocols were investigated in order to efficiently cleave the SUMO group from the pQ43 of interest. The resultant protein was concentrated, resulting in the aggregation of pQ43.

Infrared Spectroscopy was used to analyze the structure of SUMO-pQ43 and pQ43 aggregates. Bands in the amide I region of the spectra show evidence of helical and disordered SUMO-pQ43 but fibrous β -sheets in the aggregated pQ43 sample. The spectra were compared with pQ32, to study the length dependence of structure.

The author acknowledges the Fisher Fund for financial support of the project.

1. Nagai, Yoshitaka. *et al.* *Nature Structural and Molecular Biology* 14 (2007): 332-340.

Structure-Function Analysis of APOBEC3G

Michelle Arata, Justin Rucci, Melissa Farrow and Ann Sheehy
Department of Biology, College of the Holy Cross

The human cytidine deaminase APOBEC3G (apolipoprotein B mRNA editing enzymatic catalytic polypeptide 3G; hA3G) functions as a cellular innate immune response against viruses. Particularly striking is a well-characterized anti-HIV activity. However, in a viral counter-response, HIV-1 expresses Vif, (viral infectivity factor) a protein which effectively counteracts the anti-viral activity of hA3G. To provide a more comprehensive understanding of the anti-viral function of hA3G and to further characterize the precise interplay between hA3G and Vif, an unbiased alanine-scan mutagenesis of the full-length hA3G protein (384 amino acids) was undertaken, resulting in the synthesis of a catalog of 130 mutant hA3G proteins. These 130 mutants were initially evaluated for antiviral function in an infectivity assay. The results of this analysis identified 27 mutants that while stably expressed, no longer suppress an HIV-1 challenge. In an effort to investigate this loss of activity, the subset of mutants was characterized for their ability to enzymatically function as a cytidine deaminase. An *E. coli*-based assay was used to determine mutagenic capacity. Of the 27 mutants, 23 were screened in the assay which showed that 14 of them retain mutagenic capacity. The remaining 4 mutants will be screened and then further analysis of all of the mutants will begin.

We gratefully acknowledge the Simeon Fortin Fellowship Fund for financial support.

Poster 5

Carbon Monoxide Poisoning and Capture Recapture

Ela Banerjee
Hartford Hospital

Carbon Monoxide (CO) is a colorless, odorless, poisonous gas and is the product of incomplete combustion of fuels. Some common sources of CO in the home and workplace are furnaces, gas heaters, generators, and cars. From 2000-2005, 1350 cases of CO poisonings were reported in Connecticut. These cases ranged from mild to severe poisonings.

Capture Recapture Analysis is a method used in wildlife biology to estimate population numbers of a species using a mathematical model with certain assumptions. This analysis method helps create an accurate population based estimate of CO poisonings in Connecticut. The Department of Health can use this information to create better educational programs and more effective policy regarding CO in order to prevent accidental exposures to CO.

My role in the research was to collect data from 2000-2006 from three different databases using the Capture Recapture Analysis. These databases were the Connecticut Poison Control Center, the Department of Health, and the Medical Examiner. Using this data, I created a complete database with specific information regarding all the CO poisoning cases in Connecticut. After comparing the number of exposure cases between Connecticut and the US, we saw that Capture Recapture Analysis is a valid method of estimating the population exposed to CO.

I would like to thank my mentors, Dr. McKay and Dr. Delgado for helping me with this project.

I would like to thank The Hartford Hospital Division of Emergency Medicine for financial support.

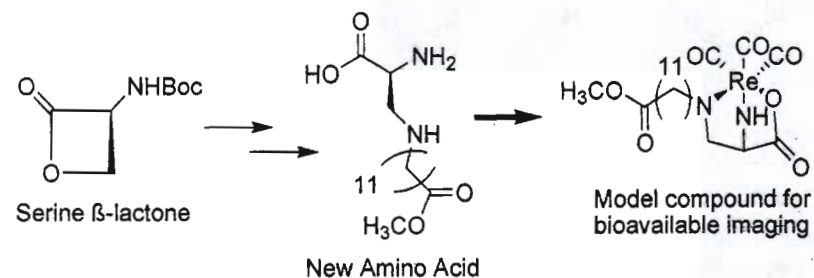
Poster 6

Synthesis of Non-Natural Amino Acids

J. Beaudoin, R. Herrick, and B. Sculimbrene,
Department of Chemistry, College of the Holy Cross

The synthesis of non-natural amino acids has been extensively studied in order to develop a facile and general synthetic method, starting from the natural amino acid, Serine. In one step, serine was converted to the serine β -lactone, a versatile synthetic intermediate. The research focused on attaching a nucleophile to the β -lactone ring through attack at the β -carbon instead of the carbonyl, which would be confirmed spectroscopically. The first nucleophile tested was 12-aminododecanoic acid methyl-ester, which was successfully reacted with the serine β -lactone to generate the new amino acid after deprotection.

In collaboration with the Herrick group the amino acid formed was tested as a tridentate ligand for rhenium metal. Once formed, this metal ligand complex can be used as a model compound for bio-available imaging.



We thank the Fischer Foundation for financial support.

Poster 7

Investigation of Metallo-enzymes and Proteins

Brittany W. Bergeron and Joshua R. Farrell
Department of Chemistry, College of the Holy Cross

The goal of our research is to model the structure and reactivity of metallo-enzymes and proteins. We are interested in synthesizing a small molecule model for the enzyme liver alcohol dehydrogenase, which is known to catalyze the oxidation of an alcohol to a ketone or aldehyde. In order to model the reactivity and structure of such a metallo-enzyme we have synthesized a library of ligands containing O, N, and S heteroatoms, examples of which are shown in Figures 1 and 2. Our synthetic schemes and other results will be presented. We acknowledge the Becton Dickinson Fund for financial Support

Figure 1.

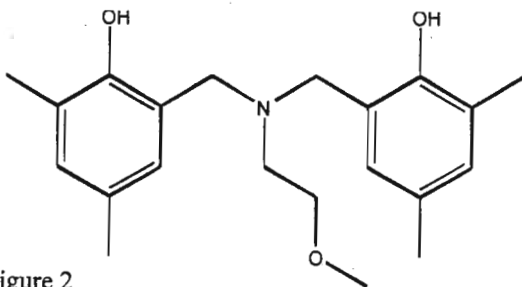
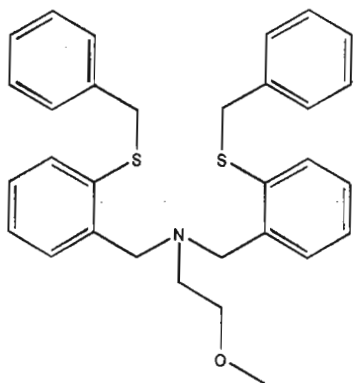


Figure 2



Poster 8

Development of a Universal Surface Coating for Microfluidic Chips

Stephen Crowley and Professor Kimberly Frederick
Department of Chemistry, College of the Holy Cross

Microfluidics is revolutionizing analytical methods by making it possible to use less sample, decrease run time, and automate sample methods. While there are various substrate materials that can be used to create microfluidic chips, each has its own set of chemical and mechanical properties. This means that chips made out of different materials will produce different results. In order to avoid this problem, a common coating for these chips is necessary. This will allow for a standard, reproducible electroosmotic flow (EOF) regardless of the substrate material.

Poly(methylmethacrylate) (PMMA), cyclic olefin copolymer (COC), poly(dimethylsiloxane) (PDMS), and glass were used to fabricate the microfluidic chips which were then modified by a semi-permanent coating method. The channels were coated with polyelectrolyte multilayers consisting of alternating cationic layers of poly (diallyldimethylammonium) chloride (PDADMAC) and anionic layers of poly(sodium-4-styrene-sulfonate) (PSS). For ease, the surface layer was always PDADMAC resulting in a positive surface charge induced on the channels themselves.

The flow was measured as a function of number of coating layers. While there was an initial effect from the microchip substrate, after nine layers the EOF was constant and determined primarily by the coating chemistry. The effect of chip material and chip-sealing methods were also evaluated. All tested chips showed relatively the same EOF on the PDADMAC/PSS-coated channels as the number of layers was increased. Therefore, it seems feasible that a universal coating of polymer microchips is within reach.

The Camille and Henry Dreyfus Foundation, Research Corporation, National Science Foundation and Fischer Summer Fellowship program provided support for this research.

Poster 11

Timing Analysis of the Neutron Star MS 1603.6+2600

Joseph Palmieri, Erica Tow and Tom Narita

Department of Physics, College of the Holy Cross

Using the Rossi X-Ray Timing Experiment (RXTE) satellite, we sought to confirm the orbital period of the neutron star MS 1603 as well as find the rotational and long term periods.

We studied the photon emission from MS 1603 over a five day period in the X-Ray energy band. A folding analysis of the data suggest a 109 minute orbital period with an uncertainty of 2 minutes. We also analyzed the data for rotational and long term periodicities using a Fast Fourier Transform. We could not draw any conclusive evidence. The data, however, contained several interesting features that will require further analysis.

We thank the Massachusetts Space Grant and Holy Cross Fisher Fellowship for financial support.

Poster 12

**A Forensic Economist's Challenge:
Assessing Personal Injury and Wrongful Death Damages in
Rhode Island**

Professor David Schap

RA: Caitlin Street

Department of Economics, College of the Holy Cross

Forensic economics is the practice of applying economic theories and methods to determine the amount of pecuniary damages in cases of personal injury, wrongful death, wrongful termination, or lost business profits. Forensic economists are often called to testify in court and their assessment of damages may play an important role in determining the amount of the settlement. Rules and practices for assessing damages differ across states. Therefore, a practicing forensic economist must be careful to derive his damage calculations based on the relevant case law and legislative codes of state in which the accident occurred. This research, focusing entirely on Rhode Island, contributes to an existing series of articles which detail the case law and legislative rules in various states. This study hopes to further inform and enlighten practicing forensic economists to the precedents established in Rhode Island for assessing monetary damages in personal injury and wrongful death law suits.

This research was supported by a grant from the May and Stanley Smith Charitable Trust .

Efforts Toward the Total Synthesis of Annonaceous Acetogenins by Tandem Olefin Metathesis

Brendan L. Mackinson, Stacy A. Powell and Kevin J. Quinn
Department of Chemistry, College of the Holy Cross

The Annonaceous acetogenins are a large family of natural products possessing a wide range of biological activities including potent antitumor activity. Typical acetogenin cores contain one or two tetrahydrofuran (THF) rings. We will describe our progress toward the syntheses of two members of acetogenin family, murisolin A and asimicin. In both cases, we make use of tandem olefin metathesis reactions to significantly simplify and shorten the synthetic routes.

We thank the Pfizer/CBIA Research Fellowship Program and the American Chemical Society Petroleum Research Fund for financial support.



Signals Against Various Simulation of a Polarized Photon Detector

S. Kondak and T. Narita

Cross Department of Physics, College of the Holy

carlo -custom C++ data structures in the monte Using simulator GEANT4, we built a working model of a polarized photon detector called PHENEX. Once PHENEX was fully constructed, we began simulating how the detector would react to photons and protons of various energies. Using this data, were were able to determine how effective PHENEX was at measuring energy deposits from both desirable signals and undesirable .backgrounds in space

This work was supported in part by NASA.

Laser Excitation of Lithium Atoms*James Daly, and Professor Paul Oxley**Department of Physics, College of the Holy Cross*

We have constructed and tested a Lithium oven and a diode laser system. Lithium atoms from the oven will be laser excited to high principal quantum number by a combination of three lasers. In the future we will study charge transfer (CT) collisions between excited Lithium atoms and ions. Understanding CT collisions is important for determining the physical properties of fusion, astrophysical, and other types of plasmas.

Our oven consists of a carefully designed stainless steel vessel containing Lithium and mounted inside a vacuum system. The oven is heated by three high temperature heaters and must reach 500°C for a sufficiently intense beam of Lithium vapor to be emitted from the oven. In our tests we reach a maximum oven temperature above 500°C and have been able to produce a beam of Lithium atoms for many hundreds of hours without replenishing the oven with Lithium. The Lithium beam is collimated to about a 10 degree spread by a 5mm long tube at the exit of the oven. We have solved an earlier problem of Lithium plugging the exit tube by keeping the tube at a higher temperature than the body of the oven.

The laser used in the first excitation step of Lithium is a diode laser operating at 671nm. Commercial electronics control the laser diode current and its temperature. We have tested the properties of the laser and use it to excite atoms from the Lithium oven from the 2S ground state to the excited 2P states. We can detect these excitations by monitoring the fluorescence emitted when the Lithium atom returns to the ground state. We have excited Lithium from both hyperfine levels present in the 2S state to all fine structure levels present in the 2P state. This is done for both naturally occurring isotopes of Lithium.

We wish to thank Dick Miller for his machining expertise, the Research Corporation and Holy Cross College for financial

Apparatus for Creation of Ion Beam*Suzy Flaherty and Professor Paul Oxley**Department of Physics, College of the Holy Cross*

We have assembled an ion gun and vacuum system that will be used in conjunction with an apparatus for laser exciting lithium atoms. In the future a beam of ions from the gun will be collided with the lithium atoms in order to study charge transfer collisions between the excited lithium atoms and the ions. Understanding charge transfer collisions is important for determining the physical properties of fusion, astrophysical, and other types of plasmas.

The ion gun is a complex piece of equipment designed to create, accelerate, and focus a beam of ions. In addition the gun can select ions with a particular velocity using a device called a velocity filter. The ions are created by electron impact ionization. They are accelerated and focused by routing them across a series of plates of varying high voltage, while the velocity filter employs both electric and magnetic fields to select the desired velocity. The gun is controlled by a six feet tall electronics tower which houses the master controls and power supplies that support the various parts of the ion gun and the required cooling and vacuum systems.

Our vacuum system is assembled from standard vacuum parts and from parts which we have designed and were built at Holy Cross. The vacuum environment is maintained by a diffusion pump which is simple to use, can reach very low pressures, and is inexpensive. It is used in conjunction with a cold water trap to keep the vacuum system free from contamination by oil used in the diffusion pump. We plan to make initial tests of the ion gun using nitrogen ions.

We wish to thank the Research Corporation and the College of the Holy Cross for financial support, and Dick Miller for machining expertise.

Quantitative Analysis of Illicit Drugs Using Raman Spectroscopy and Chemometrics

O. Fenton, D. Damiano and K. Frederick

Departments of Chemistry and Mathematics, College of the Holy Cross

Raman spectroscopy was used to develop a rapid and non-invasive means of classifying and quantifying complex drug mixtures. Drug dealers often dilute white powder drugs such as cocaine with other non-pharmacologically active powders such as dry milk to boost profits. This poses a challenge to law enforcement because it leaves the identity and mass of the illegal drug in the sample in question. This research focuses first on identifying a drug surrogate in a complex mixture and second on determining the mass percent of the drug surrogate in the sample. Two training sets were created, the first consisting of 146 samples containing 1 drug surrogate and 1, 2 or 3 cutting agents and the second consisting of 40 samples containing a single drug surrogate and 1, 2, or 3 cutting agents. The drug surrogates in the first training set were benzocaine, norephedrine, lidocaine, and isoxsuprine, and the cutting agents in both sets were corn starch, baking soda and baking powder. To increase reproducibility, the percent by mass of the drug surrogates in each sample was greater than 20% and 5 spectra of each sample were averaged. Both calibration sets underwent various forms of preprocessing, including truncation, normalizing, differentiation and autoscaling. Principal components analysis was used on the first calibration set and the resulting model successfully classified the four drug surrogates. Partial Least Squares Regression was used on the second training set to develop a chemometric model, and the resulting model was used to predict the drug concentration of benzocaine in their respective samples.

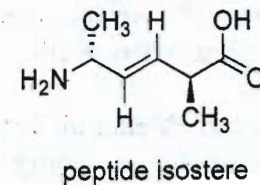
The authors would like to thank the College of the Holy Cross and the Fisher Summer fellowship program.

Utilizing Olefin Cross Metathesis for the Synthesis of Peptide Isosteres

Amelia Cianci and Professor Bianca Sculimbrenne
Department of Chemistry, College of the Holy Cross

An isostere is a compound that possesses geometrical similarities to the compound it is modeled from but differs electronically, allowing the electronic component to be studied. A common isostere for peptides is to replace the amide bond with a trans-olefin. Our initial isostere target is D-Ala-D-Ala, the peptide sequence found to interact with Vancomycin on bacterial cell walls. By studying how Vancomycin recognizes the peptide isostere versus the natural system, one can ascertain the importance of the amide bond for this interaction.

The key step in the synthesis of the peptide isostere involved utilizing olefin cross metathesis to generate the trans-olefin. Both of the termini necessary for the metathesis step have been synthesized and studies are ongoing to conduct the metathesis reaction.



The author acknowledges a Becton Dickinson Fellowship for financial support.

Overexpression of IGF-1 disrupts migration of primordial germ cells in zebrafish

Matthew Curran and Antony Wood

Vincent Center for Reproductive Biology, Vincent Obstetrics and Gynecology Service, Massachusetts General Hospital, Harvard Medical School, Harvard Stem Cell Institute

Cell-specific suppression of IGF signaling in zebrafish primordial germ cells (PGC) results in aberrant migration, suggesting that IGF ligands may play a role in guiding germ cell migration, as has been observed in other migratory cell types. We hypothesized that PGC migration is sensitive to endogenous levels of IGF ligand expression. To test this hypothesis, we designed an expression construct encoding IGF-1 fused to the 3' untranslated region of the zebrafish *nanos1* gene (*nos1*), which restricts translation of the mRNA to germline-committed cells. Our construct thus provides a means to overexpress IGF-1 in PGCs, thereby obscuring their ability to detect endogenous IGF ligand gradients. In support of our hypothesis, overexpression of IGF-1:*nos1* resulted in significant mismigration of PGCs, without affecting total PGC number. These data support our earlier work indicating that IGF signaling plays a role in guiding germ cell migration in zebrafish.

We thank the Vincent Memorial Research Funds and the Harvard Stem Cell Institute for providing financial support for this work.

The Aggregation of Human- γ C Crystallin

Amy Trojanowski and Dr. Sarah Petty

Department of Chemistry, College of the Holy Cross

Cataracts is an eye disease which affects 50% of individuals over the age of sixty-five.¹ It involves a physical clouding of the lens of the eye that interferes with the passage of light to the retina. Lens opaqueness is attributed to the formation of aggregates of Crystallin proteins composing the lens, including γ C- and γ D- Crystallin.²

By varying concentration, pH and temperature we determined environments that promote Human- γ C-Crystallin aggregation using FT-IR Spectroscopy. Analysis shows that an increase in temperature causes an increase in the amount of aggregates. If concentration is increased, aggregates form at lower temperatures. Lowering the pH leads to aggregate formation at lower temperatures whereas increasing the pH delays aggregate formation to higher temperatures; at pH 7 no aggregates are observed at temperatures up to 65°C.

Kinetic experiments were also conducted, with the ultimate goal of elucidating the mechanism of aggregation. Aggregation proceeds more rapidly at higher temperatures and concentrations, although preliminary analysis suggests the final amount of aggregate formed is independent of the concentration. Seeding experiments provide further insight into Crystallin aggregation: seeds of aggregated Human- γ C-Crystallin added to the native protein at 37°C promoted aggregation that was not seen in unseeded experiments at this temperature. These seeds act as templates for the misfolding and aggregation of native Human- γ C-Crystallin in the sample.

The author acknowledges financial support from the Simeon J. Fortin Charitable Trust.

1. Kosinski-Collins, M.S. and King, J. *Prot. Sci.* (2003),**12**:480-490.

2. Pande, Ajay *et al.* *PNAS* (2001), **98**:6116-6120.

Investigation of Aggregation Pathways of Human Lens Gamma-C Crystallin Protein

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Cataract is the opacification of the eye lens and is the leading cause of blindness worldwide. It is estimated that one in six Americans over the age of 40 has cataract (National Eye Institute, 2002). Aggregation of lens proteins has been identified as one of the causes for lens opacification. Proteins in the lens are susceptible to aggregation due to covalent damage from UV radiation and oxidative stress through the process of aging. Human Gamma-C Crystallin (H γ C-Crys) is a member of the γ -crystallin family of lens proteins. Aggregation of H γ C-Crys was studied by characterizing conformational changes in native and partially unfolded states using fluorescence spectroscopy. It was determined that partially unfolded intermediates were generated at pH3 in 50mM Acetate buffer, but similar species were only observed at pH2 in 50mM Citrate buffer. Fluorescence intensity ratios were monitored as a function of time, which elucidated the presence of different partially unfolded states in each of the different buffers. Lag times observed by fluorescence spectroscopy were well correlated with those measured by solution turbidity. Aggregation kinetics were determined by solution turbidity, which demonstrated that kinetics are affected by the ionic strength of the buffer solution. These results suggest that many different protein aggregation morphologies are accessible to the native state via a network of partially unfolded intermediates. Fluctuations in the protein macro-environment can induce measurable conformational changes in intermediate structures and influence aggregation pathways and morphologies. This research was made possible by NIH Grant GM17980 and NEI Grant EY015834 to Jonathan King.

Isothermal Dendritic Growth Experiment Archive

Marina Vornle von Haagenfels, Matthew Koss
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Dendrites are branch-like crystals formed most commonly by solidifying metals and alloys. The branch-like formation is caused when materials freeze unstably. Dendrites are how metals are formed naturally. The characteristics of size, shape, and how the side branches of the dendrites interact with each other strongly influence its mechanical, electrical, thermal, and chemical, properties. The key feature of the Isothermal Dendritic Growth Experiment (IDGE) is that dendritic growth data was obtained don orbit to reduce or eliminate energy transfer via natural (gravity driven) convection. Natural convection affects dendritic growth at lower super cooling (how far below the melting temperature the material is before it begins to solidify.. On earth the gravity driven convection energy flow disturbs the data and one cannot tell if it is the convection energy flow or an inherent phenomena that create the side branch or controls the growth. On orbit in a continual state of free-fall convection is eliminated or so reduced that dendritic growth data is easier and more productive to study then on earth. This data is critically important to archive because it is bench mark data to confirm/deny/judge the theories that have been already postulated to see if they are correct. Even proving that they are wrong is useful to us. The cost of this experiment, and it requirement to be on orbit, makes it almost impossible to be repeated. Archiving all the data makes the information accessible to the other scientists so they can draw their own conclusions from the data or make entirely new inferences.

We thank the Massachusetts Space Grant Consortium and the Fisher Summer Research Funds for support.

Patterns and variability in recruitment densities of scleractinian coral spat on Caribbean reef flats

A.C. Dempsey and A. Dikou, Ph.D

Center for Marine Resource Management, School for Field Studies

Stony corals, also known as scleractinian corals, are considered the reef-building corals; they appear in a range of shapes and sizes to form the basis of colonies. Both the recruitment and early histories of corals are important indicators of their responses to natural and anthropogenic disturbances; these disturbances may affect individuals, by imparting growth rates, or communities, by reducing the percent of live coral cover.

Establishing baseline data of coral recruitment and regenerative data is pivotal to understanding the fitness of the reef. The aims of this study are to answer the following question: (1) What is the coral recruitment density on seven different reefs? (2) Does mean coral recruitment density differ among reefs? (3) Are there significant differences between coral recruitment densities on seven different reef flat sites in conjunction with seasonal variation? (4) What is the percent size frequency distribution of coral recruits in regards to seasonal changes? This research project will census coral spat more than 2 mm to 20mm at depths between 9 and 12 meters on seven reef flats using SCUBA. One Way ANOVA revealed that the recruitment density of hard corals was found to have no significant difference between the seven different reef flat sites (**p-value = 0.072, f-value = 0.129**). The differences in coral density between the fall and winter seasons were seen as being significantly different through applying a One-Way ANOVA statistical test (**p-value= -4.662×10^{-15} , f-value=64.4617**).

There is a significantly higher density of coral recorded in the fall than in the winter. The size-frequency distributions show patterns in specific size classes between the fall and winter. Given these results the data show that the differences in recruitment density on the reef flat sites between seasons may help determine the spawning seasons that result from the sexual reproduction of coral.

We would like to thank the Department of Environment Coastal Research Center on South Caicos, Turks and Caicos Islands.

Understanding Mechanisms of Flow in Polyelectrolyte Coated Capillaries

K.Swords and K. Frederick

Department of Chemistry, College of the Holy Cross

In today's society there is a growing demand for smaller and faster analytical separations in order to increase precision and save money in both the pharmaceutical and industrial fields. Polyelectrolyte multilayers (PEMs) have been established as a successful and useful broadly-applied coating in microfluidics and in capillary electrophoresis, as well as many other applications in nanotechnology and medicine. PEMs are created based on the electrostatic attraction between oppositely charged layers of polycations and polyanions which are deposited using the layer-by-layer (LBL) or a successive rinsing method. Several theories have been published to explain how solutions flow through or over the PEM coated layers. This work details our efforts to elucidate whether the flow is established in solution above the PEMs or inside the materials. By studying the response of PEM coated capillaries to changing solution conditions, we are able to detect the location of the double layer. By increasing the number of layers, which therefore increases the thickness of the coating, we are able to determine if the flow is affected by the thickness of PEMs. In particular, we have used PEMs composed of strong cation/strong anion, weak cation/strong anion and strong cation/weak anion. We have studied the effect of changing buffer pH on the observed flow (EOF) using a real-time method based on periodic photobleaching of a neutral fluorophore.

This research was supported by the Research Corporation, the National Science Foundation and the Fisher Fund.

Poster 25

Protein Splicing of Three Inteins in *Pyrococcus Abyssii*

Adam Kerrigan, Taryn Powers, Deirdre Dorval, and Prof. Ken Mills

Department of Chemistry, College of the Holy Cross

Inteins are polypeptide sequences that interrupt the functional domains of proteins, called exteins. Inteins catalyze their own excision out of proteins to result in a sequence of joined exteins. I am studying three inteins found in *Pyrococcus abyssii*, an extreme thermophile. These inteins interrupt Ribonucleotide Reductase, and are referred to as RIR 1, 2, & 3. Our goal is to examine the necessary requirements of the polypeptide sequence to result in successful splicing of the inteins.

Previous work in the lab has resulted in the isolation and expression of the inteins in *E. coli*. To aid expression in vivo, mutations were made in the homing endonuclease gene (HE) to render it ineffective. Mutations were then made using site-directed mutagenesis at each intein insertion site and internal sites important to protein splicing. At these sites, the amino acids naturally present in the inteins were mutated to the naturally occurring amino acids from the other two RIR inteins.

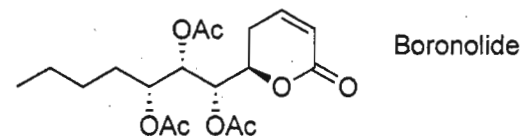
At present, I am overexpressing these mutated proteins and analyzing the effects the mutations have on splicing. The parent strains with only the HE mutation of all three inteins splice in vivo as shown by SDS-PAGE and Western blotting. The RIR 1HE and RIR 2HE mutations appear to have spliced in vivo, as confirmed by Western Blotting. I am now working on optimizing the purification conditions for our desired proteins before expressing the RIR 3HE mutations. If successful purification methods cannot be found, future work may entail genetically altering some of the affinity tags used for purification.

We would like to thank the National Science Foundation for their financial support.

Poster 26

Synthetic Studies on (+)-Boronolide

John M. Curto and Kevin J. Quinn
Department of Chemistry, College of Holy Cross.



Boronolide is a natural product possessing a six-membered, α,β -unsaturated lactone, a structural component of many biologically active natural products. We will describe an efficient approach to the synthesis of boronolide in which asymmetry is introduced by Sharpless asymmetric oxidation reactions. The key step in this approach is a tandem ring-closing/cross metathesis/alkene isomerization in which both lactone formation and side chain appendage are achieved. Financial support by the Pfizer Summer Undergraduate Research Fellowship Program is gratefully acknowledged.

Quality Control with Principal Components Analysis of Actigraph Data

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The actigraph, an electronic device that measures frequency-of-movement (FOM) over an allocated epoch, has generally been used as a tool to estimate sleep and wake times/durations in clinical and research settings. When collecting data, however, many errors have generally been attributed to the participant rather than the actual actigraph. Therefore, this pilot study assessed inter-actigraph reliability. Multiple trials were run to develop a statistical methodology for assessing reliably across the 41 actigraphs used in our lab.

All actigraphs were placed in a bubble-wrap bag, and taped to the back of a swivel chair to provide a 2-day period of movement that modeled the daily activity of a subject. The actigraphs were set to an epoch length of 1 minute over which the device measured FOM within each epoch. The FOM was our dependent measure, while our independent measure was the minute epoch intervals. Using principle components analysis, we first reduced the dimensionality of the data and then applied a multivariate *F*-test to evaluate statistically each actigraph when compared to a 95% confidence interval for the distribution. One of the 41 actigraphs was found to be statistically different when compared to the overall pool. This method of quality control can now be applied to the set of actigraphs before a full/real data collection period.

We thank the National Institute of Child Health and Human Development Grant for financial support.

Protein Splicing in Glutamine Transaminase

A. Schufreider and K. Mills

Department of Chemistry, College of the Holy Cross

Protein splicing is the process by which intervening polypeptide sequences, known as inteins, catalyze their excision from a polypeptide chain. Inteins are adjoined on both sides by exteins, so when the intein is cut out the exteins bind through ligation to form a functional polypeptide chain. The enzyme glutamine transaminase, which catalyses the first step in the hexosamine pathway, has an intein in it. In order to study protein splicing in this enzyme, we will make three forms of it. The first is the whole enzyme interrupted by the intein. The intein is flanked by exteins that might influence splicing. The second form is the enzyme lacking an intein, which we will use to study the function of the protein. The third form is the intein flanked with affinity domains in order to study splicing in a simpler context. Thus far we have amplified two selected fragments of *Methanocaldococcus jannaschii* genomic DNA through PCR that will serve as inserts into either a pET28-b(+) vector or a modified pMal-c2x expression vector. This fall we plan to ligate each set of vector and insert to form genes that will express the desired proteins. Finally, I would like to acknowledge the National Science Foundation for their financial support.

Spectral Analysis of the Neutron Star MS 1603*E. Tow, J. Palmieri and T. Narita**Department of Physics, College of the Holy Cross*

We used data from the Rossi X-Ray Timing Explorer (RXTE) satellite to obtain new information about MS 1603. The proportional counters on the RXTE satellite can detect photons between 2 keV and 60 keV, which gives a clearer view of high energy photons that is not possible to see with other satellites. We used the data to form an energy spectrum over the course of five days from July 11 to July 15, 2004. We fit the spectrum with different emission models, which gave us information about the neutron star. From these models we were able to get a better idea of the geometry and brightness of MS 1603.

In addition, we divided the spectrum into high and low intensity photons based on the peaks and troughs present in the folded lightcurve. We fit each of these spectra with different models to come to a conclusion about the affects of rim shading by the accretion disk. We also made a color-color diagram that included the results of observations of MS 1603 by other satellites in order to track the changes in flux and spectral shape over time. The color-color diagram gave some insight into the classification of MS 1603 as an atoll source or a Z source.

We thank the Massachusetts Space Grant and Holy Cross Fisher Fellowship for financial support.

Implicit Learning in Cotton-top Tamarins*Lindsey Driscoll, Lauren Nutile, Katie O'Gorman, and Dr. Charles Locurto**Department of Psychology, College of the Holy Cross*

Implicit learning can be described as the learning of information to which subjects are exposed even when learning is unnecessary. Its counterpart, explicit learning, involves actively absorbing any presented information and is the topic of widespread research. We have chosen to study implicit learning in the cotton-top tamarin (*Saguinus oedipus*) using a touch screen system. During training a single visual stimulus appeared in different locations on the screen. The tamarin was required to touch the screen to advance the stimulus to the next location. Each stimulus location possessed an equal chance of being rewarded. Following training the tamarins received pair-wise tests and chain tests. The pair-wise tests were used to determine whether they preferred some stimuli over others. The chain tests involved rearranging the order in which the five stimuli appeared on the screen.

The explicit learning in our experiment included recognizing that when stimuli in the chain were touched, a reward would be given. The implicit learning aspect included learning the order in which stimuli appeared in the original chain. If the tamarins had learned the order of the chain, their reaction times would be slowed during the chain tests. Also, if the tamarins did not show a preference for one stimulus over another in the pair tests, they will have learned that a stimulus appearing in any area of the screen was likely to provide a reward.

We thank the National Science Foundation and the Fisher Fellowship fund for financial support and the New England Regional Primate Research Center for this research opportunity.

Fishing with Worms: Using Genetics and Molecular Biology to Identify Interactors

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Department of Molecular Medicine, UMass Medical School

The two genes I studied during my fellowship are both involved in the processes of chromosome segregation and the proper development of germline cells in the *Caenorhabditis elegans*. The first gene, *csr-1* (Chromosome Segregation and RNAi deficient) encodes a conserved and key component of the RNA Interference (RNAi) machinery. RNAi is a naturally occurring process in a number of organisms that leads to the suppression of gene expression. Understanding the mechanism of RNAi is essential to harnessing this process as a disease therapy. We utilized a yeast two-hybrid screen to determine which proteins interact with CSR-1. As CSR-1 is an essential component of the RNAi machinery, and there are currently no interacting proteins identified, these studies are key to understanding the role of CSR-1 in RNAi.

The second gene, *pam-1*, encodes an ortholog of the human puromycin-sensitive aminopeptidase. In *C. elegans*, PAM-1 activates a conserved Ras/MAPK signaling pathway to promote maturation of the germline. Mutations in the human Ras oncogene and aberrant signaling from the Ras/MAPK pathway are critical effectors of carcinogenesis. Through the use of genetic screens, we have tried to elucidate which genes are involved in the PAM-1 pathway. When mutated, the gene encoding PAM-1 in *C. elegans* causes a phenotype in which only 15% of the progeny are viable. Through randomly mutating the worm's genome, suppressing mutations can be found to restore the viability of the mutated PAM-1. By determining what chromosome this gene is on and the location on that chromosome, the specific proteins that are involved in this pathway can be elucidated.

I would like to thank the American Cancer Society and the Fuller family for financial support.

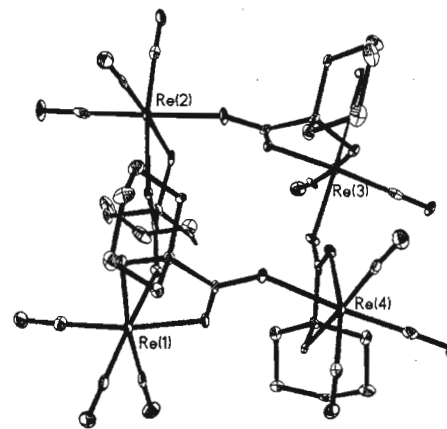
Diagnostic Imaging and the possibilities of Rhenium

Joseph Lopez and Prof. Richard Herrick
Department of Chemistry, College of the Holy Cross

In the medical world there is always need for new bioorganometallic imaging agents that are more target specific. Currently the most widely used isotope used is ^{99m}Tc , which is very similar to Rhenium in part because of the Lanthanide contraction. Although Rhenium is not used itself in imaging it does have potential to be used in therapy because its primary isotopes β -emitters. Rhenium is also safer to use for experimentation than Technetium because of its radioactivity.

The research consists of trying new reactions with either bidentate or tridentate ligands with either $[\text{Re}(\text{CO})_3(\text{H}_2\text{O})_3]^+$ or $[\text{Re}(\text{CO})_6]^+$ under the proper conditions to get crystalline complexes. Once the crystalline complex is isolated and the crystal structure the halide is replaced with a biomolecule. We successfully grown and solved five crystal structures including one tetramer, a picture included below.

We would like to thank the Simeon Fortin Fellowship for their financial support.



Investigating *gbb* expression and function in the red flour beetle

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The Transforming Growth Factor-beta (TGFbeta) superfamily consists of signaling molecules that play a critical role in establishing the embryonic body plan of organisms, as in the thoroughly studied *Drosophila melanogaster*, a species that develops its appendages from imaginal discs. Studies indicate variation in the conservation of such signaling molecules across species with different modes of appendage development. This work attempts to identify the function of *glass bottom boat* (*gbb*) in *Tribolium castaneum*, a beetle species that develops its limbs directly. Through *in situ* hybridization of embryos we plan to visualize the expression patterns of *gbb* at various stages of embryonic development. Additionally, we will observe the phenotypic effects of RNA interference (RNAi) on embryos who have had the expression of *gbb* silenced. This will enable us to draw conclusions on the role that *gbb* plays in appendage development and its overall role in the establishment of the embryonic body plan. Our work involving *in situ* hybridization and RNAi is ongoing.

We wish to thank the Becton Dickinson Fund for financial support.

Magnetic Properties of Commercial Stainless Steels

Jennifer Goodell, and Professor Paul Oxley

Department of Physics, College of the Holy Cross

The purpose of this work is to investigate the magnetic properties of ten types of magnetic stainless steel. A magnet will be built using the steel that has the best magnetic properties. This magnet will operate at cryogenic temperatures and will generate a magnetic field which can be used to influence the electron orbit in laser-excited Lithium atoms.

In order to create a magnetic field at cryogenic temperatures it is useful to employ the properties of magnetic materials. We want materials with a high relative permeability (which require less energy to produce a given magnetic field), high magnetic saturation (which allows the production of strong magnetic fields) and low coercivity (which allows the magnetic material to be demagnetized easily). The published magnetic properties of stainless steels are not comprehensive enough to allow us to choose a material for our application, and no information is available on the magnetic properties of stainless steels at cryogenic temperatures.

In our studies a stainless steel rod sample is placed inside a magnetizing solenoid and a 20Hz electrical current is passed through the solenoid to produce an oscillating magnetic field at the position of the sample. A flux coil wrapped around the sample produces a voltage indicative of the magnetic flux density (or *B* field) within the sample. Using either a Hall probe or a field coil positioned next to the sample we measure the magnetic field strength (or *H* field). Knowing these values, we can calculate the room temperature permeability, magnetic saturation, and coercivity for the ten stainless steels. In addition, we also report the maximum permeability and magnetic saturation for our steels at cryogenic temperatures (77 Kelvin).

We wish to thank the Research Corporation and the College of the Holy Cross for financial support.

The Physics of Baseball: The Importance of Weather in Baseball

J. Singleton

*M. B. Koss, T. Roach, C. Amante, M. Knierim, and D. Wirth
Department of Physics, College of the Holy Cross*

Weather conditions can postpone or even cancel baseball games, but how does the weather affect a game during play? This was one of our concerns on the Physics of Baseball Team. Our goal was to create a model to describe the trajectory of a batted ball. Once the ball is in the air the distance it travels is affected by the qualities of the air (temperature, barometric pressure, humidity) more so than one may think.

We use the qualities of the air at the time the ball is in flight to calculate the dynamic viscosity and from that the kinematic viscosity, which describes how viscous the air is. These quantities are used to calculate the Reynolds number, which we use to find the drag force on the ball.

We looked at how the weather changes over a period of a month and a day, and calculated the kinematic viscosity for each day of the month, and each hour of the specific day. We found that the kinematic viscosity could change by as much as 12% during a month, and as much as 8% during a day. This means that a hit during a summer game can have a very different result in the winter, and that a hit in mid-afternoon can even differ from the same hit at night.

The wind is also a very important contributor to the path of a baseball. We have been working on models to describe wind patterns so that our trajectory model can take into consideration differing wind speeds and directions as the ball flies through the air.

I would like to thank the Massachusetts Space Grant Consortium and the Fisher Fellowship for financial support, as well as Diane Jepson and Richard Miller for help with supplies and equipment.

Using Algebraic Geometry in the Circular, Restricted Four-Body Problem

Julianne Kulevich, Christopher Smith, and Prof. Gareth Roberts
Department of Math/CS, College of the Holy Cross

We are studying the circular, restricted four-body problem (CR4BP) in which three large masses travel along individual Kepler circular orbits as a fourth body of infinitesimal mass moves under the gravitational force of the other three. Investigation of this problem relies heavily on the software package Maple, several topics from algebraic geometry, such as polynomial ideals and Groebner bases, arrangements of bodies known as central configurations (c.c.'s), and on analytic proofs that bodies can form collinear or equilateral triangle c.c.'s. In particular, our demonstration that equilateral triangle arrangements are c.c.'s for equal masses *or* arbitrary masses is crucial to our study of the restricted four-body problem.

The overall purpose in studying this problem is to prove a version of Saari's conjecture, an important statement in celestial mechanics that was proven for the planar, three-body problem using BKK Theory. The modification of this conjecture asserts that the only solutions to the CR4BP with a constant value of the amended potential are equilibria (or critical points of the amended potential). For the equal mass case of the CR4BP, we show that the configuration of the critical points is symmetric. Previous work on the restricted three-body problem by Lisa Melanson and Prof. Gareth Roberts guides our study; however, the added dimension of this problem imposes several difficulties. After a careful assessment of our methods and calculations, we have begun to examine alternate means of proving Saari's conjecture for the CR4BP.

We would like to acknowledge the Fisher Summer Research Fellowship and the NSF Award DMS-0708741 for financial

Poster 37

Instruments and Experiments For Determining Effects of Spin on a Baseball

D. Wirth, M. Koss, T. Roach, M. Knierim, C. Amante, and J. Singleton

Department of Physics, College of the Holy Cross

The game of baseball, with all its great moments and memories all relies on one thing; the baseball. Over the last century, the game and how it has been played has changed greatly, while there have been no major changes to the ball used in the professional major leagues. Despite expert investigations, there is still some uncertainty about the interacting forces between a baseball and the air it travels through on its trajectory. We have begun several experiments to analyze the rotation rate and its effect on the forces on a baseball in flight. To do these experiments we have developed and set up several laboratory componets and methods, including a high speed digital camera system, a pitching machine, and a way to impart a known rotation on the baseball. As part of this laboratory build-up, we have designed, built and begun testing wind tunnels to make measurements in centralized, controlled air environments over longer periods of time on the rotating baseballs.

We would like thank Dick Miller and Diane Jepson in the Physics Department, Coaches Comrie and C. Ridolfi in Athletics, and Jim Long in Physical Plant. We would also like to acknowledge the Fisher Fellowship Fund for financial support.

Poster 38

Applications of Computational Commutative Algebra in Statistics

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University of Arizona University of Puerto Rico

Alexander Simao, Jr. Dr. John B. Little
Department of Mathematics and Computer Science
College of the Holy Cross

Recently, applications of computational commutative algebra and algebraic geometry in statistics have played an important role in bioinformatics and genomics. In particular, when maximum likelihood estimation is used to obtain estimates of parameters in discrete probability models, the equations to be solved can often be expressed in terms of polynomials in several variables.

Some of the most basic questions are: How many different critical points does the likelihood function have, and is there an efficient way to determine this number? The focus of this project is a certain concrete three-parameter mixture model involving two binomial random variables. Following recent results of Hosten, Khetan, and Sturmfels, the maximization of the likelihood function is recast as a constrained optimization problem for the log-likelihood, expressed as a function of several variables representing the probabilities of certain outcomes in the model.

Employing Grobner basis techniques, we prove a number of general statements concerning properties of the solutions of the Lagrange multiplier equations for the critical points. We also develop a purely symbolic method to count the number of critical points of the Lagrange multiplier equations in the probability simplex.

We would like to thank the NSA and the PREMUR program for their support of this research.

Poster 39

Solution of Laplace's Equation in an Atom-Ion Collision Chamber

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It is often desirable to study collisions in a uniform electric field. Such experiments are carried out in an atom-ion collision chamber, which consists of a series of equipotential plates with a small opening for the atomic beam. In order to determine the resulting electric field in the chamber, one must solve Laplace's equation $\nabla^2 V(\vec{r}) = 0$ with the appropriate boundary conditions. In practice, the equation is exactly solvable only for the simplest geometries and boundary conditions. For a realistic chamber, one must obtain the electric field numerically.

We have used the finite element method to obtain solutions to Laplace's equation in cylindrical coordinates. To test our code, we first applied it to an exactly solvable problem consisting of a grounded cylindrical chamber with a single plate. We then modified the boundary conditions in the finite element code to match the specifications of an atom-ion chamber used by Professor Paul Oxley to study Rydberg atom collisions. Our calculations verified that the chamber can produce a collision region where the electric field is stable to within 1%.

This work was supported by the Marlon Professorship in the Sciences and the National Science Foundation PHY-0440714.

Poster 40

BEZ235 – A New Step in Targeted Chemotherapy

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Although advances in conventional cancer treatments have resulted in small, incremental survival benefits for most common tumors, cancer researchers have long believed that the future of treatment rests in targeted therapies—"smart" drugs that, unlike the non-discriminating chemotherapy approach, take aim at individual proteins, enzymes, and pathways unique to cancer. At UCLA, under the management of Dr. Dennis Slamon, M.D., the lead investigational researcher that led to the use of Herceptin for breast cancer, and Dr. William Tap, M.D., we have been using BEZ235, a brand new drug developed by Novartis which acts as a PI3K inhibitor, against the Sarcoma cell lines to develop the IC50 for those lines and to gather a greater understanding at how it works and a baseline to work off of for future experiments with that drug in the lab.

The tests that we performed included dose response curves where we took different concentrations of the drug and drugged a known amount of cells and counted the cells remaining in the end to create an IC50 for that drug that can then be used in lycates for when we ran our Western Blots. In addition to running Western Blots and dose response curves, we also ran Flow experiments where we did Cell Cycle Analysis and Apoptosis experiments, and PCR reactions in an attempt to identify any "hot spots" for mutations in certain proteins.

We thank the drug companies, private donors, and UCLA for their financial support.

Poster 41

Insights Into the Mechanism of DNA Replication in Tumor Viruses and its Regulation.

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The replication of a number of DNA viruses depends upon the interaction of virally encoded initiators with DNA sequences called origins of replication. Our long term goal is to isolate cyclic peptide inhibitors that disrupt the assembly of initiators on viral origins of replication. Our lab uses the Simian virus 40 as our model viral system because the virus's proteins are very well characterized. Simian virus 40 encodes an initiator termed SV40 T-antigen (T-ag) whose structure, especially the origin binding domain (OBD), closely resembles the T-ag's encoded by other human pathogens.

Regarding our approach to the isolation of inhibitors of viral initiators, vast peptide libraries, can be prepared in *E. coli*. The DNA sequence of our library consists of "NNS codons" where N represents any of the four DNA bases and S represents C or G. Thirty-two codons ($4 \times 4 \times 2$), encoding all twenty amino acids, are generated by the NNS sequence. In theory, the initial library that we constructed can have any of the twenty amino acids at five positions. Therefore, it is capable of encoding 20^5 cyclic peptides, some of which may disrupt the assembly of initiators on viral origins of replication.

Inhibitors identified from this project will serve as lead components for the development of inhibitors against members of the Papovaviridae family of viruses and the herpes virus. Creating therapies against the herpes virus would help control oral and genital infections, and therapies against members of the papilloma virus would control clinical lesions ranging from warts to invasive cancer formation. We would like to thank the NIH for funding this project.

Poster 42

Cell Rearrangement: Mathematical Modeling of Branching Morphogenesis and other Biological Phenomena

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Mathematical modeling of cellular rearrangement is of interest to developmental biologists, particularly in the area of branching morphogenesis. The goal of this project is to help identify morphogenetic mechanisms, which may be capable of producing certain observed shape changes in developing tissues. In both two and three dimensions, we use a grid system to model cells as well as different cell types. Cells begin as rectangles of given dimensions surrounded by medium, a neutral non-cellular substance. The discrete stochastic model incorporates interface energies as well as random movements. In order for cells to maintain biologically realistic shapes, movements occur with greater probability if the cells will remain convex, reach a given aspect ratio, and stay with cells of their own type. The algorithm developed aids in the modeling of cell growth, mitosis, and convergent extension. This model is important because cell rearrangements are imperative in determining the shapes of tissues, which helps to explain how complex organisms grow from a single cell.

Funding for this project was provided by the National Science Foundation.

Replacing the Fragmin[®] Kjeldahl Method with the Leco TruSpec Elemental Determinator

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Fragmin[®] is an anticoagulant drug that is marketed by Pfizer and is injected to prevent thrombosis. It consists of low molecular weight heparin which is heparin extracted from porcine intestine and depolymerized into short polysaccharide chains. The current method used to measure nitrogen content in Fragmin[®] is a digestion, distillation, and titration procedure called the Kjeldahl Method. This procedure is costly, uses hazardous chemicals, and is time consuming, taking 2 to 3 hours to analyze one sample. Leco Corporation has produced an instrument called the TruSpec Elemental Determinator that can measure nitrogen in organic substances more efficiently. Analysis using the Elemental Determinator takes 3 minutes and waste is minimal and non-hazardous. At the request of the Fragmin[®] manufacturing site in Strängnäs Sweden, the objective in this series of experiments is to demonstrate that the Elemental Determinator methodology is a suitable replacement for the Kjeldahl Method in the quality control release test for Fragmin[®]. The method qualification elements evaluated during this study included accuracy, repeatability, specificity, linearity, range, and robustness. It was concluded that the Elemental Determinator method can measure the nitrogen content in Fragmin[®] with suitable accuracy, repeatability, and linearity within an acceptable analytical range. It was further demonstrated that the instrument and method are robust and specific to nitrogen.

A Selective Estrogen Receptor β Agonist Fails to Replicate the Effects of Estrogen in a Spatial Working Memory Task

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The finding that estrogen has a positive effect on working memory has led to the research examining the relative roles of estrogen receptor subtypes, ER α and ER β . Whereas our previous research found that ER β stimulation fully mimicked the effects of estrogen in non-spatial working memory tasks, this experiment focused on the role of ER β in spatial working memory. WY2000700 (0.1, 1, or 10 mg/kg) was tested relative to 17 β -estradiol (66 μ g/kg), and a vehicle control. Ovariectomized rats were tested in a radial arm maze (RAM). Twenty-four hours after the last of two daily injections (SC), animals that were previously habituated to the RAM were allowed to explore the maze for one 10 min trial on each of four consecutive days. Each arm of the maze was baited with a food pellet. Working memory errors were recorded when animals re-entered an arm from which it had already consumed the reinforcer. Performance in the RAM was not affected by either estradiol or the WY compound. Injections were repeated and testing in the RAM was conducted over four consecutive days with a 1 hr delay between the fourth and fifth correct responses. One week later, injections were again administered, and testing in the RAM was continued over four consecutive days with a 1 min delay between the fourth and fifth correct responses. Estradiol was found to significantly improve performance in both delay conditions. WY at 0.1 or 1 mg/kg also improved working memory after the 1 min delay, but not after the 1 hr delay. The highest dose of the WY compound had no effect in either delay conditions. The results suggest that stimulation of the ER β may not be sufficient to produce the facilitative effects of estrogen on spatial working memory, thus leaving the possibility that ER α may also be important in this regard. We thank Wyeth Pharmaceutical for financial support.

**Protein splicing and extein activity of the *Pyrococcus abyssi*
lon protease intein**

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Protein splicing involves the excision of an intervening sequence, called an intein, from flanking polypeptides, called exteins. This process is coupled to the ligation of the exteins. It has been suggested that the extein sequences can influence protein splicing, and that the presence of an intein interferes with the native activity of the exteins. We are studying the intein that interrupts the lon protease of *P. abyssi*. The intein lacks a highly conserved penultimate His residue. We have shown that this intein is capable of promoting efficient *in vivo* protein splicing in *E. coli* when over-expressed as a fusion protein. The in-frame fusion protein consists of an N-terminal maltose binding protein domain, the 23 C-terminal residues of the N-extein, the intein, the 29 N-terminal residues of the C-extein, and a poly-His tag. We have also generated vectors to express extein-intein fusion proteins to determine if the intervening sequence influences either the ATP-dependent or ATP-independent activity of the protease, and have designed efficient assays for protease and ATPase activity. We isolated the protease domain and found that it is able to cleave poorly folded proteins.

We thank the National Science Foundation for financial support.

**Exploiting Thermo-responsive Guanosine Gels for Sample
Pre-Concentration in Capillary Electrophoresis**

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The detection of low abundance analytes has long been a problem plaguing the use of capillary electrophoresis and microfluidic separations. This project exploits the temperature responsive properties of mixed guanosine and guanosine monophosphate gels in a selective method of protein preconcentration. The co-aggregation of guanosine and guanosine monophosphate produces thermo-responsive "g-gels" whose temperature dependence is easily dictated by adjusting the ratio of guanosine and 5'-GMP composing the gel. The majority of gels undergo conversions from a near solid state to that of a viscous liquid between 10 – 50° C, and all completely melt upon reaching 80° C. We manipulate the thermo-responsive behavior of the g-gels in conjunction with the affinity of certain proteins for the G-quadruplex motif in our method of preconcentration. Our first step calls for the gel to be inserted into the capillary in its liquid state, after which an appropriate temperature adjustment causes the gel to solidify. The protein is then introduced into the capillary, and subsequently captured by the gel. Finally, the gel is melted, allowing the protein to migrate through the capillary and to eventually be detected. Ultimately, we hope to employ this method to screen complex mixtures for the subclass of proteins possessing an affinity for the G-quadruplex motif to selectively detect and identify each protein.

We thank the Connecticut Business and Industry Association and Pfizer Global Research and Development for their support.

Poster 47

Ferrocene Chemistry: non-isotopic tracers and β -sheet mimetics

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Ferrocene is an organometallic molecule of interest due to its structure consisting of an iron atom between 2 cyclopentyl coplanar rings. With coplanar rings just 3.3 angstroms apart, the structure is extremely sturdy and can be used as a non-isotopic tracer in the body because it can not easily be broken down. Ferrocene can also be used to mimic secondary structures in proteins such as β -sheets. β -sheets and β -turns are stabilized by hydrogen bonding. Biological functions of proteins are therefore dependent upon this bonding system. Studying these interactions will offer insight into how these biological functions occur and help researchers gain a better understanding as to why these biological functions could malfunction, for example, cause a protein to misfold. Ferrocene serves as the organometallic scaffold that simulates an environment in which inter- and intramolecular interactions can be observed.

Ferrocene monocarboxylic acid was attached to lysine in the first step in creating a tracer. Future work in this area will be to remove the protecting groups on either end of the lysine and react with more amino acids. 1,1-Ferrocene dicarboxylic acid derivative was used in chemical synthesis to create peptide chains off both cyclopentyl rings. Aminobutyric, aminohexanoic, and aminododecanoic peptide chains have been synthesized. Future work in this area will be to attach an amino acid to both chains of all three synthesized product, creating dipeptide chains, which would allow for a study of the hydrogen bonding inter- and intramolecularly.

We thank the Simeon J. Fortin Foundation for financial support.

Poster 48

Localization of circadian gene expression in the brain of *Xenopus tropicalis*

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Circadian rhythms are the endogenous twenty-four hour rhythms, found in organisms ranging from bread mold to humans, which persist even under constant conditions. Each day, biochemical and physiological processes and behaviors, such as production of hormones and the sleep-wake cycle, occur rhythmically. This cycling is controlled by a central oscillator which functions through rhythmic gene expression. This gene expression that maintains the circadian clock involves several genes, including *clock*, *period1*, *cryptochrome1*, and *bmal1*, that are regulated by a negative feedback loop.

We have chosen to study the circadian rhythms of the frog, *Xenopus tropicalis*. Our aim was to identify the clock neurons in the brain of *X. tropicalis* by localizing the gene expression of *xclock*, *xper1*, and *xcry1* using in situ hybridization. We have also begun to localize gene expression in tadpole brains to compare with that of adults. Our results indicate high levels of expression for all three genes predominately in the adult forebrain and midbrain with very similar patterns of staining. The expression pattern was similar to that of PACAP, a neuropeptide known to be expressed in the mammalian central clock. The colocalization of these three genes suggests brain regions that are candidates for the central oscillator in *X. tropicalis*. Our ultimate goal is to correlate this gene expression with behavioral rhythms in tadpoles and adult frogs.

This work was supported by the Becton Dickinson Summer Research Fellowship Fund and the Holy Cross Biology Department.

Uncovering Molecular Signatures of Rapid Evolutionary Radiation in the Phylogenies of Carabid Beetles.

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Rapid evolutionary events may have driven the patterns of biodiversity we see today, especially in taxonomically and morphologically diverse groups such as beetles. The ability to document evidence of rapid radiations is critical for our understanding of the evolution of biodiversity. Many scenarios attempt to explain the evolution of mega-diverse groups of organisms but few studies have attempted to test these hypotheses in a phylogenetic context. Molecular sequence data can be used to estimate divergence times and rates of evolutionary change among and within lineages of organisms using specific models of evolution.

We worked with molecular sequence data from the nuclear gene for the ribosomal subunit 18S in the subfamily of carabid ground beetles, which consists of over 19,000 species. Informed by that data, the divergence times of major Harpalinae lineages were determined using several maximum likelihood analysis techniques. We looked for evidence of rapid evolution in the 35 species of beetles that were sampled. Most of the radiations in the phylogenies occurred approximately between 40 and 90 million years ago. Future work in this area will include work on the rDNA sequence for 28s and the wingless sequence in beetles and species in Harpalinae and we will eventually run simulations of rapid evolution to test these models.

A special thanks goes to the Simeon Fortin Fellowship for its financial support for this project.

Recruitment of Proteins to Syndecan-4 Mediated Focal Adhesions

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b1 integrin is the primary transmembrane adhesion protein responsible for the initiation of focal adhesion formation when cells attach to extracellular matrix. However, during the process of cell adhesion, syndecan-4—a transmembrane heparan sulfate proteoglycan that mediates cell adhesion—also acts cooperatively with integrins to facilitate formation of mature focal contacts. In previous studies in our lab, antibody-conjugated cover slips were used to investigate the recruitment of proteins by syndecan-4 in the formation of focal adhesions. To further explore this recruitment, magnetic beads were coated with syndecan-4 antibody and dropped on living cells. These magnetic beads were found to become physically connected to the cells independent of integrins. Specifically, vinculin was discovered to be recruited to syndecan-4 based adhesions.

In order to further develop these findings, we transfected mouse fibroblast cells and green monkey kidney cells with DNA constructs to express Green Fluorescent Protein (GFP) and GFP fused to either paxilin or talin. Using confocal microscopic analysis, we observed the recruitment of these proteins to syndecan-4 antibody-coated beads in live and fixed cultured cells. We found that both GFP and our GFP fusions were recruited to the magnetic beads, indicating that GFP may be attracted to focal adhesion sites independent of whether it has been fused to one of our studied proteins. This finding indicates that more work is needed to determine the influence of syndecan-4 on extracellular matrix and focal adhesions.

We would like to thank the Fisher Foundation, Becton Dickinson and the National Science Foundation for their financial support of our work.

Socioeconomic Status as a Potential Factor in Determining Sleep Patterns and Well-being

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The Sleep-Smart Pacesetter study (principal investigator, Prof. Wolfson¹) is a longitudinal, preventive/intervention study that aims to identify the sleep patterns and daytime functioning behaviors of 7th and 8th grade students in Worcester. Participants completed questionnaires to address sleep/wake times, school performance, and psychopathology. Using self-report and school measures we categorized our sample population into three socioeconomic status (SES) levels: High, Medium, and Low. After reviewing Time 1, baseline data, sleep pattern differences according to income level were observed to help explain the diversity and variability within our sample. We then assessed the dependent measures mental health, physical well-being, and sleep hygiene practices across the three income levels.

From previous analyses, 7th graders from low to medium income levels had an average of 35 minutes less total sleep during school nights and woke up an hour later on weekends (p 's $\leq .05$). Our study used a MANOVA analysis to detect if any of our dependent measures were statistically different across SES groups. In addition, we also evaluated correlation matrices across these dependent measures. The MANOVA analyses produced no statistically significant differences amongst the three SES levels, which allowed us to discard the idea that the differences were present due to mental health, physical well-being, and/or sleep hygiene. Increased child physical activity was associated with better/higher pupil behavior ratings by their middle school teachers ($r = .23, p < .05$).

Research supported by the National Institute of Child Health and Human Development.

Individual Differences in Regret and Maximization Moderate the Endowment Effect

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The endowment effect (Thaler, 1980) is the tendency to value an object more after one possesses it. According to prospect theory (Kahneman & Tversky, 1979), higher prices are required to sell than to acquire an object because the loss of something one has is subjectively experienced more intensely than a corresponding gain of the same amount. Although it is a fairly robust phenomenon, recent studies have identified factors such as social value orientation (Lin & Lin, 2006) and people's affective states (Lerner, Small & Lowenstein, 2004; Zhang & Fishbach, 2005), that moderate this effect. The current research examined individual differences in decision making style (Schwartz et al., 2002) as moderators of the endowment effect. College students ($N = 70$) received a DVD and indicated how much they would accept to exchange it for cash and then indicated how much they would pay to acquire a similarly preferable DVD. The endowment effect occurred more strongly for people with a maximizing decision making style, characterized by always searching for the best possible outcome ($b = .36, p = .004$), and less strongly for people who tend to experience regret about their decisions ($b = -.33, p = .009$).

We thank the Richard B. Fisher Summer Student Research Fellowship Fund for financial support.

Poster 53

Exploration of the Triassic Chinle Formation of Southern Utah

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In July 2007 we prospected and quarried Cretaceous fossil localities in the Kaiparowits Plateau of Grand Staircase-Escalante National Monument in Southern Utah, in collaboration with the Utah Museum of Natural History (UMNH). Together with the UMNH crew, we worked in several quarries and assisted in the uncovering of a near complete, articulated ceratopsian dinosaur skeleton, the first complete crocodile skull from the Monument, and a partial lambeosaur skeleton. After two weeks in the Cretaceous, we shifted our attention to the Triassic Period, seeking out Chinle Formation exposures across the monument, including the Vermilion Cliffs and Circle Cliffs, as well as Red Canyon and San Rafael Swell outside the monument. With the Yale Peabody Museum of Natural History as our skeletal repository, we prospected Chinle exposures for 4 weeks and documented 41 unique bone localities. We found several disassociated teeth, vertebrae, and armor scutes of phytosaurs, metoposaurs, and aetosaurs, some of which may be diagnostic, but did not recover any associated specimens. Bone samples were collected to expand the understanding of species distribution and mineral content of bone in the Triassic. The logged Triassic fossil sites in the Chinle provide important information for future expeditions into this promising fossiliferous formation.

We thank the College of the Holy Cross and the Yale Peabody Museum for their financial support.

Poster 54

Sequential Mannich condensations to prepare ligands with oxygen, nitrogen donors with systematic variations in steric and electronic properties to model the active site of protocatechuate 3,4-dioxygenase

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Enzyme activity is a major subject of interest in biochemistry. We are attempting to model the structure and function of metallo-enzymes and proteins using small molecules as models. Mannich condensations were employed to synthesize novel ligands with two unsymmetrical phenol rings with varying steric bulk and electronic environments. These ligands were used in reactions with anhydrous ferric chloride in an air free environment in order to produce a model for the enzyme protocatechuate 3,4-dioxygenase (PCD). PCD takes molecular oxygen and integrates both oxygen atoms into an organic product. PCD shows cleavage of organic compounds like catechol. Product study of 3,5-di-*t*-butylcatechol with iron complexes using mass spectroscopy revealed several products of catechol cleavage. Kinetic study of catechol reaction with iron ligand complex and molecular oxygen was done to investigate catechol 1,2-dioxygenase activity of iron (III) complexes.

We thank Pfizer Global Research and Development and the Connecticut Business & Industry Association for financial support.

Poster 55

The Mathematics behind the Schroedinger Equation

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The Schroedinger equation is an essential equation for studying the behavior of quantum mechanical systems. The complete Schroedinger equation has a time and space dependence. Depending on how many dimensions the equation is describing and on the potential function being used, a variety of scenarios can arise. We began our studies by examining the one-dimensional, time-independent version of the equation, and were able to progress to the three-dimensional, time-dependent version of the equation describing the hydrogen atom. We learned that the solutions for the behavior of the hydrogen atom depend on two special classes of functions called the Legendre polynomials and the Laguerre polynomials.

We then created a CD describing and depicting the mathematical concepts behind the Schroedinger equation complete with images and animations. This CD can be used as a supplement to anyone wanting to learn about the origins of the solutions.

We would like to thank the Fisher Scholarship Foundation for making this learning experience possible.

Poster 56

The Influence of an Intein on the Activity of the *Methanococcus jannaschii* UDP-Glucose Dehydrogenase

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Inteins are segments of intervening protein that excise themselves and direct the two flanking ends to ligate, thus creating a functional protein. It is not currently known whether inteins play a specific role in gene regulation or if they are vestigial remnants of prior regulatory processes. To investigate, we have focused our study on an intein produced by an extreme thermophile, *Methanococcus jannaschii*. The intein intervenes the enzyme UDP-glucose dehydrogenase. This reaction produces glucuronic acid, as well as two molecules of NADH. Through site directed mutagenesis, we have mutated the plasmid containing the gene for the intein fusion in order to prevent the splicing of the intein. We transformed the resulting plasmid into *E. coli* in order to over express the protein. We then isolated both the wild type protein that was able to splice and the mutated protein that was unable to splice. In order to compare their functionality, I have produced an NADH standard curve.

Through spectroscopy, I intend to compare the NADH production of both proteins, thus giving us insight as to whether or not the presence of the intein in the protein affects its function.

We thank the National Science Foundation for their financial support.

Aldosterone Protects Kidney Cells from Ouabain Inhibition of Gap-junction Communication

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Gap junctions between adjoining cells allow small molecules and ions to pass freely from cell to cell. These junctions are composed of a family of proteins called connexins. We studied the effects of various treatments on the expression of Connexin 43 (Cx43) in mammalian kidney cells. The drug ouabain inhibits the Na^+ , K^+ -pump, leading to elevated intracellular Na^+ . Dye transfer and immunofluorescence studies measured cell communication and expression of Cx43. We found that Cx43 levels and cell communication decrease after ouabain treatment, but addition of aldosterone protects Cx43 levels and communication even with ouabain present. The effect requires binding to the aldosterone receptor, because it is abolished by spironolactone and eplerenone, receptor antagonists. It also requires elevated Na^+ because it is abolished by amiloride. It is specific to mineralocorticoids because the glucocorticoid hydrocortisone does not influence ouabain inhibition.

We tested MDCK dog kidney cells, 293 T17 human kidney cells, and M1 mouse kidney cells. MDCK cells and 293 T17 cells communicated well and showed Cx43 at cell surfaces, and showed the above effects, while M1 cells did not. M1 cells, however, were successfully transfected with a plasmid that contained the Cx43 gene linked to Green Fluorescent Protein.

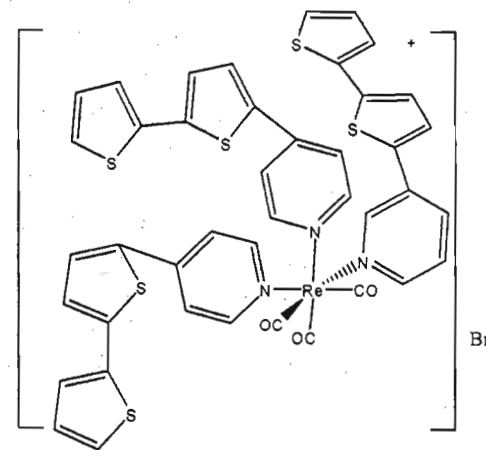
Future experiments will include confirmation of the results from dye transfer and immunofluorescence with western blotting. We will also see whether transfected Cx43 is expressed as functioning gap junctions.

We thank the National Science Foundation and the Fisher Research Fund for support of this project.

Novel Electrochemically Grown Materials

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Pyridine bithiophene hybrid ligands were used to synthesize transition metal containing conducting polymers. Using $[\text{Re}(\text{CO})_3(\text{H}_2\text{O})_3]\text{Br}$ as a starting material we prepared a molecule with three pyridine-bithiophene hybrid ligands in a facial arrangement (figure below). These complexes polymerized under oxidative conditions to form polyelectrochromic films. The synthesis, characterization, and properties of these new materials will be presented. We thank the College of the Holy Cross and the Fisher Fund for financial support.



Interactions between Chemical Treatments in Yeast

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A genetic toxicology assay in *Saccharomyces cerevisiae* strain D7 was used to explore two kinds of interactions between chemical treatments: cotreatments and sequential treatments. For cotreatments, we studied interactions between intercalating agents and bleomycin (BLM). BLM is a glycopeptide antibiotic that is used as a cancer chemotherapy drug. Among the genetic effects of BLM are the induction of mitotic recombination and mutations in yeast and chromosomal aberrations in mammalian cells. The principal DNA lesions responsible for the genetic effects of BLM are double-strand breaks. BLM is a potent inducer of gene conversion at the *trp5* locus and point mutations at *ilv1* in strain D7. The compounds whose interactions with BLM were studied include both conventional and unconventional intercalating agents. The former have three fused aromatic rings and positive charge (aminoacridines). The latter were compounds predicted to intercalate by 3-D computer modeling. Some intercalating agents are themselves mutagenic or recombinagenic in strain D7 but others are not. Independently of their own genetic activity, all the intercalating agents enhanced the genotoxic effects of BLM. Thus, the interactions fall into two categories: potentiation or synergy. The sequential treatments that were studied were small priming doses of an agent that causes oxidative DNA damage (e.g., hydrogen peroxide), followed by a larger challenging dose with the same agent or another mutagen. We found that under some experimental conditions the yeast exhibit an adaptive response in which the priming dose reduces susceptibility to a larger challenging dose.

The support of a summer fellowship from the Robert Stransky Fund is gratefully acknowledged.