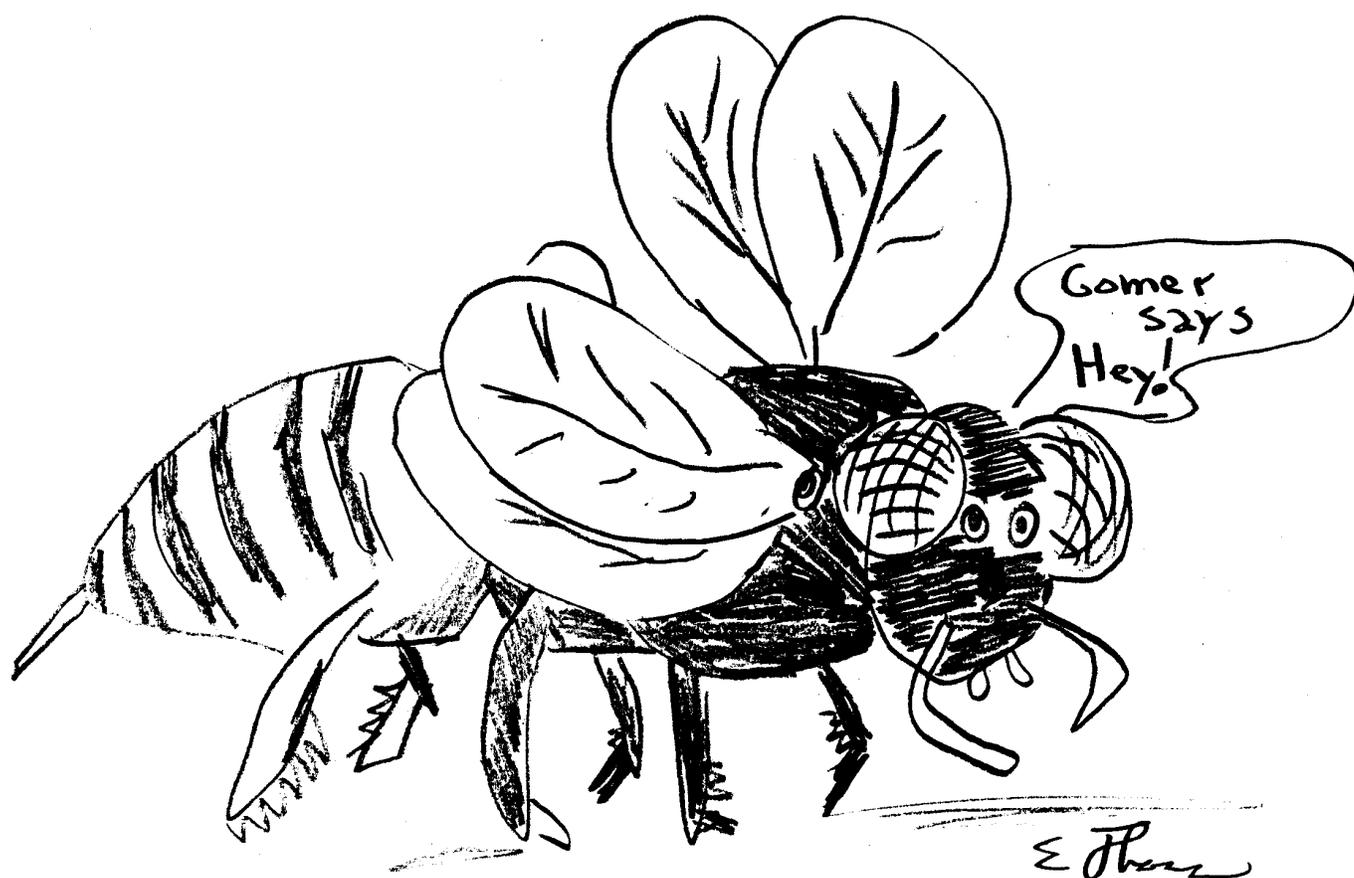




The Bulletin
of the
Virginia Section
AMERICAN CHEMICAL SOCIETY

SUMMER 2006 ISSUE



Genus Ant-Bee

A Mayberry Hybrid Arthropod

***** VIRGINIA SECTION NEWS *******VIRGINIA SECTION MEETINGS - FALL 2006**

- September 22** Virginia Commonwealth University, Richmond
Annual Awards Program (see below)
Local Contact Person: Dr. Sally Hunnicutt, (804) 828-8599
- October 24** College of William & Mary, Williamsburg
Dr. E. Ann Nalley
(Joint Meeting with the Hampton Roads Section)
Local Contact Person: Dr. Lawrence Sacks, (757) 930-2045
- November 17** Mary Washington College, Fredericksburg
Dr. Leanna Giancarlo
Local Contact Person: Dr. Roy Gratz, (540) 654-1412
- December 1** John Tyler Community College, Chester
Dr. Manfred Psiorz
Local Contact Person: Dr. Kristine Smetana, (804) 706-5143

SEPTEMBER AWARDS MEETING

The September meeting of the Virginia Section will be held in Richmond at Virginia Commonwealth University on Friday, September 22, 2006. The Virginia Section will be presenting its Distinguished Service Award to a member of the Section who has contributed significantly to the Section and to the profession. Also, one or more Industrial Awards will be presented. Meeting details will appear in the September issue of the Bulletin. For more information, please contact Dr. Sally Hunnicutt at VCU [(804) 827-0531; sshunnic @ vcu.edu] or Virginia Section Chair Elect Dr. Will Lewis at (804) 274-5869; will.h.lewis @ pmusa.com.

REPORT ON THE MARCH SECTION MEETING

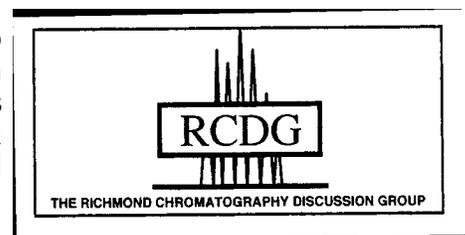
The Virginia Section met on Tuesday, March 21 at the Virginia Military Institute in Lexington. This was a joint meeting with the Blue Ridge Section of the ACS. Ten members of the Virginia Section attended. Dr. Domenic Paone of Novozyme Biologicals spoke on "Harnessing Biotechnology for a Cleaner Environment." His company utilizes natural microorganisms to degrade industrial waste. They produce Novo Surf Clean for removing oil stains from cement. Dr. Adele Addington of Radford University, Chair of the Blue Ridge Section, introduced the speaker. Thanks to Dr. Addington and to Dr. Will Lewis for organizing this meeting.

REPORT ON THE APRIL SECTION MEETING

A large gathering attended the April 14 meeting at the University of Virginia. Dr. John Butler of the National Institute of Standards and Technology (NIST) spoke on "Beyond CSI: Exciting Applications of Forensic DNA." Dr. Butler's talk was preceded by the 20th annual Poster Session that featured student research at various colleges and universities. A total of 34 posters by students from eleven colleges and universities were presented (a complete list of authors and titles and abstracts of some of the papers are included in this issue of the *Bulletin*). Section Chair Dr. Dorothy Eseonu recognized fourteen outstanding senior chemistry majors from colleges and universities within the Virginia Section (the names of the recipients are listed below). The Section thanks Dr. James Demas, Ms. Susan Collins, and others at the University of Virginia who assisted with this successful meeting. Special thanks to Ms. Collins for preparing the poster program and abstracts.

RCDG

The purpose of the Richmond Chromatography Discussion Group is to promote the interests of the chromatographic and other separation sciences by expanding the awareness and capabilities of individuals from the scientific community. To meet this goal the group publishes a newsletter and presents lectures at various locations in the Richmond area. Check out their website: www.rcdg.org.



OUTSTANDING CHEMISTRY GRADUATES

At the April meeting, the Virginia Section recognized graduating seniors from colleges and universities within the Section. Schools in the Virginia Section were invited to nominate senior chemistry majors for this honor. The outstanding students for the year 2006:

<u>College/University</u>	<u>Student</u>
Bridgewater College	Angela M. Dolph
College of William & Mary	Eleanor Brown
Eastern Mennonite University	Gregory Lamb
Hampden-Sydney College	Mithilesh Adhikari
James Madison University	Michael Peretich
Longwood University	Sarah Crane
Mary Baldwin College	Megan Huffman
Randolph-Macon College	Dana Peles
University of Mary Washington	Kirsten Studer
University of Richmond	Laura Barrosse-Antle
University of Virginia	Yogesh Surendranath
Virginia Commonwealth University	Richard B. Keithley
Virginia State University	Nikisha M. Tarver
Virginia Union University	Tierra Mayo

REPORT ON ConSOL

ConSOL, a conference on the teaching of chemistry in Virginia, was held in Richmond on June 23 and 24. Over 30 teachers joined with presenters from Virginia and other areas to consider ways to improve chemistry learning in Virginia, particularly in connection with the effect of the Standards of Learning (SOL) End of Course Chemistry Test and the Curriculum Framework. The conference received support from the Hampton Roads Section, the Virginia Section, the Virginia Blue Ridge Section, and the Chemical Society of Washington. The Local Sections Activity Committee of the ACS provided a grant for the conference. Conference participants drew up recommendations relating to the teaching of chemistry and the evaluation of students. Recommendations for improvement of the SOL tests and related materials deal with administration, construction, and content. When the ConSOL report has been finalized, it will be available on the Virginia Section website: <http://membership.acs.org/V/VA/>. Further information can be obtained from Dr. Lawrence Sacks, the ConSOL Coordinator (consolconf @ aol.com), or from Ryan Warren, Chair of the Chemical Education Committee for the Virginia Section (clwgrw @ netzero.net).

QUESTIONS FROM THE PAST

This question was asked in the April Bulletin: The Virginia Section hosted the Southeastern Regional Meeting of the American Chemical Society in November, 1959. Hiram R. Hanmer was the General Chairman for the meeting, which was held at the John Marshall Hotel in Richmond. The Chairman of the Virginia Section at the time of that meeting passed away recently. **Who was the Virginia Section Chair in 1959?** Dr. Alfred R. Armstrong was Chairman of the Section in 1959. In the program for the Southeastern Meeting, he said "Welcome to the Southeastern Regional Meeting, to Richmond, and to Virginia. May your stay with us be both professionally profitable and personally pleasant." Dr. Armstrong, Emeritus Professor of Chemistry at the College of William and Mary, died in Williamsburg on February 8, 2006, at the age of 94 years. In 1972 he received the Distinguished Service Award from the Virginia Section.



A new question from the past: The list of 50-yr members of the ACS (page 8) includes three persons who have served as Chair of the Virginia Section. Their terms were 1976, 1981, and 1982. **Who are the three former Chairs?**

DRAWING ON COVER

The cartoon on the cover of this issue of the Bulletin was done by Eddie Thomas, Councilor for the Virginia Section. Drawing is one of Eddie's hobbies. He has done cartoons for the covers of 13 issues of the Bulletin. Eddie served as Chair of the Virginia Section in 1988 and received the Distinguished Service Award in 1993. He has been a Section Councilor since 1995 and is a member of the national ACS Membership Affairs Committee and is the MAC liaison to the Committee on Constitution & Bylaws. He is retired from R&D at Philip Morris USA.

WORDS OF WISDOM FOR THE SUMMER: "All Life Is An Experiment"

**POSTER PRESENTATIONS
UNIVERSITY OF VIRGINIA - APRIL, 2006**

Banks Allen, Justin Azar, James Baldwin, Sohale Vu, and Paul Mueller; Department of Chemistry, Hampden-Sydney College - *Preparation of a Series of Proline N-Oxide Catalysts*

Luke Arbogast, Kylee Sollien, Emily Thompson, D.L. Polo, and L.M. Vallarino; Department of Chemistry, Virginia Commonwealth University - *Complexes of Co(II), Ni(II), Cu(II), and Zn(II) with 2-(N-3,5-dimethylanyline-amide)-3-naphthalenecarboxylic Acid, as Models for Metal-Doped Polyimides*

Johnese E. Bailey, Kyung-Hoon Lee, Jeff Stromberg, Loretta Tu, Robert Cicchillo, and *Squire T. Booker; Department of Chemistry, Virginia State University and *Department of Biochemistry/Molecular Biology, Penn State University - *Does the CX_2CX_2C Motif Coordinate the [4Fe-4S] Cluster of NadA?*

Laura Barrosse-Antle and Raymond N. Dominey; Department of Chemistry, University of Richmond - *Synthesis of Amino Acid Precursors to DNA-Binding Oligomers*

John P. Cicarelli, Melissa Sartin, Dan C. Fisher, Matt Coppock, Brad K. Norwood, Edith J. Banner, and John Gupton; Department of Chemistry, University of Richmond - *A Combination Strategy for the Preparation of Storniamide and pyrrolomycin Type Alkaloids*

Lisa Coletta, Joan M. Bienvenue, Carmen Reedy, Jerome P. Ferrance, *Susan Greenspoon, and *James P. Landers; Department of Chemistry, University of Virginia and *Virginia Department of Forensic Science - *Microchip-based Volume Reduction and Sample Concentration of Crude Sample Digests for Micro-Solid Phase DNA Extraction*

Christine M. Colton, Mitchell P. Maddox, and Debra L. Mohler; Department of Chemistry, James Madison University - *Dissociation of DNA-Histone Assemblies Resulting from Protein Side-Chain Functionalization*

Pamela J. Dopart and T.C. DeVore; Department of Chemistry, James Madison University - *Thermal Decomposition of Calcium Copper Acetate*

Lindsay Drennan, Emma Goldman and Raymond N. Dominey; Department of Chemistry, University of Richmond - *Synthesis of a Carbon Dioxide Reducing Catalyst*

Michael R. Edwards, Sherri L. Hensler, John M. Joyce, Christopher M. Shuford, and Melissa C. Rhoten; Department of Natural Sciences, Longwood University - *Analysis of Cucumber Plants for Use as Phytoremediators: An Instrumental Analysis Project*

Leigh A. Frame and Vladimir Garkov; Department of Chemistry, Mary Baldwin College - *Analysis of Echinacea and St. John's Wort Via High Performance Liquid Chromatography*

Lindsay C. Fuoco and Sally Hunnicutt; Department of Chemistry; Virginia Commonwealth University - *The Effects of Cyclodextrins on the Cis to Trans Isomerization of Azobenzenes*

Alex Garcia, Kevin Thompson, and Kevin Dunn; Department of Chemistry, Hampden-Sydney College - *Investigation of the Effectiveness of Antioxidant Additives in Artificially Aged Cold Process Soap*

Alex Garcia and Paul Mueller; Department of Chemistry, Hampden-Sydney College - *Preparation of a Chiral Ligand with C₂ Symmetry Based on a Substituted Proline N-Oxide*

Hilary Hott, Vladimir Garkov and *Regina Day; Department of Chemistry, Mary Baldwin College and *Department of Pharmacology, Uniformed Services University of the Health Sciences - *Bleomycin-Induced Pulmonary Fibrosis: Egr-1 and Sp3 Activation*

Karl Jackson, Courtney Williams, and Colleen Taylor; Department of Chemistry, Virginia State University - *A Student Run Experiment Designed to Enhance an Advanced Inorganic Chemistry Course*

John M. Joyce and Gary P. Lutz; Department of Natural Sciences, Longwood University - *Synthesis of Diphenylketones as Probes for Directed Metallation Experiments*

Richard B. Keithley, Sarah E.G. Porter, and Sarah C. Rutan; Department of Chemistry, Virginia Commonwealth University - *Fluoxetine Metabolism: A Chemometric Study*

Jessica Klinkenberg, Gina L. Fiore, *James M. Edwards, Brenda N. Goguen, Sarah J. Payne, *Daniel G. Gioeli, James N. Demas, Anne Pfister, and Cassandra L. Fraser; Department of Chemistry, University of Virginia and *Department of Microbiology, University of Virginia School of Medicine - *Tailoring Polymeric Ruthenium Complexes for Gene Delivery and Sensors*

Kenneth M. Knott, Genevieve H. Bulluss, Erin S. F. Ma, Eugenio Alvarado, Sheena M. Aris, and Nicholas Farrell; Department of Chemistry, Virginia Commonwealth University - *Modulation of Carboxylate Leaving Group Ability in Trans-platinum Planar Amine Compounds with N₂O₂ Ligand Donor Sets*

Yian Y. Lee, Sylvia Cechova and Carthene R. Bazemore-Walker; Department of Chemistry, University of Virginia - *Development and Optimization of a Sensitive ELISA to Measure Monocyte Chemoattractant Protein-1(MCP-1) in Mouse Urine*

Sarah J. Linke, Kate Manning, Jessica C. Voorhees, Jerome P. Ferrance, and James P. Landers; Department of Chemistry, University of Virginia - *The Facilitation of Cell Elution from Rape Kit Cotton Swabs*

Jimmy Marion and Carol Parish; Department of Chemistry, University of Richmond - *A Combined Quantum Mechanical and Molecular Mechanical Technique used in the Study of HIV-1 Protease--Inhibitor Interactions*

Carleen Morris, Kiev Blasier, and James P. Landers; Department of Chemistry, University of Virginia - *Polyethylene Oxide as a Sieving Matrix for ssDNA*

Michael E. Peretich and T. C. DeVore; Department of Chemistry, James Madison University - *Kinetics Study of the Reaction Between 1-propanol and Copper(I,II) Oxide*

Boone M. Prentice, Melissa C. Rhoten, *Lianyong Su, *Fred M. Hawkrige, **James B. Kelly, and **Steven I. Baskin; Department of Natural Sciences, Longwood University, *Department of Chemistry, Virginia Commonwealth University, and **US Army Research Institute of Chemical Defense - *The Effect of Cyanide Binding on the Electroreduction of Dioxygen by Cytochrome c Oxidase Immobilized in Electrode-supported Lipid Bilayer Membranes*

Sarah Remmert and Carol Parish; Department of Chemistry, University of Richmond - *The Spin-Flip Method: Quantum Mechanical Analysis of Eneidyne Molecules*

Austin B. Scharf, Barrett A. Little, Jonathan E. Hempel, Anastasia Kharlamova, Brad K. Norwood, Edith J. Banner, and John Gupton; Department of Chemistry, University of Richmond - *A Combination Strategy for the Preparation of Rigidin Type Alkaloids*

Christopher M. Shuford, Melissa C. Rhoten, *John B. Mangrum, and *Nicholas P. Farrell; Department of Natural Sciences, Longwood University, and *Department of Chemistry, Virginia Commonwealth University - *Real-time Monitoring of Multinuclear Platinum Drug Binding to Electrode-Immobilized DNA Using a Quartz Crystal Microbalance*

Kirsten E. Studer and Charles M. Sharpless; Department of Chemistry, University of Mary Washington - *Direct UV Photolysis and Advanced Oxidation of Estrone with Byproduct Formation*

Nikisha Tarver and Asmare Atally; Department of Chemistry, Virginia State University - *Uses of Grasses and Amendments for Nutrient Reduction During Rainfall Simulation*

Evan Wang and Carol Parish; Department of Chemistry, University of Richmond - *Quantum Mechanical Studies of Five, Seven and Eight-Membered Eneidyne*s

John Wass, Joan M. Bienvenue, Jerome P. Ferrance, James P. Landers; Department of Chemistry, University of Virginia - *Integration of Volume Reduction SPE to Increase Pre-PCR DNA Concentration and Purity*

Alexis Wells, Bradley D. Newkirk and Dr. Gordon T. Yee; Department of Chemistry, Virginia Polytechnic Institute and State University - *Dialkyldicyanofumarate Diesters as Acceptors for Charge-Transfer Molecule-Based Magnets*

GRANTS FOR K-12 SCIENCE PROJECTS

The Virginia Section is soliciting proposals for grants to support school science projects in grades K through 12. The \$50 to \$500 grants will be provided to teachers in the Virginia Section for the purchase of materials and supplies. To apply for support, request an application form from Mr. Ryan Warren, 304 N. Sheppard Street, Richmond, VA 23221; (804) 342-1323; warrencr @ vcu.edu. Or complete an application on-line by accessing the Virginia Section website at <http://membership.acs.org/VVA/grants.htm>.

SECTION BIDS FOR SERMACS MEETING

The Virginia Section is endeavoring to hold a Southeastern Regional ACS Meeting in Richmond. A Committee chaired by Dr. Joseph Pompano prepared a bid for the 2009 SERMACS Meeting. This was unsuccessful, as the meeting was awarded to the Puerto Rico section. The Section may submit a bid for the 2011 meeting. Anyone who would like to work on this should contact Dr. Will Lewis, Chair-Elect, at (804) 274-5869; Will.H.Lewis @ pmusa.com. The last SERMACS meeting hosted by the Virginia Section was in 1991.

VIRGINIA SECTION WEBSITE

Information on Virginia Section meetings, copies of the *Bulletin*, and much more can be found on the Virginia Section Website. It can be accessed via <http://membership.acs.org/VVA/>.

FIFTY-YEAR MEMBERS OF THE ACS

Congratulations to these Section members, each of whom has been a member of the American Chemical Society for 50 years:

Dr. Trevor B. Hill	Williamsburg
Mr. Franklin D. Kizer	Lancaster
Mr. William F. Kuhn	Midlothian
Dr. Beverly A. Pawson	Charlottesville
Mr. F. A. Retzke	Richmond
Dr. Hans J. L. Schuurmans	Richmond
Dr. Manie K. Stanfield	Beaverdam
Dr. James F. Stubbins	Midlothian

SOUTHEASTERN REGIONAL MEETING

SERMACS 2006, sponsored by the Savannah River Section, will be held at the Augusta Marriott Hotel & Suites in Augusta, Georgia, November 1-4, 2006. The program includes 25 symposia and a variety of special events including a vendor exposition. The deadline for submission of abstracts is September 1. Advance registration closes on October 9. Full information can be found at <http://membership.acs.org/S/SERMACS2006/>.

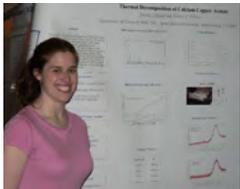
ALBEMARLE STUDENT HONORED AT CHEMISTRY OLYMPIAD

Sydney Creutz, a senior at Albemarle High School in Charlottesville, was selected as an alternate for the team that represented the United States at the 38th International Chemical Olympiad that was held July 2-11 in Gyeongsan, South Korea. The U.S. team consisted of four competitors and two alternates. They were chosen from a pool of 20 students who were invited to attend the U.S. Chemistry Olympiad Study Camp at the United States Air Force Academy in Colorado Springs, Colorado. This is the second consecutive year that Ms. Creutz was selected for the Camp. The selection is based on performance on the national Chemistry Olympiad Examination. Her chemistry teacher at Albemarle High School was Mr. Marvin Curry. The Virginia Section congratulates Ms. Creutz on her outstanding achievement. She is the only student from the Virginia Section who has ever been selected to attend the National Olympiad Study Camp.



The team from China won the International Olympiad competition. Teams from Taiwan, the Russian Federation, and South Korea finished in a tie for second place. U.S. team members were awarded one bronze and three silver medals. More than 250 students from 68 countries competed in the Olympiad which included theoretical and practical exams that each lasted five hours.





*UVA Meeting
April 14, 2006
photographs
courtesy
of Jim Demas*



ABSTRACTS OF POSTER PRESENTATIONS APRIL 14, 2006 - UNIVERSITY OF VIRGINIA

Preparation of a Series of Proline *N*-Oxide Catalysts, Banks Allen, Justin Azar, James Baldwin, Sohale Vu, and Paul Mueller, Hampden-Sydney College, Hampden-Sydney, VA.

N-cyclohexyl-(*S*)-proline was prepared by hydrogenation from the enamine of proline and cyclohexanone. After coupling reactions of the modified proline with a set of amines (3-aminoquinuclidine, 1-phenylethylamine, and phenylalanine methyl ester) the tertiary proline nitrogen of each amide was oxidized using MCPBA. These compounds are being evaluated as catalysts for Baylis-Hillman reactions.

Complexes of Co(II), Ni(II), Cu(II), and Zn(II) with 2-(*N*-3,5-dimethylanyline-amide)-3-naphthalenecarboxylic Acid, as Models for Metal-Doped Polyimides, Luke Arbogast, Kylee Sollien, Emily Thompson (CHEM 406 – Advanced Inorganic Chemistry Lab), D.L. Polo and L.M. Vallarino, Virginia Commonwealth University, Richmond, VA.

Polyimides, a class of organic polymers that possess high thermal stability as well as excellent mechanical properties, have become increasingly important as construction materials for industrial applications. Polyimides often contain an appreciable percentage of amic-acid sites that can act as ligands for metal ions, resulting in the formation of metal-containing polymers that combine the properties of the host matrix with the specific properties of the guest metal ions. As part of an ongoing project, the CHEM 406 class of 2006 at V.C.U. has undertaken the synthesis and characterization of the complexes of several metal ions, Co(II), Ni(II), Cu(II) and Zn(II), with the anion of 2-(*N*-3,5-dimethylanyline-amide)-3-naphthalenecarboxylic acid. The formulas and the suggested structures of the complexes are reported.

Does the CX₂CX₂C Motif Coordinate the [4Fe-4S] Cluster of NadA? Johnese Bailey, Kyung-Hoon Lee, Jeff Stromberg, Loretta Tu, Robert Cicchillo, and *Squire T. Booker, Virginia State University, Petersburg, VA and *Penn State University, University Park, PA.

Nicotinamide adenine dinucleotide (NAD) is a vital enzymatic cofactor present in all living organisms. NAD functions as a hydride acceptor resulting in the formation of its reduced form NADH, which is a hydride donor in redox reactions. NAD evolves from quinolinic acid, which in turn is synthesized through one of two biosynthetic pathways; prokaryotic pathway involves the condensation of L-aspartate and dihydroxyacetone phosphate (DHAP) and the eukaryotic pathway involves degradation of L-tryptophan. The prokaryotic pathway employs the enzyme L-aspartate oxidase (NadB) and quinolinate synthetase (NadA) protein (Scheme 1). The NadA protein contains nine cysteine residues, three of which lie in a motif that is characteristic of cysteines that ligate iron-sulfur (Fe-S) clusters. Through expression of the *nadA* gene from *E.coli*, and purification and characterization of its gene product, our lab is trying to verify or disprove that this motif coordinates an iron sulfur cluster. Purification of the NadA protein is done anaerobically due to the oxygen sensitive cluster. We have tangled three variant NadA proteins, which contains cysteine to serine substitutions. With the removal of each of the cysteines, we expect to prevent formation of one Fe-S cluster which should create an inactive NadA protein. Analysis of the protein will be done using iron analysis and UV-Vis spectroscopy.

Synthesis of DNA-Binding Amino Acids, Laura Barrosse-Antle and Raymond N. Dominey, Chemistry Department, University of Richmond, Richmond, VA.

Much about the way that molecules bind to DNA is unknown. For example, restriction enzymes, proteins that splice DNA at specific four to eight base pair sequences, are an integral part of genetic engineering, but the specific mechanisms associated with these proteins are still not fully understood. By synthesizing ligands engineered to bind to the minor groove of DNA and examining the ligand-DNA interactions using NMR, a better understanding of molecular interactions with DNA can be reached. These ligands, referred to as "hairpin" molecules due to their shape, are composed of five parts: *N*-methylimidazole amino acid (NMIAA), *N*-methylpyrrole amino acid (NMPAA), α -aminobutyric acid, β -alanine, and dimethylaminopropylamide. Our group's work to this point has been maximizing the purity and efficiency of the synthesis of the two amino acid components.

Microchip-based Volume Reduction and Sample Concentration of Crude Sample Digests for Micro-Solid Phase DNA Extraction, Lisa Coletta, Joan M. Bienvenue, Carmen Reedy, Jerome P. Ferrance, *Susan Greenspoon, and James P. Landers, University of Virginia, Charlottesville, VA, and *Virginia Department of Forensic Science, Richmond VA.

Microdevice research has created interest in both the forensic and clinical worlds. Current techniques utilize microdevices to carry PCR amplification, DNA separation as well as sample preparation steps that include DNA extraction. Microchip technology has many advantages including reduced sample volume, reduced reagent cost and reduced analysis time.

The small sample volumes that are used to carry out analysis on microdevices can be applied in the clinical world when the sample is not scarce or degraded and is not contaminated. However in the forensic world this is not the case, large sample volumes are common and in some cases advantageous. Larger sample volumes are needed when eluting nuclear DNA off samples with a large surface area, for example samples from fabric cuttings and cotton swabs. Large volume samples are also needed when trying to extract mitochondria DNA, links are also made to larger volumes increasing DNA yield and reducing the affects of any PCR inhibitors. These factors indicate the importance of large volumes, however, current microchip techniques can not utilize these large volumes without it significantly affecting sample analysis time.

The research presented aims to overcome this problem and develop a microchip based large volume preconcentration step. This microchip device is designed for nuclear and mitochondrial DNA extraction from large volume samples. A method developing volume reduction solid phase extraction in less than 30 minutes is described, with a preliminary investigation into the capacity and efficiency of the microchip, in addition showing elution profiles with reduction in sample volume and successful STR amplification of the elution. A microchip device and method integrating vrSPE with previously established $\bar{1}$ SPE methods to complete the DNA extraction is illustrated.

Dissociation of DNA-Histone Assemblies Resulting from Protein Side-Chain Functionalization, Christine M. Colton, Mitchell P. Maddox III, and Debra L. Mohler, James Madison University, Harrisonburg VA.

DNA-histone assemblies can be used to mimic the environment of DNA in a eukaryotic cell allowing for further research in the medicinal chemistry field. Production of methyl radicals in the presence of histone H1·DNA assemblies dissociates the H1·DNA complex, in part due to the conversion of the amines on lysine R groups in H1 into aldehydes, canceling the electrostatic attraction between H1 and DNA. In this experiment, various concentrations of three methyl radical generating organometallic compounds were irradiated for 30 minutes in the presence of the H1·DNA complex to see if dissociation or DNA cleavage would occur. The methyl radical generators used were: $\text{CpW}(\text{CO})_3\text{CH}_3$, pyridone (*N*-*tert*-butoxy-2-pyridone, $\text{C}_9\text{H}_9\text{NO}_2$), and a methyl cobalamin analogue. $\text{CpW}(\text{CO})_3\text{CH}_3$ generates a metal byproduct as well as the methyl radical, requiring further studies to verify that the methyl radical was causing the dissociation. Pyridone generates both a methyl radical and a *tert*-butoxy radical depending on concentration; during its reaction with the H1·DNA complex, only DNA cleavage was observed, leading to the conclusion that the reaction was in the concentration range of *t*-butoxy radical rather than methyl radical. The methyl cobalamin analogue will provide further evidence of whether the methyl radical is the reagent dissociating the H1 from the DNA.

Thermal Decomposition of Calcium Copper Acetate, Pamela J. Dopart and T.C.DeVore, James Madison University, Harrisonburg, VA.

The kinetics and thermal decomposition of calcium copper acetate are studied by means of evolved gas analysis (EGA) and differential scanning calorimetry (DSC). Infrared spectroscopy showed that barium acetate decomposes some carbon dioxide and acetone. From graphs of absorbance v. temperature, the activation energy, the order of the reaction, and the rate constants can be determined. These rate constants are determined by curve fitting the data to specific equations and solving for the rate constants. The activation energy is then determined using the Arrhenius equation. However, data scatter is large and further refinement is necessary.

The residue from these experiments was examined through IR and was determined to be mostly barium carbonate. DSC trials of varying heating rates ranging from 278 K/min to 293 K/min were conducted as well. The sample was heated from 323 K to 823 K and, from this data, it is apparent that barium acetate has a melting point of around 733 K.

Synthesis of a Carbon Dioxide Reducing Catalyst, Lindsay Drennan, Emma W. Goldman, and Raymond N. Dominey, University of Richmond, Richmond, VA.

There is an abundance of carbon dioxide in the atmosphere, which is a potential starting material for alternative fuel sources. Hence it would be useful to find a way to efficiently reduce carbon dioxide electrochemically. The single electron reduction of carbon dioxide is the most basic step in its conversion to other organic products. Direct single and multi-electron reductions of carbon dioxide at solid electrodes are limited by kinetics and thus exhibit very high overvoltages. Our project involves synthesizing a series of copper complexes with open α, α' -diimine ligands and evaluating their efficiency as electrocatalysts for the electrocatalytic reduction of carbon dioxide. Our work thus far has focused on the synthesis of disubstituted pyridine ligands required to make a series of copper electrocatalysts.

Analysis of Cucumber Plants for Use as Phytoremediators: An Instrumental Analysis Project, Michael R. Edwards, Sherri L. Hensler, John M. Joyce, Christopher M. Shuford, and Melissa C. Rhoten, Longwood University, Farmville, VA.

Toxic metal contamination of soil is an increasing problem in industrial settings especially in the electroplating industry. Remediation of these toxic metals can be difficult and expensive. Phytoremediation is an inexpensive and environmentally-friendly method to clean up contaminated soil. The purpose of the experiment presented here is to determine the concentration of nickel and chromium absorbed by young, growing cucumber plants to investigate the feasibility of using them as phytoremediators. The cucumber plants were grown in hydroponic media containing various concentrations of the metals of interest for two weeks. The accumulated metals were extracted from the plants via ashing and dissolution in nitric acid. Atomic Absorption spectroscopy was then used to quantify the chromium or nickel content of the plant material.

Analysis of Echinacea and St. John's Wort Via High Performance Liquid Chromatography, Leigh A. Frame and Vladimir Garkov, Mary Baldwin College, Staunton, VA.

Herbal supplements are among the most prosperous divisions in retail pharmacies, supermarkets, and general mass-market retailers, but they are not regulated. This may lead to inconsistent dosages, which can lead to unreliable results. Echinacea and St. John's Wort were chosen as the two supplements to be tested for numerous reasons, including that they were the two best selling herbs in the United States as of 1998. I have set out to verify previous studies using High Performance Liquid Chromatography. As the supplements obtained for this experiment appear to be more consistent among brands for St. John's Wort than Echinacea, the verification was obtained. Thus, parameters need to be set for the regulation of the supplements industry.

A Combination Strategy for the Preparation of Storniamide and Pyrrolomycin Type Alkaloids, John P. Ciccarelli, Melissa Sartin, Dan C. Fisher; Matt Coppock, Brad K. Norwood, Edith J. Banner, and John Gupton, University of Richmond, Richmond, VA.

Our research group recently reported the synthesis of the marine natural products polycitone A and B. Our strategy employed the conversion of a 2-substituted vinamidinium salt to a 2,4-disubstituted pyrrole, which was subsequently elaborated at the 5 and 3 positions to the desired natural product. We are currently examining a similar approach to Storniamide and Pyrrolomycin type alkaloids and ongoing work in our lab will be presented.

Bleomycin-Induced Pulmonary Fibrosis: Egr-1 and Sp3 Activation, Hilary Hott, Vladimir Garkov and *Regina Day, Mary Baldwin College, Staunton, VA, and *Uniformed Services University of the Health Sciences, Bethesda, MD.

Pulmonary fibrosis is a progressive disease characterized by the loss of alveolar architecture through fibroblast proliferation and arterial endothelial/epithelial cell apoptosis. Recent research implicates roles of angiotensin-converting enzyme activity (ACE) mediated by mitogen-activated protein kinase (MAPK) and early growth response 1 transcription factor (Egr-1) in the molecular mechanism of this disease. In this experiment, Egr-1 and Sp3 expression was qualitatively assessed using the bleomycin pulmonary fibrosis model in bovine pulmonary artery endothelial cells. Through bleomycin treatment, nuclear extraction, and Western blotting, it was found that Egr-1 expression was up-regulated but not in a time-dependent manner. Sp3 expression was not significantly altered by bleomycin treatment.

The Effects of Cyclodextrins on the Cis to Trans Isomerization of Azobenzenes, Lindsay Fuoco and Sally Hunnicutt, Virginia Commonwealth University, Richmond, VA.

We have investigated the effect of cyclodextrins on the thermal cis-to-trans isomerization of 4,4'-dimethylaminophenyl-azobenzoic acid sodium salt (p-methyl red). When irradiated with light, azobenzenes switch from the thermodynamically more stable trans to the cis isomer, which quickly returns to the trans isomer. This property of azobenzenes makes them possible candidates as molecular switches or image storage devices. UV-Vis spectra show that α -cyclodextrin interacts more strongly with p-methyl red compared to the β - and γ -cyclodextrins. Chemometric analysis of the UV-Vis spectra resolves two distinct species for p-methyl red complexes with β - and γ -cyclodextrin and three species for complexes with α -cyclodextrin. The cis-trans isomerization rate constant for p-methyl red is lower when complexed with β , γ and α -cyclodextrin. These results, along with theoretical modeling, suggest that p-methyl red may form 1:1 complexes with β - and γ -cyclodextrins and may form inclusion complexes with α -cyclodextrin.

Preparation of a Chiral Ligand with C₂ Symmetry Based on a Substituted Proline N-Oxide, Alex Garcia and Paul Mueller, Hampden-Sydney College, Hampden-Sydney, VA.

Using a procedure similar to one described in the literature, a chiral amino acid-based catalyst was synthesized and characterized. The compound, the di-N-oxide of the diamide obtained from coupling N-cyclohexyl-(S)-proline with ethane diamine, has C₂ symmetry. This new compound is being evaluated as an organic catalyst for Baylis-Hillman reactions and as a metal chelating agent. The bulky carboxyl groups on either end of the compound will potentially bind to D-orbitals of heavy metals. The flexible ethyl bridge joining the two identical constituents will allow it to conform to the symmetry of metal D-orbitals. These properties make it an excellent candidate for a metal chelator.

Investigation of the Effectiveness of Antioxidant Additives in Artificially Aged Cold Process Soap, Alex Garcia, Kevin Thompson and Kevin Dunn, Hampden-Sydney College, Hampden-Sydney, VA

The method of manufacturing cold process soap was investigated as a way for small-scale manufacturers to produce customized soap. Experiments included artificial aging of the soap at 60° C in reactive and inert atmospheres, determination of saponification value, and an extensive investigation of additives that prevent rancidity of the soap. All of these experiments together gave much information valuable to the small-scale soap manufacturer. All laboratory work was done with equipment that would be accessible to manufacturers without chemistry degrees or specialized education. This ensures that the results are realistic, and could be carried out by actual soap manufacturers.

A Student Run Experiment Designed to Enhance an Advanced Inorganic Chemistry Course, Karl Jackson, Courtney Williams and Colleen Taylor, Virginia State University, Petersburg, VA.

$[\text{Co}(\text{2,9-dimethyl-1,10-phenanthroline})(\text{H}_2\text{O})_4]^{2+}$, $[\text{Co}(\text{DMP})]^{2+}$, undergoes a change in symmetry from octahedral to tetrahedral upon introduction to sol-gel due to surface binding to inner pore walls. This process is enhanced with increasing pH but not without substantial changes in the structure of the host gel. Systematic titration of a series of $[\text{Co}(\text{DMP})]^{2+}$ -doped sol-gels with hydroxide anion produces a visually impressive data set that demonstrates to students this interplay between material structure and loading. This experiment has been incorporated in the VSU advanced one semester inorganic chemistry course as a student run exercise to reinforce and enhance the lecture course material from the *Inorganic Chemistry* text of Shriver and Adkins, 3rd ed.

Synthesis of Diphenylketones as Probes for Directed Metallation Experiments, John M. Joyce and Gary P. Lutz, Longwood University, Farmville, VA.

Enolates are important intermediates used in organic synthesis. Normally deprotonation reactions in ketones occur only at the alpha positions to form enolates. The synthesis of a series of diphenylketones designed to investigate the directing ability of an enolate ion towards the removal of a second proton that is normally not considered to be acidic is being reported. Deuterium isotope exchange reactions were used to clearly distinguish between the benzylic position and the alpha positions and these results will also be presented.

Fluoxetine Metabolism: A Chemometric Study, Richard B. Keithley, Sarah E. G. Porter and Sarah C. Rutan, Virginia Commonwealth University, Richmond, VA.

Fluoxetine is a selective serotonin reuptake inhibitor used to treat patients with depression. In this study, fluoxetine was used as a model for developing chemometric approaches for studying drug metabolism. Multivariate curve resolution with alternating least squares and kinetic modeling programs were used in the Matlab® programming environment. Several analytical methods were explored to determine the best approach to extract important pharmacokinetic constants. The kinetic constants of fluoxetine were obtained by analyzing *in vitro* CYP2D6 enzyme incubations with liquid chromatography-mass spectrometry. Using a biphasic model, K_{M1} , v_{max1} , K_{M2} , and v_{max2} of fluoxetine were calculated to be $3.3 \pm 3.2 \mu\text{M}$, $1.4 \pm 0.3 \mu\text{mol norfluoxetine} / \mu\text{mol CYP2D6} / \text{min}$, $81.2 \pm (1.0 \times 10^9) \mu\text{M}$, and $0.9 \pm (1.1 \times 10^7) \mu\text{mol norfluoxetine} / \mu\text{mol CYP2D6} / \text{min}$, respectively. The constants for the higher affinity site from the biphasic model were consistent with those of literature while the constants obtained from the Michaelis-Menten model were off by an order of magnitude. The differences in the kinetic constants between the biphasic and the Michaelis-Menten models highlight the importance of developing improved methods for obtaining this drug metabolism information.

Tailoring Polymeric Ruthenium Complexes for Gene Delivery and Sensors, Jessica L. Klinkenberg, Gina L. Fiore, James M. Edwards, Brenda N. Goguen, Sarah J. Payne, Daniel G. Gioeli, James N. Demas, Anne Pfister and Cassandra L. Fraser, University of Virginia, Charlottesville, VA.

This study seeks to develop multifunctional polymeric metal complexes (PMCs) as targeted delivery vectors for prostate cancer therapies. The target complex consists of a ruthenium tris(bipyridine) (bpy) core with pendant poly(ethylene glycol) (PEG) and poly(ethylenimine) (PEI) chains. PEG chains can be tagged with bioactive groups (e.g. antibody, carbohydrate, drug, etc.) for targeting and recognition, and the cationic PEI chains can electrostatically entrap, condense, and deliver DNA constructs. To date, Ru PEG and Ru PEI homopolymers have been synthesized as model systems. Currently polymer coupling methods are under investigation as a synthetic method for the formulation of Ru PEG. For PEI, Ru tris(bpy)-centered star-shaped polyoxazoline precursors were synthesized by metalloinitiation. Acid hydrolysis produced Ru PEI complexes with molecular weights ranging from 5,000-8,000. An alternative synthesis of a 2-arm Ru PEI complex through chelation was attempted in order to produce star systems with molecular weights comparable to commercially available linear PEI (20,000), but UV-vis data indicated ineffective conversion to the tris(bpy) 2-arm star. In gel retardation assays with Ru PEI:DNA complexes, DNA entrapment was observed for nitrogen-to-phosphate (N/P) ratios as low as 2. Transfection was studied in LNCaP prostate cancer cells, and GFP gene expression was observed at N/P ratios as low as ~18-24. Progress in synthesizing polymeric metal complex biomaterials and testing their optical and biological properties will be discussed.^{1,2}

¹Fraser, C. L.; Fiore, G. L.; Gioeli, D. G.; Goguen, B. N.; Palumbo, A. M.; Pfister, A. *Polym. Mater. Sci. Eng.* 2004, 91, 781-782. ²Fiore, G. L.; Fraser, C. L. *et al.* manuscript in preparation.

Determination of Optimal Relative and Electric Fields for DNA Separations, Carleen Morris, Kiev R. Blasier, James M. Karlinsey, Jerome P. Ferrance, and James P. Landers, University of Virginia, Charlottesville VA 22904.

Microfluidic devices (microchips) are becoming a more viable approach for performing separation analysis. The microchip is fundamentally different from the traditional mode of electrophoresis done on capillary (CE). In CE, the sample is injected directly into the capillary is quickly removed from the sample vial and paced in a buffer vial as separation and detection ensues. On microchip, the sample is introduced initially into an injection channel and then into a separation channel. As a result of the geometry of the cross-tee, the injection channel is always physically in contact with the separation channel. This makes it necessary for electrokinetic forces that confine the sample in the separation apart from the sample in the injection channel. Perfecting these conditions will allow for a small sample plug and a reduction in band broadening.

DNA sample separations with pullback were investigated on a microchip. An optimal relative field of 0.6 was determined after comparing separations at 0.4, 0.6 and 0.8. Utilizing this relative field, an ideal electric field was determined by comparing separation between 150 V/cm and 350 V/cm. An electric field of 250 V/cm was found to give the best separations.

Kinetics Study of the Reaction between 1-Propanol and Copper(I, II) Oxide, Michael E. Peretich and T.C. DeVore, James Madison University, Harrisonburg, VA.

The apparent activation energy and order of reaction for the reactions between 1-propanol and copper (II) oxide were determined at temperatures less than 700 K using flow kinetics. All of the reactions produced propanal initially and only carbon dioxide at temperatures over 585 K. The reaction order in 1-propanol changed from 2 to 1 at a temperature of ~ 515 K. The averaged values for the apparent activation energy for the production of propanal was $120 \pm 10 \text{ kJ mol}^{-1}$ at temperatures below 515 K and $30 \pm 10 \text{ kJ/ mole}$ at temperatures above 515 K. The reason for this change has not been clearly established. It could indicate a change in the rate-limiting step for the reaction or it may indicate the effect of a competing reaction that generates carbon dioxide. The apparent activation energy and order of reaction between 1-propanol and copper (I) oxide are currently being determined.

The Effect of Cyanide Binding on the Electroreduction of Dioxygen by Cytochrome c Oxidase Immobilized in Electrode-supported Lipid Bilayer Membranes, Boone M. Prentice, Melissa C. Rhoten, *Lianyong Su, *Fred M. Hawkrige, **James B. Kelly and **Steven I. Baskin, Longwood University, Farmville, VA, *Virginia Commonwealth University, Richmond, VA, and **US Army Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD.

Bovine cytochrome c oxidase (CCO) has been successfully immobilized in electrode-supported lipid bilayer membranes to investigate the effect of cyanide binding on the electroreduction of dioxygen. CCO, the terminal enzyme in mammalian respiration, is inhibited by cyanide binding because the native function of the enzyme (the reduction of molecular oxygen) is blocked. The architecture of the CCO modified electrodes used in this work is uniquely similar to its natural environment in the inner mitochondrial membrane. These electrodes also exhibit robust response and stability that mimics the *in vivo* behavior of the oxidase. Results show that the electroreduction of dioxygen by the CCO modified electrodes is inhibited by cyanide binding, and that this inhibition is both reversible and dependent on the cyanide concentration. This system could potentially be used as a biosensor for toxins that inhibit electron transfer reactions of CCO with lethal consequences.

The Spin-Flip Method: Quantum Mechanical Analysis of Eneidyne Molecules, Sarah Remmert and Carol Parish, University of Richmond, Richmond, VA.

Complete understanding of the process of Bergman cyclization is essential to the development of more effective cancer drugs. This process involves the cycloaromatization of an enediyne moiety to produce a diradical capable of abstracting hydrogen atoms from the DNA double helix, causing cell death. Bergman cyclization can be characterized through computational analysis using various levels of quantum mechanical approximations to the Schrödinger equation, such as Hartree-Fock or Density Functional Theory. These two models differ in their treatment of inter-electron repulsion terms that prohibit mathematically exact solutions to the Schrödinger equation. In addition, the spin-flip method must be employed to study the properties of the diradical reactive intermediate. A relatively new computational approach, this method enables the use of the high spin triplet state as a reference in accounting for triplet and singlet low spin states, which are indistinguishable for open shell systems. Application of this theory enables a more effective description of the electron system, and thus yields more accurate values when calculating the energy and minimized structure of the diradical reactive intermediate.

A Combination Strategy for the Preparation of Rigidin Type Alkaloids, Austin B. Scharf, Barrett A. Little; Jonathan E. Hempel, Anastasia Kharlamova, Brad K. Norwood, Edith K. Banner, and John Gupton, University of Richmond, Richmond, VA.

Our research group recently reported the synthesis of the marine natural products polycitone A and B. Our strategy employed the conversion of a 2-arylvinamidinium salt to a 2,4-disubstituted pyrrole, which was acylated at the 5-position and subsequently halogenated and cross-coupled at the 3-position to yield the key synthon. We are currently examining a similar approach to Rigidin type pyrrolopyrimidine alkaloids and ongoing work in our lab will be presented.

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CAN YOU IDENTIFY THIS PERSON?



The photograph is from 1959 when the subject was Director of Research at the American Tobacco Company in Richmond. He was born in Lincoln, Vermont and received a B.S. degree from the University of Vermont in 1918. He worked for the DuPont Company for several years before joining American Tobacco in 1921. In 1932 he became the Director of Research. He served as Chairman of the Virginia Section in 1942 and received the Section's Distinguished Service Award in 1952. In 1959 he was the General Chairman for the Southeastern Regional Meeting of the ACS that was held November 4-7 at the John Marshall Hotel in Richmond.

The "mystery person" in the April issue was Frances Burger, wife of the late Dr. Alfred Burger. Dr. Burger spoke several times at Virginia Section meeting. The photograph was taken at the March, 1992 meeting at Longwood College.

