ANTIOXIDANT ANALYSIS OF COMMERCIAL SPICES. D. Killeen and M. H. Renfroe, Dept. of Biology, James Madison Univ., Harrisonburg VA 22801. There is a growing awareness of the role of antioxidants as an important component of human health. Antioxidants have been implicated in preventing degenerative diseases such as cancer, cardiovascular and neurological diseases, and reducing the effects of aging. Spices have long been part of the human diet and are known to have antimicrobial properties. We investigated eleven spices from around the Mediterranean, southern and southeastern Asia, and the West Indies. Cloves (823 μmol TE/g dw) and cinnamon (387 μmol TE/g dw) contained the greatest hydrophilic antioxidant content. Sage (68 μmol TE/g dw) and rosemary (60 μmol TE/g dw) contained the greatest lipophilic antioxidant content. Overall, cloves (835 μmol TE/g dw) and cinnamon (397 μmol TE/g dw) contained the greatest total antioxidant content. Other spices analyzed were oregano, mint, marjoram, allspice, ginger, allspice, and turmeric. Results indicated that spices are very potent sources of antioxidants and can complement one another to provide a variety of antioxidant molecules. Spices can complement other dietary components such as fruits and vegetables to greatly increase available dietary antioxidants.

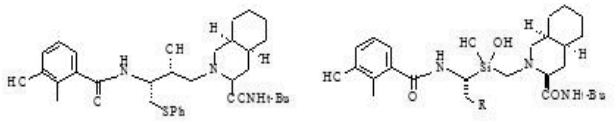
REHABILITATION OF RARE SPECIES POPULATIONS. Erin Gillin[1], Stephen W. Fuller[1] & Phillip Sheridan[2], [1]University of Mary Washington, [2]Meadowview Biological Research Station. Cell tissue culture of plant seeds has been used in previous research for horticultural and commercial purposes. This study focuses on successful seed propagation for the restoration of a variety of rare and endangered species. A standard tetrazolium test was used to determine the viability of the seeds. *Platanthera blephariglottis* (Willdenow) Lindley, white-fringed orchid, and *Tetragonotheca helianthoides* L., pinelands nerve-ray, seeds were used for both cell tissue culture and soil planting propagation. In cell tissue culture the seeds were sown aseptically on nutrient full media and stored in sealed sterile bags. Orchid protocorm development was expected, but only one vessel withstood contamination long enough to see some growth before also becoming contaminated. Failure in the aseptic processes caused loss of results for the project. Additionally, no growth was seen in the soil flats. This procedure has been successful in previous research, so we suggest further development of the methods to decrease contamination growth. With attention paid to sterile technique, plantlet development should be attainable in tissue culture for application for large scale production and wild population restoration. Further work with seed stratification and soil types is also recommended.

Chemistry

ASSESSMENT OF GUIDED INQUIRY IN GENERAL CHEMISTRY LABS: A THREE YEAR PROJECT. Heather N. Anthony & Jack K.Steehler, Department of Chemistry, Roanoke College, Salem VA 24153.This project investigates student improvements in chemistry laboratories when guided inquiry experiments are added. The project investigated student anxiety levels, content learning, and student perceptions of instruction. Three years of General Chemistry 111-112 were analyzed; the first year studied included mostly cookbook experiments, while years two and three

included a mixture of cookbook and guided inquiry experiments.Lab anxiety decreased after completing the course.The years in which guided inquiry experiments were incorporated saw a smaller decrease in anxiety about time availability. Students gained content knowledge during each experiment, regardless of pedagogy. For most experiments in which pedagogy changed, student content learning did not change significantly when the guided inquiry format was used. Students perceived *designing experiments yourself* as least helpful to their learning; however, as guided inquiry was added, their perception of helpfulness on this topic increased. This study was funded by the National Science Foundation.

COMPUTATIONAL EVALUATION OF SILICON-BASED HIV PROTEASE INHIBITORS, Chynna Blaker, Latricia Bowman, Victoria Parker & Wondwossen Arasho, Dept. of Chemistry and the Center for Biotechnology and Biomedical Sciences, Norfolk State University, 700 Park Avenue, Norfolk, VA 23504. There is no known cure for HIV/AIDS and it is imperative to develop a drug that will prevent the replication of the virus, without the stressing concern for resistance. Scientists across the globe struggle to create a mechanism that will slow down the mutations of the virus and suppress viral load in the infected human.This study focuses on HIV-1 inhibition therapy and utilizes the drug Nelfinavir (Viracept®) as a starting platform for preparation of a newly improved silicon-based drug. SYBYL software was used to test and compare the effectiveness of Nelfinavir against the silanediol analogue and other modified silanediol analogues. The original silanediol analogue (4.48p/l) proved to more effective than Nelfinavir (2.68p/l) according to the Surflex dock calculations from the SYBYL software.



THERMODYNAMICS OF THE SN2 VERSUS E2 COMPETITION. Charles M. Bump, Department of Chemistry, Hampton University, Hampton, VA 23668. Reactions between alkyl halides and strong bases give a mixture of both substitution (S_N2) and elimination (E2) products. The major product is usually discerned by students of organic chemistry on the basis of rote memorization of generalizations such as "2° halide plus strong base = elimination". The "answer" is technically correct, but an analysis of the factors that influence the major product is frequently sacrificed in favor of a quick answer to a complex question. Thermodynamics and kinetics are two major driving forces for organic reactions. We will describe how calculated thermodynamic properties (Gaussian 98, B3LYP) predict whether substitution or elimination is favored in these reactions.

THERMAL DECOMPOSITION OF METAL HYDROXIDES, A.Bagley, G.Berman & T.C. DeVore, Dep. of Chemistry and Biochemistry James Madison University, Harrisonburg VA 22897. Serious concerns about the quality of decomposition dynamics measurements obtained using standard thermal analysis methods have been

expressed over the past 25 years. The thermal decomposition of $Al(OH)_3$ has been investigated under a variety of experimental conditions to further explore the cause of these concerns. The results of these investigations indicate that while analysis using standard techniques such as those developed by Ozawa, Kessinger, and others appear to give describe the dynamics well, they give different answers as experimental conditions change. For example, the apparent activation energy increases by ~ 10 kJ mol^{-1} is decreased from 10 mg to 0 mg (determined by measuring the dynamics at several sample masses and extrapolating to zero mass). These results clearly indicate that this decomposition does not follow a one step mechanism and clearly indicate the need to use several sets of experimental conditions to determine the reaction dynamics for the process.

3,4:3',4'-BISBENZO[B]THIOPHENE AND RELATED DERIVATIVES: SYNTHESES AND INVESTIGATION OF THEIR ELECTRO-OPTICAL, CHELATING, AND BIOLOGICAL PROPERTIES. Marissa L. Estep, Diego S. Suarez Boscan, Matthew VanTil, Zachary R. Rhodenizer, Garth McGibbon & Michael R. Korn, Dept. of Biol. & Chem., Liberty Univ., Lynchburg, VA 24502. 3,4:3',4'-Bisbenzo[*b*]thiophene (BBT) was prepared following a published patent protocol. Molecular modeling computations of BBTcalculated itsbandgap (i.e. the energy difference between the HOMO and of LUMO) to be 3.61 eV (343 nm) (DFT, B3LYP, 6-31G*); to test for the accuracy of these computations, UV-vis spectroscopy of BBT was performed. The resultingspectrum (in dichloromethane) showed two maxima at approximately 383 nm and 365 nm, and two smaller peaks at 349 nm and 332 nm (shoulder); the UV-vis cut-off wavelength was at396 nm (3.13 eV). BBT was tested for intercalation into DNA because of its planar structure. Agarose gels were run in the presence of BBT and a DNA ladder (0.5-10 kb); however, no intercalation of BBT was observed as determined by the absence of fluorescence when gels were exposed to wavelengths of 254 and 365 nm; additional experiments are planned to further investigate the interaction of BBT with agarose gels as well as with DNA. BBT was also tested for antibacterial activity because of its two sulfur atoms; two strains of *Pseudomonas aeruginosa* were investigated which were grown in the presence of small paper discs soaked with BBT (from water and from DMSO). No growth inhibition was observed. Chelating properties are still under investigation as well as improved synthetic pathways to increase yields and reduce overall synthetic steps.(Supported in part by a $500 award from the Virginia Academy of Science).

A LUMINESCENCE DEMONSTRATION REACTION. Susan Hannegan & H. Alan Rowe, Department of Chemistry, Norfolk State University, Norfolk, VA 23504.Luminol ($C_8H_7N_3O_2$), also known as o-aminophthalylhydrazide, 5-amino-2,3-dihydro-1,4-phthalazinedione,and 3-aminophthatichydrazide, is used in popular luminescent chemical demonstration reactions as well as in forensic science for the detection of blood. Luminol added to a metal catalyst in a basic solution is oxidized resulting in the release of energy as light (maximum wavelength of 424 nm). Light from the oxidation of luminol is the basis for a sensitive method for the detection of blood. A popular chemistry luminescent lecture demonstration involves the addition of two solutions in the dark creating a dramatic glow. In one popular version, the solutions are noted as "A-1", consisting of luminol, in a complex salt solution, and

"A-2" a hydrogen peroxide solution. To establish the optimum conditions for this reaction each component wasvaried and the response evaluated using a computer-interfaced light sensor. De-oxygenation of both solutions resulted in an increase in both intensity and half-life presumably due to the elimination of quenching. Inclusion of cobalt instead of copper as the metal catalyst increased bothparameters. Alteration of the hydrogen peroxide concentration did not significantly improve the results, while exclusion of some components had a reciprocal effect: increasing intensity and decreasing half-life (sodium bicarbonate) and vice versa (sodium carbonate).

OYSTER RESTORATION AND WATER QUALITY ANALYSIS IN AN URBAN SUB-ESTUARY. Melinda Hopper, Matthew Boyce, & Dr. Maury Howard, Chemistry Department, Virginia Wesleyan College, 1584 Wesleyan Drive #B314, Norfolk, VA 23502. This study was conducted to monitor a local body of water and to determine the effect of oysters on water quality. The purpose is to determine whether oyster restoration can help the quality of the water and whether this site is an ideal location for restoration. Water samples were collected over a year long period at 3 different sites. Each sample was tested for various water quality indicators, including chlorophyll a, total phosphorus, temperature, pH, BOD and salinity. Sediment samples and oyster tissue samples were also collected and run through an ICP-MS to identify the toxic metals found within them. High concentrations of lead, mercury, arsenic, and other heavy metals were some of the main components. The water contained very low levels of metals due to the tidal influence. However, the sediments and oyster tissue contained high concentrations of many of them, showing the effects of bioaccumulation. It also shows the value of the oysters as filters for the system, removing toxins and nutrients from the ecosystem.

NEW SULFONE-DERIVATIVE PHENYLENEVINYLENE-BASED CONJUGATED POLYMERS FOR OPTOELECTRONIC APPLICATIONS. Thuong H. Nguyen & Sam-Shajing Sun, Department of Chemistry., Norfolk State University., Norfolk VA. 23504. A series of stable, processable, and end functionalizable sulfone-derivatized phenylenevinylene based conjugated polymers (SFPVs) containing different donor type co-monomers have been synthesized and characterized. The polymer main chains consist of a sulfone-phenylene electron accepting unit coupled with an electron donating unit derived from one of the dialdehyde co-monomers based on benzene, thiophene, and pyrrole. The solution optical energy gaps and the electrical energy gap (thin films) of these polymers are in the range of 1.94 - 2.45 eV and 2.04 – 2.51 eV respectively. The lowest energy gap was obtained from the polymer containing pyrrole unit due to the smallest resonance energy. The vinylene bounds on the polymer main chain are still chemically stable to survive strong basic conditions as compared to the S,S-dioxo-thiophene based PTV polymers developed earlier. These polymers also have very good thermal stability (onset decomposition temp, in N_2 gases, >270 ^{o}C). The lower energy gap P(Pyrrole-SFPV) exhibited ten times better photoelectric power conversion efficiency than the higher energy gap P(TV-SFPV). The diphosphonate ends functionalized and frontier energy level engineered of these conjugated polymers are very attractive in development of supramolecular block copolymers for the next generation of optoelectronic devices particularly in solar energy conversion applications.

BLUING OF *HYDRANGEA MACROPHYLLA* SEPALS BY INTRODUCING ALUMINUM IONS THROUGH ROOTS, CUT STEMS, AND SEPAL SURFACES. Henry D. Schreiber, Corinne M. Lariviere, Andrew H. Jones, Kelly M. Mayhew & Judith B. Cain, Department of Chemistry, Virginia Military Institute, Lexington, VA 24450. Sepals of many *Hydrangea macrophylla* are red when grown in basic to neutral soils, blue in acidic soils, and shades of purple in soils of intermediate pH. Delphinidin-3-glucoside that provides the red color to the sepals is transformed to a blue complex in the presence of molar Al(III). Al(III) is only mobile in acidic soils so the roots can only assimilate aluminum as a citrate complex into the plants under acidic soil conditions. The threshold Al(III) content for bluing is about 40-80 μg/g fresh sepal. If the Al(III)-citrate complex is introduced into cut stems of red hydrangea inflorescences, several orders of magnitude more Al(III) must be distributed to the sepals before bluing occurs. In addition, the bluing is not homogeneous throughout the sepals, but instead results in unique patterns in which the blue color advances from the center and outer edges. Evidently, the diffusion of Al(III) to the reaction centers, or pigment location, in the cell vacuoles is slow. An aqueous spray of a pH-adjusted Al(III)-citrate solution was also directly applied to the sepals over a period of time. The rapidity of the bluing was related to the pigment concentration of the sepals; the cultivars with the lighter sepals and less pigment blued faster as less Al(III) was required for a molar excess. The threshold Al(III) contents were about the same as when obtained through the roots.

HETEROGENEOUS OPENING OF EPOXIDES AND EPISULFIDES WITH AMINO ACIDS – AN APPROACH TO THE SYNTHESIS OF THIOLS. Marc-Antoine Tremblay, Eric P. Ginsburg, Chelsea L. Brown, Ellen R. Simmons, Dylan J. Jamieson & Jeffrey M. Carney, Department of Molecular Biology and Chemistry, Christopher Newport University, Newport News, VA 23606. Cystinuria is a metabolic disorder that results in the accumulation of insoluble and reoccurring cystine stones in the kidneys. Only a few methods for the treatment of cystinuria exist and surgery to remove the stones is frequently required. Further research is necessary to determine how to best prevent and treat this painful disorder. One known treatment involves the use of thiols to break up cystine and increase solubility of the stones through disulfide exchange. Our vision is to develop a small library of thiol compounds via the nucleophilic opening of episulfides with amino acid derivatives. Epoxide ring-opening with amino acids represents a simpler model system, but it has also not been extensively studied under heterogeneous conditions. We report our progress in the development of both epoxide- and episulfide-ring opening using amino acids and a solid catalyst.

MEASURING STUDENT COMPREHENSION OF LEARNING OBJECTIVES IN ORGANIC CHEMISTRY COMPUTATIONS EXPERIMENTS, M.K. Waddell, C. Bump, E. Ndip, and G. Nwokogu, Dept. Of Chemistry, Hampton University, Hampton, VA 23668. The incorporation of computation macromodels into several organic chemistry laboratory experiments has been an ongoing endeavor. As a result, the measurement of student comprehension of these computational experiments has been assessed. Students were surveyed on their perceptions of the learning objectives of an organic chemistry computation experiment. Pre and post surveys were administered through the BlackboardTM course webpage. Results were compared to identify trends and key areas of learning deficiencies.

Computer Science

ALERT: AN ARCHITECTURE FOR THE EMERGENCY RETASKING OF WIRELESS SENSOR NETWORKS. Syed R. Rizvi, Stephan Olariu, & Michele C. Weigle, Dept. of Computer Science, Old Dominion University, Norfolk, VA 23529. When an emergency or disaster strikes, first responders work as part of a complex emergency management network that calls upon many functions, resources, and capabilities. The objective of our research is to design a real-time information system to improve emergency-response functions by bringing together information to respond to a terrorist attack, natural disaster or other small or large-scale emergency. We call this system *ALERT: An Architecture for the Emergency Retasking of Wireless Sensor Networks*. The novel contribution of this research to the emergency response strategies is the seamless integration of various wireless sensor networks by *retasking* them with explicit missions involving a dynamically changing situation. Preliminary results have shown that retasking sensor networks for emergency response is a promising new paradigm that can not only promote a wider adoption of sensor network systems in support of guarding our national infrastructure and public safety, but can also provide invaluable help with disaster management and search-and-rescue operations.

DENSE UNSTRUCTURED AND STRUCTURED MATRIX COMPUTATIONS USING MPI. Stephen V. Providence, Dept. of Computer Science, Hampton University, Hampton, Virginia 23668. Computations with dense unstructured general matrices requires $O(n^3)$ operations and $O(n^2)$ words of storage for $n \times n$ input matrices. Such matrices are encountered in applications to solving integral equations. The best algorithms involving computations with dense structured matrices require $O(n \log^2 n)$ operations and $O(n)$ words of storage with small overhead constants. MPI or the message passing interface binds to the C programming language and is used to implement parallel algorithms. The time and space complexity estimates above are for sequential algorithms involving matrix computations. We have interest in the complexity estimates for parallel implementation of the sequential versions. For p processors where $p << n$, straightforward complexity estimates are proportional to $O(n^3)/p$ operations and $O(n^2)/p$ words for parallel implementation of dense unstructured general matrix computations. Analogously, computations with dense structured matrices require $O(n \log^2 n)/p$ operations and $O(n)/p$ words for parallel implementation. We conduct experiments on a high-performance computing cluster computer system to obtain the hidden constants in the O-notation of the estimates given.

Education

THE IMPROVING GROUNDS EXHIBITION. E. G. Maurakis, R. Conti, and D. Hagan. Science Museum of Virginia. Objectives of the Improving Grounds exhibition project are to create exhibits, programs, audio and video media for mass communication, and web-based curriculum materials on how to improve health and fitness. The overarching theme is a science perspective on understanding, testing, and measuring self-improvement in health and fitness. Exhibits and programming will be