

inflorescence surfaces via scanning electron microscopy (SEM). LM and SEM images were pooled with macrophotographs and line drawings from the literature to create an image bank. In class, each student then created, from scratch, a short PowerPoint presentation designed to analyze/interpret flower and inflorescence structure, drawing as needed from the image pool. At first students balked at the relatively open-ended and unstructured nature of the assignment, but soon began to engage with the challenge of making sense of the flowers and the different ways that the same structure can appear when rendered by different imaging techniques. Students discovered for themselves the peculiar flowers of *Dorstenia*, thus broadening their understanding of the fundamentals of flower structure and floral diversity.

### Chemistry

IS  $\text{TiF}_2$  REALLY LINEAR? T.C. DeVore, Department of Chemistry and Biochemistry, James Madison University, Harrisonburg VA 22807. The molecular geometry of the first row transition metal difluorides has been of interest to experimentalists and theorists for over 40 years. Recently, Wilson et al. concluded that there was no evidence that any of these compounds were non-linear. Density functional theory (DFT-B3LYP with a 3-611G++ (3df,3pd) basis set) has been used to determine the molecular geometry and the vibrational frequencies for  $\text{TiF}_2$  and  $\text{Ti}_2\text{F}_6$ . These calculations indicated that the  $^3\text{B}_2$  ground state of  $\text{TiF}_2$  was non-linear with a bond angle of  $\sim 139.2^\circ$ . The bond length was 180.6 pm. The  $^3\text{B}_{2u}$  ground state of  $\text{Ti}_2\text{F}_6$  has  $\text{D}_{2h}$  symmetry with terminal and bridging bond lengths of 178.3 and 180.3 pm respectively. The terminal F-Ti-F bond angle is  $125.1^\circ$ . The IR active Ti-F stretching frequencies are 728.19 and 625.13  $\text{cm}^{-1}$  for  $\text{TiF}_2$  and 755.9, 681.0 and 513.0  $\text{cm}^{-1}$  for  $\text{Ti}_2\text{F}_6$ . The calculations indicate that in contrast to the recent conclusions reached by Wilson et al., the ground state of  $\text{TiF}_2$  is non-linear.

THE SYNTHESIS OF NITROGEN-AND SULFUR-CONTAINING HETEROCYCLES FROM CYCLO-PROPANOL FRAGMENTATION. Georgia T. Stoyanov, Kelly L. George & Kevin P.C. Minbiole, Department of Chemistry and Biochemistry, James Madison University, Harrisonburg VA 22807. The prevalence of heterocycles as the backbone of common pharmaceutical entities has created a demand for simple reactions to prepare them. Our research aimed to create six- and seven-membered heterocycles containing both a carbonyl group and either sulfur or nitrogen in the ring. This is modeled after a cyclopropanol fragmentation approach to the formation of oxepanes developed previously in our group. Our current endeavor is to synthesize nitrogenous heterocycles, specifically piperidines and azepines, as well as sulfur-containing thiepanes. The nitrogenous approach begins with suitably protected  $\alpha$ - or  $\beta$ -amino acid ethyl esters which were transformed by cyclopropanols via the Kulinkovich reaction. The resulting  $\alpha$ - or  $\beta$ -amino cyclopropanols were then reacted with various aldehydes to form an aminal. Subsequently, various Lewis acids were investigated to promote the rearrangement of the aminal into the piperidine or azepine. Analogously, a seven-membered sulfur-containing heterocycle was formed, albeit in low yields.

ANTHOCYANIN AND ALUMINUM CONTENT OF RED AND BLUE SEPALS FROM SELECTED *HYDRANGEA MACROPHYLLA* CULTIVARS. Henry D. Schreiber, Samantha E. Wade, Kelly M. Mayhew, Andrew H. Jones & Judith B. Cain, Department of Chemistry, Virginia Military Institute, Lexington VA 24450. The primary pigment in sepals (modified leaves comprising the inflorescences) of hydrangea is an anthocyanin, delphinidin-3-glucoside. In red sepals, this anthocyanin occurs as its red flavylium cation. In acidic soil, aluminum as  $Al^{3+}$  is incorporated through the roots into the shrub and is transported to the sepals where  $Al^{3+}$  forms a complex with the blue quinoidal base anion of this anthocyanin. Analyses of the red and blue sepals of numerous hydrangea cultivars show that whereas red and blue sepals of the same cultivar have the same anthocyanin content, individual cultivars can be classified by their unique anthocyanin contents. For example, the popular remonant or cold-hardy cultivars have 80-120  $\mu\text{g}$  anthocyanin per g fresh sepal, while the most vibrantly colored cultivars have over 300  $\mu\text{g}$  anthocyanin per g fresh sepal. The anthocyanin content of a particular cultivar is typically proportional to its perceived intensity of coloration. Bluing of the sepals on the average require about a 10-fold molar excess of aluminum over anthocyanin, meaning that the threshold aluminum content for bluing is also cultivar dependent. Experiments have also shown that greater aluminum contents than the threshold for that cultivar do not result in bluer sepals, in agreement with a chemical model for bluing.

CHEMICAL CONTROL OF PAPERWHITE (*NARCISSUS TANZETTA ZIVA*) GROWTH AND FLOWERING. Timothy V. Johnson & Henry D. Schreiber, Department of Chemistry, Virginia Military Institute, Lexington VA 24450. Paperwhites, *Narcissus tanzetta* Ziva, are plants that are commonly grown from bulbs for winter blooming indoors. They are known for their stunning white flowers, but these flowers are often perched on top of a much too-tall stem that seems out of proportion to the flowers. In a previous study, paperwhite bulbs were grown in alcoholic solutions (optimal 5 vol% ethanol) instead of water, resulting in shorter stems to remedy the plant's "floppiness" without sacrificing floral quality. This study expanded the prior work by testing a wider variety of alcohols and other common laboratory and household chemicals. Growing paperwhites in a 5 vol% solution of ethanol in water indeed stunted the stems of the plants, but also lessened the number of flowers, in contradiction to the previous study. 5 vol% solutions of ethanol, methanol, isopropanol, ethylene glycol, glycerol, and acetone in water were all effective at stunting the stem growth by 33-50%, but the number of flowers also tended to be about 33% less than the control (water). The size of the blooms as well as the bloom period remained unaffected by the chemical additives. The chemical additives appeared to stunt but not kill the paperwhites, for which the additives acted as a mild toxin. Thus, although alcoholic solutions are effective in producing dwarf paperwhites, the previous conclusion that floral quality remains unaffected is misleading.

SUBUNIT INTERACTION OF THE CAP METHYLTRANSFERASE. Joolan Saroor, Jessica N. Skeeter, Jeanhee Chung & Thomas O. Sitz, Dept. of Biochemistry, Virginia Tech, Blacksburg, VA 24061. The 5'-end of eukaryotic mRNA is capped and

methylated in the N-7-position of the guanine base generating a fully functional cap structure. If the cap is not methylated at this position, the mRNA is not translated, i.e. this methylation is essential for gene expression. The enzyme that methylates the N-7 position, Guanine-7-methyltransferase, has been expressed as a His-tag protein in *E. coli*. The addition of histidines at the N-terminus allows the enzyme to be purified on a Nickel column. The full length enzyme, 476 amino acids long, and the deletion mutation, 120 amino acids removed from the N-terminus, are about 80% pure after the nickel column. To further purify the enzymes, a positively charged ion-exchange column (Mono Q-Sepharose) was used resulting in greater than 95% purity. This purified guanine-7-methyltransferase (full length and deletion mutation enzyme) was then applied to a FPLC-Superose 12 gel exclusion column and two major peaks of protein were observed for both the full length and the deletion mutation enzyme which corresponded to about 90% homodimer and 10% monomer for each respectively. The purified enzymes were also analyzed by blue-native polyacrylamide gel electrophoresis and the deletion of 120 amino acids had no effect on the subunit interaction, i.e. about 90% dimer. The enzyme samples were then subjected to cross-linking with 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and N-Hydroxysuccinimide (NHS). Both the full length and deletion mutation were not cross-linked, suggesting that dimers were not formed by charge interaction (electrostatic interaction).

POLYCEPHALIC (MULTI-HEADED) CATIONIC AMPHIPHILES AS NOVEL SURFACTANTS AND ANTIMICROBIAL AGENTS. Robby Davis<sup>1</sup>, Christian Schwantes<sup>1</sup>, Devon Flaherty<sup>2</sup>, Kevin Caran<sup>1</sup>, Kevin Minbiole<sup>1</sup> & Kyle Seifert<sup>2</sup>, <sup>1</sup>Department of Chemistry and Biochemistry, James Madison University, Harrisonburg VA 22807 and <sup>2</sup>Department of Biology, James Madison University, Harrisonburg VA 22807. We recently reported the synthesis and colloidal study of a novel series of biscationic bicephalic amphiphiles, each with two charged head groups and a single nonpolar tail connected via an arene core. Initial biological testing showed that six of seven amphiphiles tested were antibacterial and/or antifungal; several inhibited bacteria more effectively than ampicillin. We aim to build on this preliminary data and investigate the structure dependence and mechanism of antimicrobial activity of a wide range of cationic multiheaded amphiphiles. We will incorporate different substitution patterns as well as vary the cationic and hydrophobic groups to access a diversity of related amphiphilic structures. Colloidal characteristics of these surfactants will be assessed. We plan to determine the MIC and mechanism of action of each synthesized compound. Then, correlation of monomeric structure, aggregation tendencies, and mechanism of action will be examined.

AMPHIBIAN CHEMICAL DEFENSE: IDENTIFICATION AND APPLICATION OF ANTIFUNGAL METABOLITES FROM JANTHINOBACTERIUM LIVIDUM AND PEDOBACTER CRYOCONITIS. Jacob Smith & Kevin P. C. Minbiole, Department of Chemistry and Biochemistry, James Madison University, Harrisonburg VA 22807. To develop a probiotic antifungal treatment against the deadly fungus *Batrachochytrium dendrobatidis*, anti-fungal metabolites from bacteria on the amphibians' skin were identified. As a preliminary step, metabolites from *Pedobacter*

*cryoconitis* separated through HPLC are currently being tested against *B.d.* A previous study of the mountain yellow-legged frog (*Rana muscosa*), infected with *B.d.*, provides a model for the probiotic treatment of amphibian populations with *Janthinobacterium lividum*. A study is underway to measure the effects of *Janthinobacterium lividum* against Chytridiomycosis on the extirpated Panamanian golden frog (*Atelopus zeteki*). A soil extraction protocol to detect violacein, currently under development, will allow for the identification of *J. lividum* in soil samples. If successful, this could simplify the transition from the lab to the wild.

THREE *ARABIDOPSIS THALIANA* MYO-INOSITOL 1-PHOSPHATE SYNTHASE GENES ENCODE BIOCHEMICALLY SIMILAR ENZYMES. Xinyi Huang, Marcy Hernick & Glenda E. Gillaspay,

Dept. of Biochemistry, Virginia Tech, Blacksburg, VA 24061. Inositol L-*myo*-inositol 1-phosphate synthase (MIPS; EC 5.5.1.4) catalyzes the conversion of D-glucose 6-phosphate to 1L-*myo*-inositol 1-phosphate. The expression pattern and metabolite function of three MIPS genes from *Arabidopsis thaliana* have been characterized. In order to prove that these proteins were similar enzymes with similar catalyzing ability, MIPS1, MIPS2 and MIPS3 ORFs were cloned into vector pDEST17 and induced in *E. coli* BL21(DE3) strain. The N-terminal his-tagged MIPS proteins were purified by Ni-IMAC (Fig.1). The yield of MIPS proteins were among 4 to 20 mg/L culture. The catalytic activity of MIPS proteins was measured under steady-state conditions, by coupling reaction with excessive amount of *myo*-Inositol monophosphatase (IMP, EC 3.1.3.25) at 30°C. The kinetic parameters ( $k_{cat}$ ,  $K_M$ ,  $k_{cat}/K_M$ ) were obtained by fitting the Michaelis-Menten equation to the initial linear velocities measured at the various substrate concentrations. The kinetic properties of MIPS1, MIPS2 and MIPS3 were not significantly different among each other ( $\geq 2$  fold) Thus, we concluded that MIPS proteins were similar enzymes in plants, and the different impact on growth and cell death was due to the developmentally and spatially regulation of MIPS genes expression.

EXPRESSION AND PURIFICATION OF Rv0323c, A HYPOTHETICAL MYCOBACTERIAL PROTEIN. J. Boggia & M. Hernick, Dept. of Biochemistry, Virginia Tech, Blacksburg, VA 24061. Mycothiol is the primary reducing agent used by mycobacteria to prevent against oxidative damage. Consequently, enzymes involved in mycothiol biosynthesis are targets for antibiotic development. One of the key steps in this pathway is the hydrolysis of GlcNAc-Ins to form GlcNH<sub>2</sub>-Ins and acetate. Under normal conditions, this reaction is catalyzed by the enzyme MshB. However, the MshB knockout is capable of producing some, albeit decreased, mycothiol indicating that there are one or more redundant enzymes. Based on sequence alignment data, there are two potential enzymes that may fulfill this function, mycothiol-conjugate amidase (MCA) and the hypothetical protein Rv0323c. We have cloned the genes for both of these enzymes into vectors that allow for the recombinant expression of these proteins in *E. coli*. We have been able to express and purify the protein encoded by the Rv0323c gene. Current efforts are focused on characterization of the Rv0323c function, and determination of whether it possesses GlcNAc-Ins deacetylase activity.

SOLUTION-PHASE SYNTHESIS OF CuPt BIMETALLIC CATALYSTS AND THEIR APPLICATIONS IN CO OXIDATION. Q. Liu<sup>1</sup>, D. W. Goodman<sup>2</sup>, J. D. Batteas<sup>2</sup> & R. E. Schaak<sup>3</sup> <sup>1</sup>Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807, <sup>2</sup>Department of Chemistry, Texas A&M University, College Station, TX 770842 and <sup>3</sup>Department of Chemistry and Materials Research Institute, The Pennsylvania State University, University Park, PA 16802. A mixture of CuPt nanospheres and nanorods was directly synthesized in liquid phase. The characterization of Transmission electron microscopy (TEM) and X-ray diffraction (XRD) demonstrated that the atomic ratios of Cu/Pt in both spheres and rods are very close to 1. Moreover, the length of the nanorods can be tuned by changing reaction conditions in the range of 10 to 55 nm and a possible formation mechanism for these nanorods was hypothesized. To investigate the catalytic activities of resulted CuPt nanoparticles, the nanospheres and nanorods were separately deposited on Al<sub>2</sub>O<sub>3</sub> and then used as catalysts probing the light-off temperature for oxidation of CO to CO<sub>2</sub> in a closed system.

METHOD DEVELOPMENT FOR ELEMENTAL ANALYSIS OF FOLIAR BLUEBERRY (*VACCINIUM CORYBOSUM* L.) SAMPLES. Allison E. Glick, Denay M. Fuglie, Braydon P. Hoover & Roman J. Miller, Dept. of Chem., Eastern Mennonite Univ., Harrisonburg, VA 22802. Nutrient levels in blueberry leaves from established Blueray, Coville, and Jersey cultivars were analyzed by flame atomic absorption spectroscopy (FAAS) in a method development to use in research for a model organic blueberry farm. Foliar samples were oven-dried or oven-dried and dry-ashed at 450° C, then digested with 6 M HCl or concentrated HNO<sub>3</sub>, and compared for higher extraction of the elements Fe, Zn, Mn, Cu, Ca, and Mg. There were no differences in which acid is used to digest nor whether the sample is ashed. However, the blueberry cultivars did differ in elemental concentrations and cannot be grouped together for nutrient evaluation. Older leaves also had different elemental concentrations as measured by FAAS than younger leaves gathered from the same bush. FAAS could also detect difference between a healthy bush and one recovering from stress. Using oven-dried leaf samples digested with 6 M HCl is the method of choice to measure the nutrients Fe, Zn, Mn, Cu, Ca, and Mg. (Research supported in part by USDA Specialty Crop Grant # 2008-427, Commonwealth of Virginia, Department of Agriculture and Consumer Services.)

SPECIFIC ION EFFECTS ON PROTEIN AGGREGATION. Yanjie Zhang<sup>1\*</sup>, Branden Deyerle<sup>1</sup>, Justin Hagerman<sup>1</sup>, Paul S. Cremer<sup>2</sup>, <sup>1</sup>Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807 and <sup>2</sup>Department of Chemistry, Texas A&M University, College Station, TX 77843. Specific ion effect was first noted by a protein chemist, Franz Hofmeister, over a hundred years ago that ions showed varying abilities to precipitate protein molecules out of solution. This effect is known as a recurring trend in a variety of physical and biochemical processes such as protein stability, enzyme activity, and colloidal assembly. Despite its generality, the understanding about the mechanism of the Hofmeister effect on molecular level is far from complete. In this presentation, interactions between ions and

protein molecules were investigated in a temperature gradient microfluidic setup and the mechanism of the Hofmeister effect was elucidated.

**BIOMINERALIZATION TEMPLATED BY AMINO ACID-BASED CHIRAL MOLECULES.** Justin Hagerman, Branden Deyerle, Yanjie Zhang, Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807. Biomineralization is an extremely widespread phenomenon in the biological world. Examples of biominerals include silicates in algae and diatoms, carbonates in invertebrates, and calcium phosphates and carbonates in vertebrates. The functions of biominerals range from magnetic sensing to structural support. Herein, amino acid-based chiral molecules were employed as model systems to direct the growth of biominerals. The role of chiral molecules and the mechanism for the nucleation and crystallization of biominerals will be discussed.

**HOFMEISTER EFFECTS ON THE PHASE BEHAVIORS OF THERMAL RESPONSIVE POLYMERS.** Branden Deyerle, Justin Hagerman, Yanjie Zhang, Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807, Over the last 120 years, a wide variety of phenomena from protein folding and enzymatic activity to colloidal assembly and protein crystallization have been shown to follow the Hofmeister series. Despite its ubiquity, a molecular level understanding of the Hofmeister series is still lacking. Herein, we will employ a model system, phase transitions of thermoresponsive triblock copolymers, to investigate the mechanism of the Hofmeister series on the molecular level. The phase transition temperatures of these triblock copolymers were measured in the presence of Hofmeister anions and the data were correlated with the properties of anions.

**EXPERIMENTAL AND COMPUTATIONAL APPROACHES TO IDENTIFY SELECTIVE INHIBITORS OF CASEIN KINASE 1 FROM *TRYPANOSOMA CRUZI*.** Sahil Khanna, Pablo Sobrado & David Bevan, Department of Biochemistry, Virginia Tech, Blacksburg VA 24060. *Trypanosoma cruzi* casein kinase 1 (TcCK1) is a multifunctional Ser/Thr protein kinase that catalyzes the phosphorylation of key proteins in regulation pathways. Its function in cell growth makes TcCK1 a potential drug target to prevent the growth of *T. cruzi*. Infection by *T. cruzi* parasite results in Chagas disease, known to cause sudden cardiac failure. Human casein kinase 1 delta (hCK1 $\delta$ ) is important to proper physiological function of human cells, therefore the drugs developed need to be selective towards TcCK1 over hCK1 $\delta$ . Computational docking experiments of 14 potential inhibitors to both TcCK1 and human casein kinase 1 delta (hCK1 $\delta$ ) were performed using Dock6. Analysis of the ATP binding pocket of TcCK1 and hCK1 $\delta$  showed exploitable structural differences, particularly spacing between residues E49/D149 in TcCK1 and E50/D149 in hCK1 $\delta$ . The resulting grid scores have indicated 5 inhibitors for *in vitro* study, (R)-DRF053, Purvalanol B, CKI-7, PF670462, and D4476. TcCK1 was cloned into Top-10 *E. coli* cells and co-expressed along side chaperone protein complexes DnaK-DnaJ-grpE and GroEL-GroES. TcCK1 was partially purified utilizing an Immobilized Metal Affinity Columns (IMAC). A  $\gamma$ -<sup>32</sup>P-ATP assay was used to determine a  $K_m$  value of  $2.3 \pm 0.72$  mg/mL for  $\alpha$ -casein as

a substrate. A method to obtain active enzyme was formed, and can be used for further inhibition studies.  $K_i$  values for selective inhibitors determined by the *in silico* study can be obtained.

### Computer Science

USING SECOND LIFE FOR COMPUTER SCIENCE EDUCATION. Robert A. Willis Jr. Department of Computer Science, Hampton University. Over the past few years, I have noticed that our students are reluctant to approach learning computer science in the traditional ways. Computer science requires beginning students to learn the concepts of computer science and the art of programming. While disparate, both of these facets require a good deal of study using texts and practice. Second Life is used to implement a number of innovative interactive tutorials tailored for this generation of students. Furthermore, the environment is conducive for instruction in a number of other areas in computer science (and other disciplines). Second Life is a three dimensional virtual world. It is a social environment that allows people to “live” much as they do in real life. People (represented as avatars) can purchase land, build houses, work, play, and participate in many other activities. It is an ideal environment to reach all levels of students.

INTERACTIVE PARAPHRASE TRAINING: THE DEVELOPMENT AND TESTING OF AN ISTART MODULE. Chutima Boonthum. Department of Computer Science, Hampton University Hampton University. Comprehension of science texts is challenging, particularly when the reader lacks the skills or knowledge necessary to fill in conceptual gaps in the text content. The iSTART system was developed to help readers learn and practice reading strategies to improve their ability to comprehend challenging text. This study describes a new iSTART module recently developed and tested, called Interactive Paraphrasing (IP), in which students are interactively and adaptively taught how to paraphrase sentences. We compared the effects of iSTART to iSTART with IP (IP-iSTART) with high school students on their strategy use and ability to comprehend text. IP-iSTART increased skilled readers’ self-explanation quality, improved their ability to answer online comprehension questions, and increased their use of paraphrases after training. Less skilled readers benefited most in self-explanation quality from the original version of iSTART. Results are discussed in terms of tailoring reading strategy training to the needs of the reader.

GENERATION Y AND COMPUTER LITERACY/EDUCATION. Angela Hayden. Department of Computer Science, Hampton University Hampton University. The generation of Americans born between 1977 and 1994 are affectionately known as Generation Y. They hold to similar values of their parents, but will challenge authority and the information given them in any setting. They possess a variety of skills including computer skills, making them the most computer literate of all generations prior to them. They can be stimulated through a variety of means, most of which are visual and audio. They also appreciate having fun more than just learning facts. Strategies for both study and pedagogy offered as suggested means to help students learn have not changed