

is not sister to *M. pratense*. Rather, this analysis provides mixed support for the competing hypotheses of European versus Asian ancestry.

### Chemistry

CHEMICAL PROBES FOR PROTEIN N-TERMINAL METHYLTRANSFERASE. Rong Huang, Gang Zhang, Yunfei Mao, & Stacie Lynn Richardson, Department of Medicinal Chemistry, Institute for Structural Biology and Drug Discovery, Virginia Commonwealth University, Richmond VA 23219. The objective of this study is to develop chemical probes for N-terminal RCC1 methyltransferase (NRMT1). NRMT transfers methyl groups from S-adenosyl methionine to the N-terminal alpha-amine of proteins. It plays an important role in regulating protein-DNA binding and protein-protein interactions. However, there is no chemical tool available to further characterize NRMT biological and pharmacological roles. We have characterized the kinetic mechanism of NRMT1 using recombinant NRMT1 via a MALDI-MS method. Our results indicated that NRMT1 catalysis underwent a formation a ternary complex. Based on this mechanism, we adopted a bisubstrate strategy to design NRMT inhibitors to covalently link an N-adenosyl methionine (NAM) to a peptide derived from N-terminal protein substrate. We have successfully synthesized a series of bisubstrate analogues and determined their inhibitory activities via a fluorescent competitive assay. Among them, SPKR-NAM exhibits a highest inhibitory activity with an  $IC_{50}$  of 13.4  $\mu$ M. As negative controls, both NAM-triazole and triazole-peptide did not show any significant inhibition at 100  $\mu$ M. In conclusion, our bisubstrate inhibitors showed more than 10-fold inhibitory activities and they can be used as chemical tools for future study of NRMT1.

THE BLACK POLYMORPH OF TTF-CA: TTF POLYMORPHISM AND SOLVENT EFFECTS IN MECHANOCHEMICAL AND VAPOR DIGESTION SYNTHESSES, FT-IR, CRYSTAL PACKING AND ELECTRONIC STRUCTURE. Silvina Pagola<sup>1</sup>, Saul H. Lapidus<sup>2</sup>, & Amit Naik<sup>3</sup>, <sup>1</sup>Department of Applied Science, College of William and Mary, Williamsburg, VA, 23187, <sup>2</sup>Dept. of Physics & Astronomy, Stony Brook University, Stony Brook, NY, 11794, & <sup>3</sup>Thomas Nelson Community College, Hampton, VA, 23666. Tetrathiafulvalene-chloranil (TTF-CA) was synthesized by liquid assisted grinding (LAG) and vapor digestion (VD), largely reducing the use of reaction solvents. The effects of the small quantities of LAG and VD solvents towards the formation of a particular TTF-CA polymorph were studied from the orange and brown tetrathiafulvalene (TTF) polymorphs as reactants. A high solvent polarity favors the formation of the ionic (black) TTF-CA vs. the quasi-neutral green form, whereas the crystal structure and crystal habit of the orange TTF also favors the formation of the black TTF-CA. The crystal structure of the black TTF-CA was determined from synchrotron X-ray powder diffraction and it consists of dimerized  $TTF^{\bullet}$  and  $CA^{\bullet}$  radical ions, in agreement with room temperature magnetic susceptibility measurements indicating the material is diamagnetic. The black TTF-CA does not undergo a phase transition in the range 298K-20K. FT-IR showed that the compound is a semiconductor with a band gap of  $\sim$ 0.198 eV and it remains ionic at low temperatures. Band structure calculations are in good agreement with the measured band gap.

TESTING FOR INTERFERING SUBSTANCES USING OIML RECOMMENDED CONCENTRATIONS ON VIRGINIA INTOX EC/IR II BREATH TEST INSTRUMENTS. T. L. Neece, Jr., M. S. Kennedy & A. B. Lohmann, Virginia Department of Forensic Science, Richmond VA 23141. The International Organization for Legal Metrology (OIML) has established recommendations for breath alcohol testing related to the interference of chemicals that may occur in human breath at the time of sampling. Acetone, methanol, and isopropanol are currently listed as possible interferents and were tested on the Intox EC/IR II by the Virginia Department of Forensic Science. Acetaldehyde was also tested in this study as it was previously listed by OIML and examined by the laboratory. These chemicals were tested at, above, and below the levels recommended by OIML. Results of this testing demonstrate the Intox EC/IR II with Virginia firmware meets the OIML interfering substance recommendations to ensure accurate and precise testing of evidential breath samples in the Commonwealth of Virginia.

EVALUATION OF THE EFFECT OF INVISALIGN ON MOUTH ALCOHOL RETENTION ON THE INTOX EC/IR II BREATH TESTING INSTRUMENT. M. M. Billeter, M. S. Kennedy & A. B. Lohmann, Virginia Department of Forensic Science, Richmond, VA 23219. The presence of an Invisalign device was evaluated to determine if it will retain mouth alcohol and interfere with the accuracy of a breath test. The rate of mouth alcohol elimination was observed in one subject wearing Invisalign. The subject was tested under two conditions. The first test was while wearing the device. The subject rinsed her mouth with a 43% ethanol solution and was tested immediately on the Intox EC/IR II Breath Instrument. In the second test, the subject rinsed with the alcohol beverage and then placed the Invisalign in her mouth and was again tested immediately. It was observed that after 10 minutes, no residual mouth alcohol remained. This confirmed that the 20 minute observation period prior to performing a breath test ensures that there is no effect from residual mouth alcohol when wearing an Invisalign device.

THE EFFECT OF STORM WATER RETENTION PONDS ON WATER QUALITY IN AN URBANIZED AREA AS INDICATED BY ANION CONCENTRATIONS. C. Aneroussos & M. Howard, Department of Chemistry, Virginia Wesleyan College, Norfolk, VA 23502. The focus of the current study is to establish a baseline of sampling and analysis methods for future research while simultaneously collecting and analyzing preliminary data for the long term goal of increasing storm water pond efficiency through the use of vegetation. Storm water retention ponds act as collection points (or buffer areas) for run-off water, before the water travels to natural water sources such as streams, lakes or oceans. Past research suggests that storm water retentions ponds affect anion concentrations, and therefore water quality in an urbanized area. The anion concentrations present in the runoff water of urbanized areas is largely influenced by human activity. Major anions such as chloride, phosphate and sulfate come from a number of sources including farming activity, pollution emission, natural ecological activities such as excretion and many more. Significant imbalances in the anion concentration can cause a plethora of negative from harmful algal blooms, to dead zones, to ecosystem (resource) distortion. The research being discussed took place over the course of approximately 4 weeks. Water samples were collected from

storm water retention ponds located on the campus of Virginia Wesleyan College and were analyzed by ion chromatography to determine anion concentrations. The research was conducted during the winter season in order to limit the effect of biological activity (which is severely reduced in the winter months) and explores sampling methodology, methods of analysis and establishes a baseline for reference as the project continues.

AN INVESTIGATION OF THE COMPOSITION OF GLAZE AND CERAMIC PIECES FROM NICARAGUA. A. Ibarra & M. Howard, Department of Chemistry, Virginia Wesleyan College, Norfolk, VA 23502. The purpose of this experiment is to examine the compositional variation in glazed and unglazed ceramic samples from collection sites in Nicaragua. Physical and chemical properties are compared using scanning electron microscopy and energy dispersive spectroscopy (SEM-EDS). Trace elements are also analyzed using flame atomic absorption spectrometry (FAAS). Glazes and ceramics used in commercial production of pottery versus traditionally produced vessels and those sold by local Nicaraguan street vendors are compared to identify similarities and differences in composition.

PROGRESS TOWARDS THE SYNTHESIS OF A SERIES OF TPA CENTROSYMMETRIC VINYLENE-BRIDGED ARYL STYRYL HETEROCYCLIC D-PI-D SYSTEMS. Michelle K. Waddell, Department of Chemistry, Hampton University, Hampton, VA 23668. As a result of their unique delocalized  $\pi$ -electron systems and fascinating optical and electro-optical properties, conjugated organic molecules and polymers are making significant contributions to the emerging technologies of molecular electronics and photonics. One area of research interests is the design, synthesis, and investigation of conjugated organic compounds with new molecular architectures to be used as electronic and photonic materials – multichromophoric benzenes. Organic molecular systems with large multi-photon absorption, MPA, in particular, Two Photon Absorbance (TPA) cross-sections, have a broad spectrum of technological applications. The use of organic methods for the synthesis of these compounds is ideal: it permits not only the tailoring of molecular structures to enhance specific properties, but also the tuning of physical characteristics via changes in functionality. Progress towards the synthesis of 2,5-bis(4'-N,N-diethylaminostyryl)thiophene (BEST), 2,5-bis(4'-N,N-diethylaminostyryl)furan (BESF) and 2,5-bis(4'-N,N-diethylaminostyryl) pyrrole (BESP) was performed with characterization of these compounds. These compounds were synthesized in a three step process which readily allows for the interchange of reagents to generate a library of compounds. Fluorescence absorption spectra of these compounds will be compared to computational models to validate the results of theoretical studies.

INTERACTION OF METAL NANOPARTICLES WITH THIOL AND THIOETHER-CONTAINING COMPOUNDS. S. Babu<sup>1</sup>, Jaetae Seo<sup>2</sup> & M. O. Claville<sup>1</sup>, <sup>1</sup>Department of Chemistry and <sup>2</sup>Department of Physics, School of Science, Hampton University, Hampton, VA 23668. Gold nanoparticles (Au NPs) have vast applications in drug therapy because of their unique optical, electronic and molecular properties. We present preliminary findings regarding the interaction of Au NPs with methionyl compounds, L-Methionine (Met), D/L-Met, N-Acetyl-L-Met, L-Met Ethyl Ester, and Met-Glycine. The average sizes of the eight Au NPs used in the study are ~5, ~10, ~15, ~20, ~30,

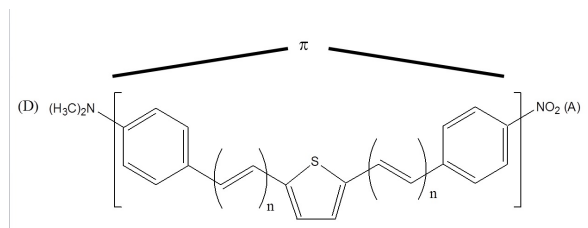
~32, ~35, and ~40 nm diameters. The UV-Vis spectral studies showed that Au NPs exhibit a strong plasmon at ~530 nm while the methionyl compounds displayed an additional plasmon band at ~785 nm, indicating the formation of Au NPs aggregates. Methionine was found to aggregate Au NPs (conc.  $3.487 \times 10^{-10}$  M) with size ~35 nm at higher concentration (final 0.125 M) with the color change from red to blue. While lower concentration of L-Met and D/L-Met did not aggregate immediately, N-terminal (N-Acetyl-L-Met) and C-terminal protected Met (Met Ethyl Ester) readily formed Au NPs aggregates. Methionine-Glycine dipeptide was only slightly better than D/L-Met at inducing aggregation of Au NPs. The results provide insight into the impact of NP size, peptide sequence, and concentration of NPs, on aggregation. We strongly believe aggregation size and kinetics may have a role in the etiology of cellular response which needs to be systematically evaluated. [Supported by the National Science Foundation-Faculty Early Career Development (CAREER) Award, CHE-0847742 and ACE Implementation Award NSF HRD-1238838]

LEAVING GROUPS IN SUBSTITUTION AND ELIMINATION REACTIONS: AN UNEXPECTED JOURNEY. Charles M. Bump, Department of Chemistry, Hampton University, Hampton, VA 23668. Calculated (B3LYP – 3-21G) thermodynamics of competing  $S_N2$  and E2 reactions are consistent with textbook descriptions of the competing reactions in concluding that elimination is thermodynamically favored at higher temperature. This is not a surprise since the entropy change for substitution reactions is small while the entropy change in eliminations is large. At higher temperatures, the TΔS term in the definition of Gibbs free energy ( $\Delta G = \Delta H - T\Delta S$ ) is of minor importance in substitution reactions since ΔS is nearly zero while that term becomes increasingly larger in elimination reactions. A plot of ΔG as a function of temperature reveals a common temperature above which elimination is favored – regardless of leaving group. A steeper (more negative) slope of the ΔG vs. T plot is indicative of a “better” leaving group. Or is it?

THE EFFECT OF THE PRESENCE OF Ag ON HOMO-LUMO VALUES OF THIOPHENE. C. S. McKinney & S. M. Black, Center for Materials Research, Norfolk State University, Norfolk, Virginia 23504. Transforming solar energy into electricity using photovoltaic devices provides clean, abundant and renewable energy for readily use. The alignment of HOMO and LUMO levels of donor and acceptor moieties in organic solar cells can enhance the efficiency of photovoltaic devices. We use Density Functional Theory to determine the effect of the presence of a silver dimer on the frontier orbitals of Thiophene. HOMO and LUMO energy levels and gap were obtained for the isolated Thiophene molecule, and in the presence of a silver dimer, Ag<sub>2</sub>, at different distances. Calculations were performed using the B3LYP functional, with the 6-31++G\*\* basis set chosen for the Thiophene, and cc\_pvdz\_pp for the silver dimer. Preliminary results show that the presence of Ag lowers the HOMO LUMO energy values, but no changes occur in the energy gap.

POLARIZABILITIES AND HYPERPOLARIZABILITIES OF VINYLENE - BRIDGED ARYL STYRYL SYSTEMS – SUBSTITUENT AND EXTENT OF CONJUGATION EFFECTS. E. M. N. Ndip & J. M. McCormick, Department of Chemistry, Hampton University, Hampton, VA 23668. An understanding of the

structure-property relationship of molecular systems of interest is important for the design of efficient organic semiconductors based on p-conjugated molecules for the fabrication of various optoelectronic devices. We have investigated the charge transport properties (band gaps and polarizabilities and hyperpolarizabilities) of forty (40) molecular systems based on varying the vinylene bridge lengths as well as permutations of three donor – acceptor pairs. Specifically, we have studied the effect of varying the donor / acceptor functionality on optoelectronic and charge transport properties was studied in donor-acceptor-thiophene systems with 1 – 10 vinylene bridges at the semi empirical level using MOPAC2012. These molecules all exhibit a reduced band gap, and excellent NLO properties.



THE FOUNDATION FOR DESIGNING EFFECTIVE ANTI-CANCER PRODRUGS: A QUANTUM MECHANICAL STUDY OF THE RELATIONSHIP BETWEEN MOLECULAR STRUCTURE AND THE ENERGETICS OF BERGMAN CYCLIZATION. Arjun K. Jaini & Carol A. Parish, Department of Chemistry, University of Richmond, Richmond VA 23173. Enediynes cyclize via Bergman Cyclization to form para-benzyne, a diradical that destroys cancer cells by extracting hydrogen atoms from tumor cell DNA. Bergman Cyclization can be initiated with light or heat. An efficient way to trigger Bergman Cyclization solely in the presence of cancer cells has yet to be discovered. In year one of this study, it was concluded that tautomers were possible triggers for activating Bergman Cyclization solely in the presence of cancer cells. Using computational modeling and quantum mechanical methods, the current study focused on further characterizing the relationship between molecular structure and the energetics of Bergman Cyclization. It was found that the number and type of tautomeric sites did not have an effect on activation barriers and endothermicities. Also, the data showed that the incorporation of the enediyne into a ten-membered ring increased endothermicity and that the addition of two carbonyl groups to the ten-membered ring system caused activation barriers and endothermicities to decrease. The theory presented throughout this research utilizes fundamental chemistry principles in order to create a unique solution.

ADVENTURES IN THE INVESTIGATION OF THE THERMAL DECOMPOSITION OF METAL CARBONATES. T. C. DeVore, Rafael Snell-Feikema, & Neil Mehta, Department of Chemistry and Biochemistry, James Madison University, Harrisonburg VA 22807. The thermal decomposition of magnesium oxalate differs from the other group 2 oxalates in that a stable magnesium carbonate intermediate ( $MgCO_3$ ) is not observed during the decomposition process. Attempts to establish the thermal stability of  $MgCO_3$  was thwarted when commercial samples of " $MgCO_3$ " from two different suppliers (Acros and Fisher) were identified as

hydromagnesite ( $\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2 \cdot 4 \text{H}_2\text{O}$ ) using Attenuated Total Reflectance – FTIR and powdered X-Ray diffraction. The thermal decomposition under normal conditions occurred in two steps. The waters of hydration were lost between 450- 550 K to form  $\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2$  which then decomposed between 600 – 800 K to produce MgO. However, if the pattern changed drastically when experimental conditions were changed to hinder the removal of the gaseous products from the cell by placing a top on the cell or increasing the sample size and or the heating rate. Under these conditions, the transition at 700 K split into two partially resolved transitions and a new transition above 800 K was observed. It is hypothesized that the increased pressure of  $\text{CO}_2$  in the cell slows the decomposition of the amorphous  $\text{MgCO}_3$  phase produced by the loss of water from  $\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2$  allowing it to be observed. If stabilized enough, this phase is converted to a new phase at 808 K. The decomposition of this phase produced the transition above 800 K.

### Posters

CONSERVATION STUDIES OF GB1 SEQUENCE AND STRUCTURE. J. Bedford, J. Collins, & L. Greene, Dept. of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529. The objective of this project was to perform a bioinformatics study of the immunoglobulin G-binding domain 1 of *Streptococcal* protein G (GB1) as well as a biophysical analysis of the wild-type protein. The hypothesis of this experiment proposes that evolutionarily conserved residues are key for the formation of protein structure. The bioinformatics investigation was carried out using the Dali-Lite server to find proteins from a wide range of organisms that retain a similar structure but have different functions. Of the proteins found thirteen different proteins were selected from various species. Conservation analysis was performed and showed that twelve of fifty-six positions are highly conserved. Hydrophobicity analysis was performed and showed that eight of the twelve residues are hydrophobic. A three-dimensional image shows that all eight of these hydrophobic residues could be in the core of the protein. To investigate the importance of these conserved residues a characterization of wild-type GB1 using biophysical techniques must be performed. The biophysical studies that were carried out were near- and far-UV circular dichroism, equilibrium fluorescence, and stopped-flow fluorescence. These techniques specifically allow for the characterization of GB1 under a specific set of conditions which will be used as a reference when mutations are done in the future.

THE INFLUENCE OF SYNTHESIS ENVIRONMENTS ON NANOPARTICLES. Perrin Godbold<sup>1</sup>, Brigitte Wendell<sup>1</sup>, Kiara Pontious<sup>2</sup>, Hilary Benedict<sup>2</sup>, Gail Moruza<sup>2</sup>, & Dr. Kyle Gipson<sup>2</sup>, <sup>1</sup>Dept. of Chemistry and <sup>2</sup>Dept. of Engineering, James Madison University, Harrisonburg VA 22807. In the field of optical materials, polymers are studied as an alternative to silica glass, which is currently the dominant matrix. Polymers have the advantage of being lighter than silica glass, but have issues with attenuation caused by high vibrational energy. Attenuation limits the effectiveness of the fiber optic cables and reduces the emissions of the rare-earth ions if dispersed without a protective polymer. To reduce attenuation, fluorescent nanoparticles are added into the polymer. This research explores the factors that impact the luminescent properties of rare-earth ions when the rare-earth ions are a part of low vibrational

energy structure such as a nanocrystal within the polymer matrix. Rare earths ions Terbium<sup>3+</sup> and Europium<sup>3+</sup> (Tb<sup>3+</sup> and Eu<sup>3+</sup>) are doped into Lanthanum Fluoride (LaF<sup>3+</sup>) to form light emitting nanoparticles and then combined with acetylsalicylic acid, (an organic ligand which aids in dispersing the nanocrystals within the polymer matrix). This research focuses on varying synthesis environments for rare-earth doped nanoparticles. The main objective is to analyze the composition of the nanoparticles to determine the effects of the various synthesis environments on the luminescent properties, size and distribution of the agglomerates. This part of the project has looked at the characterizations of four samples of nanoparticles using a scanning electron microscope (SEM), electron dispersion x-ray spectroscopy (EDX), power x-ray diffraction (PXR) and a rheometer.

#### BONDING PATTERNS OF PHENALENE AS A LIGAND BONDED TO METALS.

Ting Li, Huiling Shao, Alan DeLorenzo, Emma W. Goldman, & Donald Kelling, Department of Chemistry, University of Richmond, Richmond, Virginia 23173. Phenalene is an interesting organic compound with three fused rings. This project investigates the bonding patterns of phenalene as a ligand bonded to metals. Results of a theoretical study will be presented that indicate that the shape and structure of the computed sandwich metal complex modify dramatically along the periodic table. We will discuss our results thus far in our synthesis of the interesting transition metal compounds.

#### OXIDATION OF HISTIDINE AND CARNOSINE USING HYPOCHLOROUS

ACID. A. B. Nzesi, S. Babu, & M. O. Claville, Department of Chemistry, School of Science, Hampton University, Hampton, VA 23668. Peptides and proteins are prone to oxidation by means of reactive oxygen species such as hypochlorous acid (HOCl). These oxidized substrates may promote disease in different organs. Hypochlorous acid is a powerful oxidant that is produced and utilized by the body during the immune response. The presence of an imidazole ring in histidine and carnosine make these biomolecules (amino acid and dipeptide, respectively) instrumental in protecting against oxidative damage. Our interest in the role of these two molecules in defending against oxidative damage, has led us to investigate the mechanism of chemical oxidation with biochemical oxidants. Reactions were performed with 0 to 4  $\mu$ mol of hypochlorous acid in 2 mL of 0.1 M phosphate buffer, pH 7.0, and 0.1 mM DTPA, while keeping the concentration of histidine or carnosine (2  $\mu$ mol) constant. All reactions were monitored using a UV-Visible spectrophotometer. Both histidine and carnosine were oxidized in the presence of HOCl. In the case of histidine, UV data showed a decrease in the absorbance at 292 nm and an additional peak at 210-230 nm, with increasing concentration of oxidant. Interestingly, carnosine showed spectral shift from 292 nm to 300 nm with increasing concentration of HOCl. This absorption increased with increasing concentration of oxidant, suggesting the formation of a new species. [Supported by the National Science Foundation-Faculty Early Career Development (CAREER) Award, CHE-0847742 and ACE Implementation Award NSF HRD-1238838]

#### SYNTHESIS OF DICYSTEINE AND DIMETHIONINE PEPTIDES. D. Oliver, S.

Babu, & M. O. Claville, Department of Chemistry, School of Science, Hampton

University, Hampton, VA 22668. Dipeptides Methionine-Methionine (Met-Met) and Cysteine-Cysteine (Cys-Cys) were synthesized using solid-phase peptide synthesis with an automated peptide synthesizer (Tribute, Protein Technologies, Tempe, Arizona). The syntheses were executed from C- to N-terminus, and utilized the 9-fluorenylmethoxycarbonyl (Fmoc) protecting group to prevent polymerization of the N-terminus of the amine group (Scheme 1). The syntheses involved the following consecutive steps: (1) swelling of the appropriate resin containing the C-terminal amino acid; (2) deprotection with 20% piperidine; (3) washing with dimethyl formamide (DMF); (4) coupling with the second amino acid using HBTU (O-(Benzotriazol-1-yl)-N,N,N,N-tetramethyluronium hexafluorophosphate), or HCTU (2-(6-Chloro-1H-benzotriazole-1-yl)-1,1,3,3-tetramethylammonium hexafluorophosphate) in the presence of N-methylmorphine; removal of the dipeptide from the resin; and (5) washing of the product. The crude products were analyzed using Delta Jeol NMR (400MHz) and Infrared Spectrophotometer (Varian 1000 FT-IR). Future directions for this project involve the optimization of the syntheses followed by oxidation with peroxyxynitrite. [Supported by the National Science Foundation-Faculty Early Career Development (CAREER) Award, CHE-0847742 and ACE Implementation Award NSF HRD-1238838]

POLYELECTROLYTE MULTILAYER FILMS: UV-VISIBLE STUDIES OF METHYLENE BLUE LOADING AND RATES OF RELEASE. Alison M. Washington, & Kevin W. Kittredge, Department of Chemistry, Virginia Wesleyan College, Norfolk, VA 23502. A study of the rates of release of methylene blue (MB) from hyperbranched poly(acrylic acid)/poly(allylamine hydrochloride) (PAA/PAH) films at 38 °C and pH 7.15 is reported. Hyperbranched were synthesized in a layer-by-layer fashion with an intercalated organic dye, methylene blue, and cured at 150 °C for 15 min. The films were approximately 575 Å in thickness as measured by profilometry. The rates of release were measured by UV-visible spectroscopy by monitoring the appearance of methylene blue at 665 nm. Two processes have been observed, the first is for the release of methylene blue from the film and the second, slower process is undetermined. We are examining two potential processes to determine which corresponds to the slower rate, hydrolysis of the free methylene blue in solution or decomposition of the film.

RATIONAL DESIGN OF CHEMICAL INHIBITORS FOR PROTEIN N-TERMINAL METHYLTRANSFERASE. Gang Zhang, Yunfei Mao, Stacie Lynn Richardson, & Rong Huang, Department of Medicinal Chemistry and Institute for Structural Biology and Drug Discovery, Virginia Commonwealth University, Richmond VA 23219. The objective of this study is to develop potent inhibitors of N-terminal RCC1 methyltransferase (NRMT). NRMT is upregulated in a variety of cancers and plays an important role in regulating protein-DNA binding. Depletion of NRMT increases multipolar spindle formation during cell mitosis. Thus, NRMT plays an important role in cell growth and may be a potential anticancer target. However, there is no chemical tool available to characterize NRMT function. Hence, we aim to develop potent inhibitors for NRMT, which can be applied as chemical probes to validate the role of NRMT function in cancer cell growth and as lead compounds to develop novel anticancer therapeutic agents. We used a mechanism-based approach to design NRMT inhibitors



to mimic the transition state. They have three components: an N-adenosyl methionine (NAM), a peptide derived from N-terminal protein substrate, and a linker. We adopted a fluorescence-based assay to evaluate the activities of bisubstrate analogs. We have successfully synthesized a series of bisubstrate analogues and determined their inhibitory activities. Among them, SPK-NAM and SPKR-NAM have an  $IC_{50}$  of 51.9 and 13.4  $\mu$ M, respectively. As negative controls, both NAM-triazole and triazole-peptide did not show any significant inhibition at 100  $\mu$ M. We have synthesized the first NRMT inhibitors using a mechanism-based strategy. These inhibitors showed inhibitory activities in the micromolar range. These results suggest the possibility of developing potent NRMT inhibitors using a bisubstrate approach.

### Computer Science

ADOPTING SECURITY ASPECTS INTO THE SOFTWARE DEVELOPMENT LIFE CYCLE. Yen-Hung Hu, Department of Computer Science, Hampton University, Hampton, VA 23608. Our research has found that security vulnerabilities exist in most undergraduate capstone and programming projects that are mainly caused by ignorance of security aspects in coding. This raised our concern about adopting security aspects into the teaching of the software development life cycle in undergraduate software engineering and programming courses. To emphasize this concern, we developed a security assessment table to identify vulnerabilities and security breaches in such projects. The assessment table consists of 13 critical questions which are derived from several prominent institutions including Oracle, CERT, and CMU. We also adopt three security characteristics: confidentiality, integrity, and availability, from the McCumber Cube framework, as the measurement criteria for each critical question in the assessment table. For every captured security vulnerability and breach, we identify solutions that follow Oracle and other secure coding guidelines.

FROM SCRATCH TO JAVA. Bruce Chittenden, Department of Computer Science, Hampton University, Hampton VA. Our high schools are failing us because students entering college today have few courses in Computer Science. Many students have no idea what Computer Science is about or think Computer Science is about creating video games. Most students also lack critical thinking and problem solving skills which are essential to Computer Science. For the past three years, we have used the Scratch programming language in an entry-level course to introduce students with no background to Computer Science. Scratch is a 2-dimensional drag-and-drop Lego-like programming language from the Lifelong Kindergarten Group at MIT. Students spend a semester learning the concepts of programming languages through Scratch. The final project for this course is to create a Scratch Program that implements a Children's Story. This year we created a series of fifteen labs that demonstrated most of the programming constructs of the C-based Programming Languages (specifically, Java). The labs are structured so that the student first writes the program in Scratch, make sure it works, and then writes the same program again in the Java. Since Scratch gives a visual representation of the program, students can more easily visualize the program when implementing it in Java. The titles of the fifteen labs are listed below to show the various programming constructs that are presented in this approach: "Hello World!",