

and *M. roseum* sister to this grouping. If *M. lineare* is indeed descended from Asian species of *Melampyrum*, this implies a drastically different migration history than previously hypothesized. Inclusion of another widely distributed Asian species, *M. laxum*, and phylogenetic analysis of other markers will further elucidate the relationships between *M. lineare* and other members of *Melampyrum*.

A PRELIMINARY CHECKLIST OF THE FRESH-WATER PLANKTONIC MICROALGAE OF THE NORTH LAGOON AT CROOKED TREE, BELIZE, C. A. Stephen W. Fuller, Dept. of Biol., Univ. of Mary Washington, Fredericksburg, VA 22401. Tucked in on the south end of the Yucatan peninsula, on the east side, is the small country of Belize. The northern half of the country consists of low, flat habitats, generally not exceeding 330 feet in elevation, and including lagoons, and flat plains. The lagoons vary tremendously in volume, and hence water level, with the seasonal change from the rainy to the dry season. The fresh-water algal plankton of Belize is relatively unknown, with only two studies, in 2003 and '04, reporting on plankton from two lagoons in southern Belize. In March of 2013 the North Lagoon at Crooked Tree Wildlife Sanctuary was sampled, and 31 taxa were identified. The sample was dominated by Desmids, the Chlorophyta having the most diverse representation at 15 taxa. Species of *Pediastrum* and members of the Cyanobacteria were also prevalent. But frequently, specimens of *Synura*, *Scenedesmus*, and *Dinobryon* were observed, and less frequently, specimens of diatoms and *Euglena*. A thorough investigation of the fresh-water phytoplankton throughout the country and the seasons would provide an interesting exposition of this part of the community.

A PHYLOGENETIC TREE OF THE PEANUT GENUS *ARACHIS* (FABACEAE) BASED ON *TRNT-F*/ITS VS. ALLERGEN GENES. Jenna Sackenheim, Sheena Friend, Chandra Shrestha & Khidir Hilu, Department of Biological Sciences, Virginia Tech, Blacksburg, VA 24061. The legume genus *Arachis* L. (Fabaceae) contains 80 annual and perennial, diploid and polyploid species, including the economically important crop peanut (*Arachis hypogaea*). We are exploring the usefulness of the nuclear allergen genes in *Arachis* phylogenetics. Sequence information from two allergen orthologs Ara h 2 and Ara h 6 for 17 species of *Arachis* were analyzed with RAxML to assess the phylogenetic relationships among the species. The tree based on Ara h 2 was highly congruent with the ITS/*trnT-F* tree obtained by Friend et al. (2010). In contrast, the Ara h 6 tree, although resolving some of those relationships, failed to discern others. This shortcoming might be due to either differences in amount of phylogenetic signals or varying selection pressures operating on the orthologs. Our future study will focus on addressing the issues stated above.

Chemistry

PROGRESS TOWARDS THE SYNTHESIS OF DRAGOMABIN. Michelle K. Waddell, Dept. of Chem., Hampton University, Hampton, VA 23668. Malaria is a degenerative disease caused by a parasitic infection transmitted by infected female *Anopheles* mosquitoes. Worldwide 350-500 million cases have been reported with an attributed 1 million deaths. Currently, Artemisinin is the last line of defense against

Chloroquine-resistant malaria parasites. Due to the pressure on governments to switch to more effective treatments, it is conceivable that Artemisinin-resistant parasites are on the horizon. There has been an increased interest in developing new drugs due to the danger of transmission of anti-malarial resistance in malaria parasites. Dragomabin is one of a class of lipopeptides with anti-malarial activity isolated from a Panamanian strain of the marine cyanobacterium *Lyngbya majuscula*. While it is known that Dragomabin can bypass a cellular membrane, the mechanism of incorporation is unknown. The lipopeptides Carmabin A, Dragomabin, and Dragonamide A have IC_{50} = 4.3, 6.0 and 7.7 μ M respectively. The goal of this research is to perform the first synthesis of Dragomabin in its enantiomeric pure form. The aliphatic side chain will be synthesized in solution phase. Standard Wang solid phase protocol will be used to synthesize the tetrapeptide. Results of the synthetic strategy are presented. Once the synthesis has been completed, structural analogs will be constructed by varying the substituents on the core molecule. These analogs will be used to determine the structure activity relationships of these molecules in order to increase their biological activity against Chloroquine-resistant *Plasmodium falciparum*.

EXPLORING THE COORDINATION CHEMISTRY OF CURCUMINOIDS: SYNTHESIS AND BIOPHYSICAL REACTIVITY. Floyd A. Beckford, Shylene A. Scott, Kinsey L. Hall & Samantha Smith, Dept. of Natural Sciences University Virginia College at Wise, Wise, VA 24293. Curcuminoids are diarylheptanoids which contain a β -diketone group and are analogs of curcumin an important polyphenol long-known for its biological activity. These molecules exhibit many therapeutic properties being applied as antioxidant, anticancer preventive, antibacterial and anti-inflammatory agents. Despite the fact that the diketone moiety can act as a chelating site the coordination chemistry of curcuminoids have not been extensively studied. Recent research into ruthenium-based organometallics suggests potential medicinal use due to ruthenium's low toxicity to healthy cells and good selectivity for malignant cells when compared to competing metals. In this paper a set of structurally diverse curcuminoids were synthesized by the reaction of 2,5-pentanedione with the appropriate aldehyde in the presence of tributylborate and n-butylamine as catalyst. These curcuminoids were used as mono-anionic bidentate ligands in the synthesis of half-sandwich organometallic ruthenium complexes of the type $[(\eta^6\text{-arene})\text{Ru}(\text{curcuminoid})\text{Cl}]$ where arene = benzene or *p*-cymene. The complexes have been characterized and initial investigations of reactions with DNA as well as some model proteins have been carried out. A number of the complexes show a weak ability to uncoil pBR322 plasmid DNA but this ability disappears under irradiation with 365 nm UV light. Spectroscopic and viscometric experiments suggest that the complexes interact with DNA via weak intercalation. On the other hand the interaction, as measured by the binding constant, with human serum albumin is strong.

INVESTIGATION OF COPPER RUNOFF IN SOIL SAMPLES. Darren Driscoll & M.E. Howard, Dept. of Chem., Virginia Wesleyan College, Norfolk, VA. 23502. With rain being naturally acidic and with the continuance of acid rain throughout industrial areas; the leeching of metals into the water and soil of industrial areas is an important topic. This research was geared towards looking at how copper siding would be affected by this acidified rain on a small scale. Copper siding or cladding is used to

cover two external walls on Clark Hall, one of the buildings on the campus of Virginia Wesleyan College. The objective of this research was to develop a method to investigate the effects of rain on the copper building material. This was done by determining if copper concentrations were greater in areas of high probability for copper runoff and by investigating whether the copper runoff had high mobility through the soil, possibility impacting the groundwater systems. An exchangeable ion method of extraction was used and the solutions were analyzed using Flame Atomic Absorption Spectrometry (FAAS). It was found that soil concentrations of copper were significantly higher in areas of high copper runoff probability (adjacent to the wall with copper siding) compared to control locations. The highest value of copper near the build was found to be $31.8 \pm 0.5 \mu\text{g} / \text{g}$ of soil. It was also found that the copper runoff had a little mobility through the soil which suggested that the copper is accumulating in the soil underneath the building.

SUBSTITUTION VERSUS ELIMINATION: THE INFLUENCE OF THE LEAVING GROUP. Charles M. Bump, Dept. of Chem., Hampton University, Hampton, VA 23668. A survey of the competition between $\text{S}_{\text{N}}2$ and E2 reactions is an important part of the study of mechanistic organic chemistry. Generalizations are presented with little theoretical background in support of those statements. We present a review of the calculated (DFT-B3LYP – 3-21G) thermodynamics of different leaving groups as a factor in determining the favored product in the reaction between sodium hydroxide and an ethyl group bonded to a leaving group. We considered the halides (F, Cl, Br, I), acetate, tosylate, hydroxide ion, and methoxide ion as leaving groups. The favored pathway ($\text{S}_{\text{N}}2$ or E2) appears to be independent of leaving group. All substrates share a common “crossover temperature” above which elimination is favored and below which substitution is favored.

BORON-ACRIDINE CHIMERAS: FUNCTIONALIZING BRANCHED PEPTIDES TOWARD TARGETING HIV-1 RRE RNA. Jessica Wynn, Wenyu Zhang & Webster L. Santos, Dept. of Chem., Va. Polytechnic Inst. and State Univ., Blacksburg, VA 24061. While human immunodeficiency virus type 1(HIV-1) is manageable with current antiretroviral therapies, the majority of FDA approved drugs for HIV-1 target enzymes that are prone to high rates of mutation, such as HIV-1 reverse transcriptase. This leads to drug resistance over time, creating the need for therapeutic alternatives. Our research focuses on targeting a conserved region of the HIV-1 genome, the rev response element (RRE). Branched peptides are utilized as a scaffold for multivalent binding to RRE IIB with the incorporation of boronic acid side chains to increase binding affinity via possible interaction with the 2'-OH group of RNA. A high-throughput screening assay of a 3.3.4-branched peptide boronic acid library revealed a hit compound that selectively bound to RRE IIB RNA in the submicromolar range, and was both cell permeable and non-toxic up to $30 \mu\text{M}$. To further improve the binding affinities of our peptides, acridine was incorporated into a new 3.3.4-branched peptide boronic acid library. Our findings indicate that a hit compound containing boronic acid and acridine resulted in an improved binding affinity in the low nanomolar range.

DEVELOPMENT OF SPHINGOSINE KINASE II SELECTIVE INHIBITORS: DESIGN, SYNTHESIS AND BIOLOGICAL ACTIVITY. Molly D. Congdon¹, Neeraj Patwardhan¹, James Gumkowski¹, Elizabeth Childress¹, Emily Morris¹, Yuges Kharel², Kevin Lynch² & Webster L. Santos¹, ¹Dept. of Chemistry, Virginia Tech, Blacksburg, VA 24061 & ²Dept. of Pharmacology, University of Virginia, Charlottesville, VA 22908. Sphingosine-1-Phosphate (S1P) is formed naturally through the phosphorylation of sphingosine (Sph) by the two isoforms of Sphingosine Kinase (SphK1 and SphK2). Increased concentrations of S1P have been implicated in a variety of diseases including cancer, fibrosis, multiple sclerosis and diabetes through intracellular and intercellular targets. SphK1 and 2 differ in size, cellular localization, and possess different intercellular roles. The highly studied SphK1 has been shown to be proliferative while the less known SphK2 has been shown to be pro-apoptotic. Selective inhibitors could aid in the understanding the physiological roles of these kinases. While a wide variety of SphK1 selective inhibitors have been synthesized, there exists an absence of high affinity, SphK2 selective inhibitors. This presentation will discuss the continuation of a tail region structure-activity-relationship based upon a novel SphK2 selective scaffold, SLR080811.

STRUCTURE ACTIVITY RELATIONSHIP STUDIES OF NOVEL GUANIDINE BASED INHIBITORS OF SPHINGOSINE KINASE-2. Neeraj N. Patwardhan¹, Mithun R. Raje¹, Emily A. Morris¹, Kenneth Knott¹, Yuges Kharel², Ming Gao¹, Kevin Lynch² & Webster L. Santos¹, ¹Dept. of Chemistry, Virginia Tech, Blacksburg, Virginia 24061 & ²Dept. of Pharmacology, University of Virginia, Charlottesville, Virginia 22908. Sphingosine kinase (SphK) has emerged as an attractive target for various therapeutics due to its prominent role in processes such as cell proliferation, apoptosis etc. EN.CITEEN.CITE.DATA¹ SphK exists in two isoforms: SphK1 is localized in the cytosol while SphK2 is localized in the nucleus. These enzymes phosphorylate sphingosine to sphingosine-1-phosphate, which has been shown to signal intracellularly via HDACs and BACE1, and extracellularly via interactions with the five G-protein coupled receptors S1P₁₋₅. This signaling pathway has recently been associated with a variety of different diseases. Recently, the Santos group has developed a novel guanidine based lead compound SLR080811 that selectively targets SphK2 with good selectivity and potency at a low micromolar K_i . The structural scaffold contains three regions that could be diversified into a variety of derivatives to improve selectivity: the head, linker and tail regions. In this presentation, we will highlight our current efforts towards developing different head-group analogs of SLR080811. The *in vitro* and *in vivo* activity of these inhibitors will be discussed.

BIOPHYSICAL ANALYSIS OF THE ACTIVE SITE LOOP OF BACTERIAL BETA-GLUCURONIDASE. Suzanne Hengeli & Kimberly Lane, Dept. of Chemistry, Radford University, Radford, VA 24142. β -glucuronidase has been associated with the side effects related to the cancer treatment drug CPT-11 (irinotecan hydrochloride), which is primarily used for colon cancer treatment. CPT-11 is converted in the body to the active form of the drug, SN-38, which is further metabolized into SN-38G (by addition of a glucuronide group). SN-38G is transported to the intestine for elimination, where it is hydrolyzed to SN-38 by bacterial β -glucuronidase. This release of SN-38 causes damage to the intestinal lining, leading to side effects such as severe

diarrhea. Recent studies have produced an inhibitor that is specific for the bacterial form of β -glucuronidase and have demonstrated that this specificity is due to the presence of an active site loop found in the bacterial form of the enzyme, but not the human form. In this study, point mutations in the residues found in the active site loop of the enzyme, which are residues 360 through 376, were modeled using Win-Coot and Argus Lab. Residues in the active site loop were mutated to see the how the binding energies would be affected, the tighter the binding energies the estimated better the inhibitor would bind to that active site.

THERMAL DECOMPOSITION OF METAL OXALATES. T. C. DeVore, Dept. of Chemistry and Biochemistry, MSC 4501, James Madison University, Harrisonburg, VA 22807. Although the dynamics of thermal decomposition of metal oxalates have been investigated for well over a century and hundreds of papers have now been published on the topic, the mechanism for this decomposition has not been established with certainty. DFT-B3LYP calculations using the 6-311G++ (3pd, 3df) basis set have been used to investigate the mechanism proposed by Boldyrev. The first step of this mechanism is the splitting of the C-C bond in the oxalate anion to form two CO_2^- anions. The activation energy calculated for this process (178 kJ/mol) agrees well with experimental activation energies measured for many transition metal oxalates. The CO_2^- anions can rearrange and form a stable intermediate ($\text{CO}_3\text{CO}^{2-}$) that decomposes to produce the observed products. The activation energy for the production of CO was calculated to be 94 kJ/mol. Molecular geometries and vibration frequencies for each intermediate have also been determined.

PSEUDOROTAXANES AS PRECURSORS OF MECHANICALLY LINKED ASSEMBLIES. Harry W. Gibson, Zhenbin Niu, Minjae Lee, Terry L. Price, Jr., Mason A. Rouser, Arun Murugan, Hanlie Wessels, Daniel V. Schoonover & Carla Slebodnick, Dept. of Chem. & Macromolecules & Interfaces Institute, Virginia Tech, Blacksburg, VA 24061-0212. Over the past 25 years we have utilized pseudorotaxane and rotaxane self-assembly to control the structures and properties of macromolecules. Suitable bisphenylene crown ethers, such as bis(*p*-phenylene)-34-crown-10 and bis(*m*-phenylene)-32-crown-10, complex 4,4-bipyridinium compounds ("paraquats" or "viologens") have association constants, K_a , of 500 to 1000 M^{-1} . Our use of these systems as models for construction of polymeric pseudorotaxanes and rotaxanes of various architectures will be reviewed briefly. Efficient formation of pseudorotaxanes for supramolecular polymerization and formation of block, graft and star polymers from cyclic host and guest components requires high association constants ($K_a > 10^4 \text{M}^{-1}$). We have prepared cryptands with association constants in the range of 10^4 to 10^6M^{-1} with 4,4-bipyridinium compounds ("paraquats" or "viologens") and have developed several efficient ways to functionalize the most powerful versions of these hosts, the pyridino cryptands. These functionalized hosts now enable new avenues to create supramolecular polymeric structures beginning with both functionalized polymers as well as properly functionalized monomeric species. Combined with modern polymerization methodologies these systems enabled our recent work directed toward formation of star, block, graft and brush copolymers and also supramolecular polymers. These procedures will be discussed along with characterization of the resultant novel materials.

DESIGN AND SYNTHESIS OF ROMP IMIDAZOLIUM POLYMERS FOR USE AS ACTUATORS. T. L. Price Jr.¹, U. H. Cho², D. Wang³, Arunachalam Murugan¹, D. V. Schoonover¹, M. Zhang¹, R. H. Colby², J. R. Heflin³, R. B. Moore¹ & H. W. Gibson¹, ¹Dept. of Chem., Virginia Tech, Blacksburg, VA, 24061, ²Dept. of Materials Science & Engineering, Penn State University, University Park, PA, 16802, & ³ Dept. of Phys., Virginia Tech, Blacksburg, VA, 24061. Previous work conducted by our group has established that properly designed poly(meth)acrylates containing imidazolium pendant groups will exhibit high single ion conductivities ($\sim 10^5$ S/cm). Polymers of this type are known to be capable of electromechanical actuation. In this presentation we will describe our design criteria for poly(norbornene)s containing imidazolium pendant units and discuss advantages of the system; additionally, single ion conductivities ($\sim 10^5$ S/cm) and preliminary studies of their actuation behavior will be presented. (Supported by: U.S. Army Research Office grant number W911NF-07-1-0452: Ionic Liquids in Electro-Active Devices (ILEAD) MURI).

DESIGN OF MULTICHROMOPHORIC SYSTEMS FOR MOLECULAR ELECTRONICS. E. M. N. Ndip, N. Pandey & K. Cole, Dept. of Chem. Hampton University, Hampton, VA 23668. This work is part of our ongoing research on the design, synthesis, and laser spectroscopy of multichromophoric (aryl styryl heterocyclic (thiophene, furan, and pyrrole) π -centered compounds) systems for molecular electronics. Theoretical studies have elucidated the effects of tuning on several electronic properties and determined their suitability as materials for molecular electronic devices. Ground state geometries of various derivatives were optimized using both semi empirical (PM3) and DFT-B3LYP with the 6-31G** basis set. The linear absorption spectra, and energy gaps were computed for the various molecular systems in vacuum at both the semi empirical (ZINDO-CI) and *ab initio* (TDDFT) methods on the optimized ground state geometries. The computed maximum wavelengths for representative systems are in good agreement with the experimental data (405-438nm) obtained from fluorescence experiments cited in the literature. The data also shows reasonable agreement between the semi-empirical and *ab initio* calculated ?. Band gaps determined from the TDDFT/B3LYP calculations are more consistent with the experimental values for the thiophene derivatives. (Supported by NSF CREST (HRD-0734635, HRD-0630372, and ESI-0426328/002))

ELECTROCHEMICAL INTERACTIONS OF ACTIVATED CARBONS WITH AQUEOUS AND BIOLOGICAL MEDIA: AN ACID-BASE MODEL. M. M. Goldin¹, G. R. Garaeva², & N. V. Sklifosovky², ¹Dept. of Biol. & Chem., Liberty University, Lynchburg, VA 24502 & ²Institute for Emergency Medicine. The adsorption of metal ions and organic compounds on activated carbons was measured in 0.10 M Na₂SO₄ against Ag/AgCl. Activated carbon samples caused a drift in the pH of distilled water, 0.10 M sodium sulfate, and other solutions in which they were immersed. For carbons with positive OCP, the pH drifted toward acidic values, while for negative-OCP carbons, toward basic values. If the carbon/electrolyte heterogeneous equilibrium is considered as an Usanovich acid-base pair, the electron acceptor is an acid, and the electron donor is a base. The "acidic" positively charged carbon immersed in a solution acidifies it, while the "basic" negatively charged carbon makes it more basic, which is in agreement with empirical data. Identical unmodified AKU and AG-3

activated carbon samples were immersed in phosphate buffer solutions; the acidic solution caused a positive shift in the OCP of carbon, while the basic solution produced a negative OCP shift, also consistent with the Usanovich model. Finally, unmodified and oxidized SKT-6A carbon, as well as an iodide-doped polypyrrole (PPy) composite based on SKT-6A and pure chloride-doped PPy, were titrated by the Boehm method to determine surface functionalization. The amount of carboxyl groups on the surface of these materials gives a strong linear correlation with OCP and overall functional group data corroborates the increase in Brønsted-Lowry acidic groups on carbon surface with increasing potential. This study is supported by funds from the Center for Research and Scholarship Fund of Liberty University.

η^2 -DEAROMATIZATION: MODIFICATIONS OF ANILINE AND 2-(DIMETHYLAMINO) PYRIDINE. J. A. Pienkos¹, A. Knisely¹, B. Liebov¹, V. Teran¹, V. E. Zottig¹, M. Sabat² & W. H. Myers³, ¹Dept. of Chem., University of Virginia, Charlottesville VA 22903, ²Nanoscale Materials Characterization Facility, Dept. of Materials Science and Engineering, University of Virginia, Charlottesville VA 22903, & ³Dept. of Chem., University of Richmond, Richmond VA 23173. Organic scaffolding with a transition metal fragment allows for rapid access to new compounds. η^2 -coordination of an arene to a π -basic {TpW(NO)(PMe₃)} fragment renders the aromatic molecule “dearomatized.” A dearomatized arene exhibits reactivity that is different than the reactivity of the free, unbound ligand. Ligand exchange between {TpW(NO)(PMe₃)(η^2 -benzene)} and 2-(dimethylamino) pyridine or *N,N*-dimethyl aniline derivatives, in the presence of acid, affords new η^2 complexed cationic species. These species can react with various electrophiles, generating allyls, which can react with aromatic molecules to form a carbon-carbon sp³-sp² center. Additionally, the η^2 -coordinated *N,N*-dimethyl aniline derivative can be cyclopropanated and further modified through ring opening reactions. Liberation of the bound ligands affords novel α,β -unsaturated cyclohexenones.

STEP: SOLAR THERMAL ELECTROCHEMICAL PROCESS, A COMPREHENSIVE PROCESS FOR UTILIZING RENEWABLE ENERGY TO REDUCE ANTHROPOGENIC CARBON DIOXIDE EMISSIONS. Stuart Licht, Baochen Cui, Baohui Wang, Jason Lau & Jessica Stuart, Dept. of Chem., The George Washington Univ., Washington, DC. 20052. STEP is a new process that converts and stores solar energy. STEP has been shown experimentally to function at much higher efficiencies than photovoltaic solar cells and to support current densities that are 1 to 3 orders of magnitude greater than those achieved by photoelectrochemical water splitting or photoelectrochemical solar cells. STEP utilizes a portion of sunlight to drive photovoltaic charge transfer, while the remainder of the sunlight is applied as solar thermal energy to heat and decrease the energy of endothermic electrolysis reactions. By taking the reactants to a higher temperature, the voltage needed to drive the endothermic electrolysis reaction decreases improving the efficiency of the reaction. A secondary advantage of going to these higher temperatures is the ability to use molten salts as the medium for electrolysis. Molten salts can support very high molecular concentrations at the electrode surface allowing for higher current densities with greater efficiencies. Select molten salts can support very high voltages, are resistant to poisoning and can act as a thermal buffer to maintain the high temperature

needed for the reaction. STEP has been shown to be a suitable alternative for a variety of carbon dioxide releasing processes such as the production of iron, cement, hydrogen, desalination, fuels, and wastewater treatment giving STEP the potential to be a comprehensive approach for reducing anthropogenic carbon dioxide emissions.

Posters

CHEMO- AND REGIOSELECTIVE DIBORATION OF ALLENES. Xi Guo, Amanda Nelson & Webster L. Santos, Dept. of Chem., Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061. Organoboron compounds are important synthetic intermediates in organic synthesis. Metal-catalyzed diboration reaction with commercially available diboron reagents is a traditional method to introduce boron moiety. However, most of the previous work was focused on symmetrical diboron reagents such as bis(pinacolato)diboron and bis(catecholato)diboron, a differentially protected diboron reagent is employed in this work. Diboration of different allenes with it provides the borylated product chemo- and regioselectively. This work is funded by Department of Chemistry, Virginia Polytechnic Institute and State University and ACS Petroleum Research Fund.

DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF NOVEL INHIBITORS OF SPHINGOSINE KINASE 2. Emily A. Morris¹, Neeraj N. Patwardhan¹, Mithun R. Raje¹, Yugesh Kharel², Kevin Lynch² & Webster L. Santos¹, ¹Dept. of Chem., Virginia Tech, Blacksburg, Virginia 24061 & ²Dept. of Pharmacology, University of Virginia, Charlottesville, Virginia 22908. Sphingosine kinase (SphK) has become a prevalent target for many disease states in recent years. SphK phosphorylates sphingosine to sphingosine 1-phosphate (S1P). SphK can be found in two isoforms, SphK1 and SphK2, and differ in their cellular location. In mouse studies, inhibition of SphK2 showed an increase in the circulating levels of S1P in blood. This increase of S1P has been shown to be anti-fibrotic, as it leads to a decrease in the extracellular-matrix formation. Our lead molecule, SLR080811, is shown to have a K_i of 1 μ M and 5-fold selectivity for SphK2 over SphK1. SLR080811's structural motif contains a tail group, linker, and head group. In this poster, we will review the structural modifications that have been performed to the linker and head group regions of SLR080811 in an attempt to improve inhibition of SphK2.

MUTAGENIC ANALYSIS OF BACTERIAL BETA-GLUCURONIDASE. Skye Hickling, Gina Burchett & Kimberly Lane, Dept. of Chem., Radford University, Radford, VA 24142. Camptothecin-11 (CPT-11) is used for chemotherapy in cancer patients. It gets converted to the topoisomerase inhibitor SN-38. SN-38 is metabolized in the liver to SN-38-glucuronide. Bacterial β -glucuronidase hydrolyzes the glucuronide re-releasing SN-38 into the intestines. This reformed SN-38 is toxic to the body and β -glucuronidase is the key to the toxicity of the drug CPT-11. The use of inhibitors of *E. coli* β -glucuronidase decreases the amount of damage to intestinal cells. Deficiencies in the human form of β -glucuronidase may lead to the onset of Sly syndrome, a lethal disease with no current treatment. Previous studies has shown that a stable dimer of the enzyme may exist. This current study has been using WinCoot

and ArgusLab to develop mutations *in silico* of the active site in β -glucuronidase and subunit interfaces. Active site mutations were performed at residues that have shown to be of some importance through the enzyme related to β -glucuronidase called β -galactosidase. These active site mutations were developed at the following residues: H296, E297, S360, F365, N412, E413, Y468, and E504, D163, V274, Q507, F281, K277. The subunit interface mutations were performed at the following residues to reduce electrostatic interactions: E6, R71, K13, D16, D319, R43, D77, T7, D477, K157, Y517, D53, R10, K77, N308, E523, H514, K576, and S579. In the future, MC-PRO by Schrodinger will be used to determine feasible mutations for laboratory testing. Through these calculations, mutations will be developed and studied for the interactions between *E. coli* β -glucuronidase and ligands in hopes of learning more about the enzyme mechanism and dimer stability.

Computer Science

NONTRADITIONAL APPLICATIONS OF AUTOMATA THEORY. Bruce Chittenden, Department of Computer Science, Hampton University, Hampton, Virginia 23668. Automata theory is typically taught as a mathematical theory of computation with applications in compiler construction, specifically in the area of lexical analysis. Typically computer science students do not encounter automata theory outside of a course on programming languages or compiler construction, and are therefore left with the impression that automata theory is a fairly abstract mathematical theory which only applies in these areas. I would like to put forward the argument that we should expand how we teach automata theory to include several practical applications such as the specification and verification of protocols. Automata theory provides a rich set of abstractions and tools that every student should learn to apply to many situations that they will encounter in the development of complex software. I have found that automata theory is well suited for the specification and verification of many types of protocols. Any software situation where communications is occurring and state is maintained over a period of time lends itself to a software design and implementation based upon automata theory. The finite state machine is specified symbolically, that is the *inputs*, *outputs*, *states*, and *transitions* are defined in terms of symbols easily understood by humans but difficult in that form, to be used directly by a computer. An Analyzer Program can easily be created that processes the *description* of the Finite-State Machine and generates two tables of integers, *outputs* and *next state*, representing the machine behavior. These tables can be used directly by the computer. The software implementation becomes completely table driven. Using today's programming languages such as C, C++, or Java, this is easily implemented using a switch statement. The significant benefit of this approach is that it pushes the debugging of the protocol from coding and testing phase back into the design phase, therefore reducing the time to deliver working software.

OPEN QUESTIONS REGARDING UPPER BOUND ON MATRIX MULTIPLICATION OF $O(n^w)$ FOR $w < 2.374$. S. V. Providence, Department of Computer Science, Hampton University. Matrix multiplication is a fast algorithm that can be distributed and has fast performance on modern computer systems. A lower