study examines the moss *Dicranium scoparium*. From Bader et al. (unpublished) it is expected that this terrestrial moss gametophyte should show facilitated diffusion. (Supported by: Jeffress Memorial Grant).

Chemistry

DOES CO_2 WARM THE ENVIRONMENT? T.C. DeVore & D. Havey, Deptartment of Chemisdtry and Biochemistry, MSC 4501, James Madison University, Harrisonburg VA 22807. A series of laboratory exercises have been developed that let students investigate three postulates related to global warming: 1. burning fossil fuels creates CO_2, 2. CO_2 absorbs IR radiation, and 3. increasing the amount of CO_2 in the atmosphere increases the temperature of the environment. To test the first postulate, students use GC-MS and FTIR to compare the amount of CO_2 in a sample of automobile exhaust to the amount of CO_2 in ambient air. A vibrational and a rotational analysis of the spectrum for CO_2 and preparing a Beer's Law plot for CO_2 are used to test postulate 2. The Boltzmann distribution to determine the rotational temperature of the CO_2 in the cell is used to test postulate 3. By measuring the temperature of several different concentrations of CO_2, the effect of the concentration of CO_2 on the temperature inside the cell is established. If all parts of this project were done, students would learn about the combustion of hydrocarbons, the IR spectra and rotational analysis of linear tri-atomic molecules, Beer's Law, the measurement of rotational temperatures based on the Boltzmann distribution and the Greenhouse Effect.

DESIGN, SYNTHESIS AND INTERACTION STUDIES OF SULFATED ALLOSTERIC MODULATORS OF THROMBIN. Preetpal Singh Sidhu, Aiye Liang, Akul Y. Mehta, May Abdel Aziz, Qibing Zhou, & Umesh R. Desai, Dept. of Medicinal Chemistry, Virginia Commonwealth University, Richmond, VA-23219. We have synthesized a library of potent, small, aromatic allosteric inhibitors of thrombin. The sulfated benzofuran scaffold was designed from the structure of sulfated lignin and contained charged, polar and hydrophobic substitutions at the 2,3,5,6 positions, which provide diversity to the library of 15 sulfated monomers and 13 sulfated dimers. Due to presence of negatively charged sulfate and carboxylate groups, these molecules are completely water soluble. Synthesis of the library of benzofurans derivatives was achieved through a multiple step, highly branched strategy, which culminated with the introduction of sulfate group(s) using microwave-assisted chemical sulfation reaction. From the library of 28 potential inhibitors, 11 inhibited thrombin with reasonable potency. Structure activity relationship studies showed sulfation at the 5-position of the benzofuran scaffold was essential for targeting thrombin. The *t*-butyl derivative was found to be the most potent with an IC_{50} of 7.3 μM under physiologically relevant conditions. Michaelis-Menten kinetic studies showed that these inhibitors do not affect the affinity of chromogenic substrate for thrombin ($_{Km}$) but greatly reduce the maximal velocity (V_{max}) of reaction, indicating the allosteric mechanism of inhibition. The results of plasma clotting assays suggest that these inhibitors prolong both the activated partial thromboplastin time and prothrombin time, of which the former is more affected in a manner similar to the heparins and hence affect the intrinsic pathway more effectively.

DEVELOPMENT OF A METHOD FOR WATER PURIFICATION UTILIZING THE ELECTROCHEMICAL PROPERTIES OF POROUS CARBON MATERIALS. Mikhail M. Goldin[1], B.M. Grafov[2], A.D. Davydov[2], Mark M. Goldin[3], & V.A. Kolesnikov[4], [1]Dept. of Bio. and Chem., Liberty University; [2]Frumkin Inst. of Phys. Chem. and Electrochem; [3]Sklifosovky Inst. for Emergency Medicine; [4]Mendeleev Univ. of Chem. Tech. of Russia. The traditional methods for decontamination of water have limitations and are relatively expensive to use. The goals of the present work were to develop a prototype electrofilter. AG-3 brand activated carbon samples were electrochemically pre-modified to initial open-circuit potentials (OCP) between –775 and +475 mV and then placed in aqueous 2.20 M *t*-butanol and 0.100 M $CuSO_4$ solutions. Concentrations were measured on an SRI Instruments 310C gas chromatograph for *t*-butanol and on a Genesys 10uv spectrometer at 808 nm for Cu^{2+}. Effective charge transfer for each experiment was calculated using the equation $n = (C \cdot \Delta E)/(F \cdot \Delta\Gamma)$, where n – effective number of electrons, C (F) – differential capacitance of the sorbent electrode, ΔE (V) – OCP change during the experiment, F (= 96500 C mol^{-1}) – Faraday's constant, $\Delta\Gamma$ (mol) – net adsorption. The effective charge transfer for *t*-butanol (n <0.1) did not vary appreciably with potential, which pointed to a mechanism not involving electrooxidation or electroreduction. n for Cu^{2+} was near 2 for potentials more negative than –470 mV and gradually decreased until +475 mV, where it reached $n \approx 0$ indicating a major contribution from Faradaic electroreduction. Preliminary microbiological results also indicated a dependence of bacteria counts on carbon potentials. This study is supported by funds from the Center for Research and Scholarship Fund of Liberty University.

MEASUREMENT OF DOPAMINE TRANSPORTER ACTIVITY IN THE LARVAL *Drosophila* CNS USING FAST-SCAN CYCLIC VOLTANMETRY AT CARBON-FIBER MICROELECTRODES. T. Vickery & B.J. Venton, Dept. of Chem., University of Virginia, Charlottesville, VA. *Drosophila melanogaster* is homologous to mammals in primitive neurobiology making it an advantageous model system in which to study the dynamics of dopamine regulation. Here we report a new method to measure dopamine transporter activity in isolated, *Drosophila* ventral nerve cords. A carbon fiber microelectrode is implanted into a larval ventral nerve cord, while a micropipette is simultaneously implanted approximately 10 µm away. Dopamine is pressure ejected into the neuropil region, rich with dopaminergic neurons, and dopamine diffusion and clearance observed. Various concentrations of dopamine were applied and maximal uptake (V_{max}) was calculated. Clearance of exongenously-applied dopamine significantly decreased in the neuropil region following treatment with 50 µM cocaine, a dopamine transporter inhibitor. Dopamine clearance also significantly decreased in fumin mutants lacking a functional dopamine transporter. The effect of acute cocaine application on dopamine clearance is in good agreement with previous real-time, endogenous dopamine clearance measurements in Drosophila larvae as well as measurements made in adult

Drosophila. This method further validates the use of Drosophila as a model system to study dopamine regulation and the role of the dopamine transporter in the underlying mechanisms of drug addiction. This work was funded by NIH R01MH085159.

SUBSTITUTION VS. ELIMINATION – THERMODYNAMICS VS. KINETICS. Charles M. Bump, Department of Chemistry, Hampton University. The competition between substitution and elimination reactions is central to the study of organic chemistry. It is a challenge to both the classroom teacher and to the student. When reaction mechanisms are described in textbooks, generalizations are made such as "Primary alkyl halides react with strong base / nucleophiles principally by an S_N2 mechanism and secondary alkyl halides react with strong base / nucleophiles primarily by an E2 mechanism. Such generalizations correctly predict the reaction product and mechanism, but leave the student without a clearly defined chemical principle for the reaction path. We describe a systematic analysis of some thermodynamic and kinetic parameters of substitution and elimination reactions using the semi-empirical program MOPAC 2009. Free enthalpies of formation of starting materials and products as well as free enthalpy of formation of substitution and elimination transition states form the basis of the analysis.

CALCULATIONAL ORGANIC CHEMISTRY – A SUPPLEMENT TO TRADITIONAL WET CHEMISTRY EXPERIMENTS. Charles M. Bump, Edmund M. Ndip, Godson C. Nwokogu & Michelle K. Waddell, Department of Chemistry, Hampton University. The ready availability of calculational chemistry software and its widespread use in graduate education and industry presents a clarion call for calculational chemistry to be taught with other fundamental lab techniques such as distillation and recrystallization. The web site "Molecules in 4-D" (http://wetche.cmbi.ru.nl//organic//) provides an easy-to-use graphical interface to the MOPAC semi-empirical calculation engine with pre-defined starting materials to be edited for investigations by "users", not just theoreticians. We will describe our record-keeping requirements, procedures, and results in using this free resource for teaching calculational chemistry with representative examples from the first and second semester of the organic chemistry sequence. We will demonstrate that calculations are fast enough that they can be conducted as real-time class demonstrations by the teacher or assigned by the teacher to small groups or individuals who report back to the class in five to ten minutes.

O_2 DEPENDENCE of SINGLET OXYGEN YIELDS FROM NATURAL DISSOLVED ORGANIC MATTER (DOM). Charles M. Sharpless, Department of Chemistry, University of Mary Washington, Fredericksburg, VA. Natural dissolved organic matter (DOM) is a heterogeneous mixture produced by decay of plant and plankton biomass. Irradiating DOM in aqueous solution produces a suite of photoreactants including singlet oxygen ($^1O_2$), superoxide (O_2^- and its dismutation product, H_2O_2), hydroxyl radical (OH), solvated electrons, and DOM triplet states (^{3}DOM*). These photoreactants can degrade aquatic pollutants and likely play a part in the conversion of DOM to inorganic carbon (i.e., CO_2). Much of the chemistry involves O_2, and it is important to establish how the rates of the various reactions depend on dissolved O_2 concentrations. Such studies can also provide insight into the DOM photochemical mechanism, allowing determination of such properties as the excited state lifetimes of DOM precursors to various photoreactants. This talk covers relevant background and presents the results of experiments showing that DOM $^1O_2$ quantum yields vary in approximate proportion to dissolved O_2 over environmentally relevant concentrations (DO ~ 50 to 250 □M). Modeling $^1O_2$ production as arising from diffusion based reaction between ^{3}DOM* and O_2 indicates that ^{3}DOM* has a lifetime of approximately 5 to 10 □s, regardless of the DOM source.

ALUMINUM'S CONTROL IN THE BLUING OF HYDRANGEA SEPALS. Henry D. Schreiber, Andrew H. Jones, Corinne M. Lariviere, Kelly M. Mayhew, & Judith B. Cain, Department of Chemistry, Virginia Military Institute, Lexington, VA 24450. The pigment in *Hydrangea macrophylla* sepals is the anthocyanin delphinidin-3-glucoside. The color of this pigment provides a red color to the sepals, as the delphinidin-3-glucoside is in its flavylium cation structure. When grown in acidic soil, hydrangeas readily assimilate aluminum which results in blue sepals. A chemical model has been developed that attributes the blue color to Al^{3+} complexing with delphinidin-3-glucoside in its quinoidal base anion structure along with a stacked flavylium cation structure. The role of Al^{3+} is to aid in H$^+$ transfer and act as an anchor for this stacked complex. The chemical model also predicts that the bluing plateaus once a specific excess of Al^{3+} over the delphinidin-3-glucoside is achieved. In the natural system, the color change from red-to-blue with aluminum can be duplicated spectrophotometrically by this Al^{3+}-delphinidin-3-glucoside complex without recourse to co-pigments. The threshold aluminum content in hydrangea sepals is 40 µg Al^{3+}/g fresh sepal for bluing to occur; this threshold is relatively cultivar independent, despite the cultivar sepals having different delphinidin-3-glucoside contents. More aluminum than the threshold did not enhance the hue or intensity of the blue color of the sepal, in agreement with the chemical model.

COMBINING COMPUTATIONAL AND EXPERIMENTAL APPROACHES TO INVESTIGATE THE CATALYTIC MECHANISM OF GLYOXYSOMAL MALATE DEHYDROGENASE- PART I. H. Guterres, S. Hedrick & E. Bell. Deptartment of Chemistry, University of Richmond, Richmond, VA 23173. Geometry optimization calculations have been used to find the minimum total energy and structure of the transition state during the conversion of malate to oxaloacetate catalysed by the enzyme glyoxysomal Malate Dehydrogenase. The proton abstraction is suggested to precede hydride transfer due to the activity of the arginine residues around the active site. To test this, two truncated models were built; model A included Histidine 220, malate and NAD+, and model B included these three moieties from model A with the addition of three arginine residues around the active site, R124, R130, and R196. Gaussian 03W was used to build the structure of the compounds, arrange their atoms, and run the geometry optimization calculations. For model A, the result shows a single imaginary frequency that vibrates to the hydride transfer. In contrast, for model B there is a single imaginary frequency that vibrates to the proton transfer. The result suggests that the arginine residues around the active site play important roles in facilitating the proton transfer. In silico mutation of these arginine residues is being correlated with the effects of in vitro site directed mutations to ascertain the precise roles of individual arginines in binding and catalysis.

INVESTIGATING DIRECT PHOTOLYSIS MECHANISMS OF POLYCYCLIC AROMATIC HYDROCARBONS IN NON-POLAR SOLVENTS. Jonathan S. Williams & Charles M. Sharpless, Department of Chemistry, University of Mary Washington, Fredericksburg, VA 22401Polycyclic aromatic hydrocarbons (PAHs) are toxic components of oil spills whose fate is often controlled through photochemical reactions. PAH photolysis mechanisms in hydrophobic media are not known, hampering efforts to predict their removal rates from oil in the event of a spill. One hypothesis is that singlet oxygen ($^1O_2$) generated by excited state PAHs is an important intermediate that contributes to PAH photolysis. In order to test this hypothesis, we are studying whether PAHs undergo a self-sensitized photolysis mechanism involving $^1O_2$ in solvents of similar polarity to oil. We employed a $^1O_2$ probe, α-terpinene, to determine whether $^1O_2$ is produced during irradiation of four PAHs: benzo[a]pyrene, benzo[e]pyrene, benz[a]anthracene, and chrysene. Loss of α-terpinene in irradiated PAH mixtures revealed that $^1O_2$ is sensitized in hexane. Additionally, $^1O_2$ quantum yields were measured in hexane using a Stern-Völmer analysis, yielding previously unknown values for benzo[a]pyrene and benzo[e]pyrene at 0.84 and 0.70 mol Es^{-1}, respectively. To determine if this self-sensitized mechanism was occurring, we investigated whether the direct photolysis quantum yield (ϕ_D) was linearly dependent on PAH concentration as predicted by our kinetic model. Experiments showed non-linear plots of ϕ_D with increasing PAH concentration, suggesting that another mechanism is contributing to PAH photolysis in non-polar media.

DETERMINATION OF AN HPLC METHOD FOR THE QUANTITATION OF ESTRADIOL AND ITS SEVEN DEGRADATION PRODUCTS. J. Chris Maxwell & Geoffrey C. Klein, Department of Molecular Biology and Chemistry, Christopher Newport University, Newport News, VA. Estradiol is an endocrine disrupting compound that mimics endogenous estrogens found in humans and can directly interact or interfere with and alter the normal growth, reproduction, or other physiological function of an organism. The need for a highly sensitive and accurate technique to measure the presence and concentrations of endocrine disrupting compounds has generated several analytical approaches for the analysis of these compounds. This work aims to determine an analytical method for the separation and quantitation of estradiol and its 7 main degradation products. The HPLC method determined to facilitate the most ideal separation used a 15-cm C16 Polar Advantage column (Dionex Corporation) with an isocratic mobile phase composed of 10% tetrahydrofuran, 63% Phosphoric Acid Dilution (0.085%), and 27% Acetonitrile at a constant flow rate of 1.5 mL/min for a total run time of 60 minutes. The detection method used was UV/Vis spectroscopy which measured absorbance at a wavelength of 225 nm. Each compound was identified individually using the developed method but peak overlap of two compounds does not support the development of a clear separation of estradiol and its degradation products. Future research will aim to create a more complete separation where each component is indicated by a distinct non-overlapping peak and will explore the kinetics of estradiol photodegradation under various environmental conditions.

Computer Science

A MINIMAL WORKING CONFIGURATION FOR THE ASTERISK VOIP SERVER. Luke D. Acree & Robert M. Marmorstein, Dept. of Computer Science, Longwood University, Farmville, VA 23909. We present a fixed-point algorithm for reducing a large set of configuration lines to a *minimal working configuration*. A *minimal working configuration* is the smallest set of configuration lines that allow an application to provide a pre-defined level of service. We apply our algorithm to the Asterisk voice-over-IP server using a baseline of one *SIP* and one analog phone connection. Using the algorithm, we are able to reduce a configuration with more than eighty files and 12, 000 lines of configuration to a simpler system containing only four files and fifty-six lines. The algorithm finds a *local minimum* configuration which, in practice, is usually the smallest working configuration set. Reducing the number of lines of configuration makes teaching and training easier and also makes it easier to customize a server to provide exactly the desired functionality without introducing security flaws.

BIT PARALLEL SEARCH ALGORITHMS OF MOTIFS IN DNA USING TVCA. S.V. Providence, Deptartment of Computer Science, Hampton University, Hampton, VA 23668. Time-varying cellular automata (TVCA) are a form of cellular automata CA where the transition functions vary over time or are time dependent. The DNA motif search problem is a well-known problem in bio-informatics. Essentially it is the problem of searching for patterns in biological sequences. Two classical approaches utilize computation theory to exploit the power of deterministic finite automata (DFA). A third approach uses a filtering technique. CA is novel in motive searching. We view a CA as an aggregate of NFAs or cells where the NFA transitions are modified to account for neighboring cell states. There is a large body of literature on CA and large body of literature on NFA in motif searching. In this paper we extend work done in a previous paper by the author and the classical approach and explain the usage of a TVCA in motif searching further.

CAN ILLEGAL AND UNETHICAL USE OF TECHNOLOGY BE EFFECTIVELY DETERRED? Angela B. Hayden, Department of Computer Science, Hampton University, Hampton VA 23668. Modern society is advancing at such a high rate of speed that it is virtually impossible for an individual to keep up with the latest technological advancement. The worst part is the rampant disregard for ethics and ethical behavior when using technology. In an attempt to stay current with latest technology, many individuals engage in illegal and unethical practices such as illegal downloading of music or software piracy. These activities can be seen as socially acceptable behaviors. However, as computer scientist, we are well aware of the laws and policies warning against such practices. Therefore, we ask ourselves, what is the