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Heptadentate tetraazamacrocyclic pyridinophane bearing four pyridine donors

Emily Burgess, Tim Hubin, & Sierra Long

Abstract

Pyridinophanes are amine ligands containing at least one pyridine donor as part of a macrocyclic ring. Pyclen is the most well-known pyridinophane and is so named due to its twelve membered ring matching the size and spacing of nitrogen donors found in the ubiquitous 12-membered Cyclen tetraazamacrocyle. Many pendant-arm analogues of Pyclen have been published, including some with pendant arm pyridine donors added. However, we believe that our work represents the first Pyclen analogue having three pendant arm pyridines. The new pyridinophane contains seven donor atoms, four of which are pyridine nitrogen atoms. We will present the synthesis and characterization of this new pyridinophane and its coordination chemistry with a range of first-row and some second-row transition metal ions. A designed feature of this ligand is its seven nitrogen donors, which allow for the possibility of heptadentate coordination. We will discuss the characterization of our metal ion complexes with special attention to ligand denticity and complex coordination geometry.

Primary amine pendant arm cross-bridged tetraazamacrocycles and their transition metal complexes

Tim Hubin

Abstract

Cross-bridged tetraazamacrocycles form extremely stable transition metal complexes due to their topological constraint and rigidity. These stable complexes can be used in applications where complex stability is desirable, such as oxidation catalysis or biomedical applications. We have previously described a number of mono-pendant armed cross-bridged tetraazamacrocycles where the pendant arm can function to change the electronic properties of the metal complex with respect to the parent ligand, or provide a site for linking of the ligand to other moieties. Such pendant arms have included carboxylate, amide, pyridine, and phenolic donors. This work details our progress in the synthesis of cross-bridged tetraazamacrocycles having a single primary amine pendant arm. Several related routes involving Phthalimide protection/deprotection have been attempted with mixed results. A route involving the reduction of a primary amide has proven to be more reliable and will be detailed. Multiple transition metal complexes of the resulting ligands have been synthesized and their characterization will also be outlined.

Structural and kinetic stability studies of cross-bridged pentaazamacrocycles

Tim Hubin

Abstract

Ethylene cross-bridged tetraazamacrocycles have been known for multiple decades and have two primary attributes in their transition metal complexes that have made them increasingly popular for as ligands to stabilized transition metal ions for applications as diverse as oxidation catalysis and inorganic drug molecules: 1. their topological constraint and rigidity makes their transition metal complexes extremely stable even under harsh conditions, and 2. their folded structures place free coordination sites on their metal ions cis to one another as required for specific catalytic and biological binding events. Our work has recently produced pentaaazamacrocyclic analogues of these ligands which we have named cross-bridged pentaazamacrocycles. This presentation will outline the structural and kinetic stability data we have gathered on this new family of topologically constrained macrocyclic ligands. In particular, the crystal structure of a Cu(II) complex will be correlated with its ability to survive under harsh acidic aqueous conditions.

Towards controlling the alkylation of cross-bridged pentaazamacrocycles

Tim Hubin

Abstract

We have recently introduced a new class of topologically constrained ligand called cross-bridged pentaazamacrocycles. We have produced these ligands by two different synthetic paths. One involves regioselectivity of alkylation controlled by condensation of the parent unbridged pentaazamacrocycles with glyoxal to form aminal functional groups that limit alkylation and direct it to preferred nitrogen atoms which are all tertiary amines. The other follows a patent procedure involving tosyl protection, ring skeleton formation via classic Richman-Atkins strategies, and deprotection to form secondary amines. The latter approach allows addition of a range of alkyl groups and/or pendant arms to the cross-bridged pentaazamacrocyclic skeleton. In this presentation, we will describe the two synthetic pathways and their advantages and disadvantages. We will also present our recent attempts at pendant arm addition to this new topologically constrained parent system.

Electronic structure and oxidation catalysis of phenol pendant armed cross-bridged tetraazamacrocycle transition metal complexes

Tim Hubin

Abstract

We have previously presented synthetic pathways to cross-bridged tetraazamacrocycles with a single phenolic pendant arm. The pendant arm was intended to modify the electronic properties of the transition metal complexes formed, with respect to the parent cross-bridged ligand complexes. These complexes can be used as oxidation catalysts, so control of their electronic properties should allow fine tuning of reactivity in this realm. We present a detailed study of the electronic properties of the phenol-bearing complexes in comparison to published cross-bridged ligand complex analogues. Cyclic voltammetry and UV-Visible spectroscopy were used to investigate how the addition of the phenolic pendant arm modified those electronic properties. We also have obtained initial screening data in hydrogen atom abstraction screening reactions for some complexes, which will be correlated with the electronic properties presented.

Can protein crystal growth techniques be applied successfully to intermediate-sized polyamine ligands and their transition metal complexes?

Tim Hubin

Abstract

Our work with tetraazamacrocyles, and their bridged analogues, has led to some larger analogues that have not been successfully crystallized using our usually reliable small-molecule and transition metal complex crystallization methods, such as organic solvent diffusion and evaporation. A current student spent the past summer in a biological lab learning protein and nucleic acid crystallization techniques that are more suited for these larger biological polymers and oligomers. Based on our lack of success with our largest amine ligands and their complexes, we have begun to explore these biopolymer crystallization techniques, such as hanging drop techniques, and the addition of various buffers, salts, and other additives for primarily aqueous solution crystallization attempts. We will report on the techniques we have put into practice in our transition metal azamacrocycle lab and how successful they have been.

Sterically hindered cross-bridged tetraazamacrocyles

Tim Hubin

Abstract

Ethylene cross-bridged tetraazamacrocycles have found particular success in complexes used in catalytic oxidation of organic substrates. Several ligand derivatives have the two unbridged nitrogen atoms alkylated with different substituents, including methyl, benzyl, and ethyl groups. However, more extremely sterically bulky groups have not yet been utilized. The purposes of the proposed sterically bulky substituents are three-fold: (1) To prevent dimerization, allowing the study of monomeric complexes. Previous Mn and Fe work indicates that lack of steric bulk on the non-bridged nitrogens may allow dimers to form, which will alter the chemistry. Both dimers and monomers should be studied, thus the need for steric bulk. (2) In similar systems, bulky tBu groups lengthen and weaken M-N bonds and cause macrocycle twisting to keep the tBu groups far apart. Modification of the electronic properties of the complexes caused by these sterically induced complex deformations may help realize the specific properties needed for catalysis. (3) To encourage dissociation of one or more macrocyclic nitrogen due to steric bulk. These structural changes may lead to electronic and reactivity changes which should be explored. In this project, we have successfully synthesized an isopropyl substituted ethylene cross-bridged cyclen and its transition metal complexes. Synthetic details of the ligand synthesis and selected properties of the resulting metal complexes will be presented.

Modified tetraazamacrocycles as improved CXCR4 antagonists

Tim Hubin

Abstract

CXCR4 chemokine receptors are found on the surface of immune, and other, cells, and together with the specific natural ligand, stromal cell-derived factor-1α (SDF-1α, also known as CXCL12), have been revealed to play a role in a number of disease states. Within the last ten years the CXCR4 and CCR5 co-receptors have been revealed as the entry route for HIV into cells, generating interest in a new therapeutic approach to treatment via fusion inhibitor drugs rather than the current preference for reverse transcriptase and protease inhibitors. CXCR4 expression has also been reported in at least 23 different cancers. CXCL12 stimulation of tumor growth, angiogenesis, and metastasis of breast cancer cells has been described. Target organs for breast metastases such as liver, lung, and bone have high levels of CXCL12, triggering the specific migration of breast tumor cells that express the CXCR4 receptor. Due to the wide-ranging potential biomedical applications that might result, our aim is to develop new antagonists for the CXCR4 co-receptor. They are conformationally fixed macrocyclic compounds where the unrestrained equivalent is a known CXCR4 antagonist. The SWOSU-Hull collaboration has produced well over 50 metal complexes of bis-tetraazamacrocycle ligands for screening as CXCR4 antagonists. The bis-linked complexes are highly efficient antagonists, while single-macrocycle analogues are much less effective.

Using Bridged Nucleic Acids for Detection of Phosphatidyl 3-Kinase Catalytic Subunit Alpha Mutation

Rachel Hoffmeister & Sung-Kun (Sean) Kim

Abstract

PIK3CA is responsible for producing the catalytic subunit (p110) of the lipid kinase heterodimer phosphoinositide 3-kinase (PIK3 or PI3K). The E545Q mutation, which is due to single nucleotide mutation (c.1633G>C) and found in the highly conserved helical domain of PIK3CA, has been linked to cases of non-small-cell lung carcinoma (NSCLC). Bridged nucleic acids (BNAs) are modified nucleic acid analogs that have the ability to bind DNA with high affinity so that the resulting Tm values are altered. Moreover, the BNA's resistance to nucleases leads to increased stability in vitro and in vivo. We designed several BNA probes to bind more tightly to wild-type DNA than to mutant DNA. Thus, using BNA we observed lower resulting Tm values of samples of DNA containing the mutant sequence than that of the wild-type DNA. The Tm values of the mutant were significantly lower than that of the wild-type. Using BNAs a greater difference between Tm values was observed than that of the control, (e.g., solely DNA used, with no BNAs involved). This method of using BNAs for the detection of PIK3CA mutations was successful and could be utilized for earlier and more accurate diagnosis of NSCLC.

Inhibition of Metallo-beta-lactamase from Klebsiella pneumoniae by Hydroxamate Compounds

Destiny Morris & Sung-Kun (Sean) Kim

Abstract

Antibiotic resistance is a growing problem not only for scientists but for consumers worldwide. A very pertinent antibiotic resistance we are faced with is caused by metalloβ-lactamases. These enzymes catalyze the hydrolysis of β;-lactam antibiotics and have no clinically accepted inhibitor for their resistance. Consequently, it is critical that an inhibitor is discovered so this kind of antibiotic resistance can be treated. This research is concentrated on determining if the hydroxamate functional group is a viable inhibitor for the metallo-β;-lactamase, NDM-1 from Klebsiella pneumoniae. We found several commercially available compounds containing hydroxamate functional groups and tested their binding interactions using the computer software, AutoDock 4. Then the top three inhibitors will be tested experimentally in the lab to determine if they are acceptable inhibitors.

The Effect of EWG's and EDG's on HOMO-LUMO Gaps of Polycyclic Aromatic Hydrocarbons

Daniel McInnes

Abstract

This study will determine the relationship between the HOMO-LUMO gap in various PAH's and the largest number of disjoint aromatic pi sextets in the compound. The greater the number of sextets, the larger the PAH’s HOMO-LUMO gap is expected to be. Unsubstituted PAH's will be compared with those substituted with electron withdrawing groups and electron donating groups with regards to the predicted ionization potential of the molecule.

Development and validation of a High-Performance Liquid Chromatographic Method for the Determination of Metabolomic Biomarkers associated with Type 2 Diabetes

Sanjeewa Gamagedara

Abstract

Quantifications of the biomarkers associated with Type 2 Diabetes (T2D) are important in disease diagnosis and prognosis, identification of responses to the treatments, and to investigate the mechanisms of drug action. In this study, a novel High-performance liquid chromatographic (HPLC) method with diode array detection (DAD) was developed to quantify urinary hippuric acid, phenylalanine, phenylacetylglutamine and creatinine T2D biomarkers. Creatinine was included to account for the renal dilution of urine. The above biomarkers in urine samples were separated in an Agilent Eclipse XDB- C18 column using 6% acetonitrile and 94% 15 mM phosphate buffer (pH= 3.3) as the mobile phase. The detection wavelengths were 210nm and 225 nm. The Snyder's solvent strengths were constructed all four compounds showed the classical reverse phase liquid chromatographic (RPLC) hydrophobic behavior. The developed HPLC method was validated in synthetic urine matrix using analytical method validation parameters such as linearity, accuracy, reproducibility, limits of detection (LOD) and quantitation (LOQ) for accurate quantification. This validated method can potentially be used in a large scale clinical study. The detailed experimental conditions and results will be presented at the conference.

Numerical Modeling and Simulation of a Microfluidic Platform for Enrichment of Low Abundance Proteins

Mohammad Hossan & Sanjeewa Gamagedara

Abstract

Circulating TGF-β;1 is one of the key regulators of cardiovascular health. The extremely low abundance of circulating TGF-β;1 in the blood is one of the major challenges in on-chip purification and extraction. This paper reports numerical modeling and simulation of more than 25000 folds concentration gain of TGF-β;1 in a 2D cascade microchannel using isotachophoresis (ITP). The 4.3 cm long microfluidic channel with 250 times reduction in cross-sectional area from inlet to outlet was used for ITP simulation. The initial cross-sectional area was 1250 micrometer x 100 micrometer and the final cross-sectional area was 50-micrometer x 10 micrometer with 2D step changed. The reduction in the cross-sectional area was used to complement ITP concentration gain. COMSOL Multiphysics 5.2 was used to simulate the separation and concentration of two proteins- TGF-β;1 and albumin. The model used the Nernst-Planck equations to predict protein stacking and separation in the sample solution. Microchip with 1D and 2D step changed microfluidic channels were also explored using numerical simulations. The initial concentration of TGF-β;1 and albumin was 1.25 microgram/ml and after ITP concentration, each protein exhibited more than 25000 folds (~33 mg/ml) concentration gain. This is a significant improvement in the protein concentration factor compared to our previous report in an ITP microchip. This study can be utilized to develop an integrated microchip to detect proteins

Evaluating and Isolating Marine Invertebrate Extracts Based on Biological Activity

Michelle Pham & Kendra Brogden

Abstract

Natural products are defined as small molecules isolated from a source found in nature and are useful in applications such as medicine, agriculture and cosmetics. Due to their chemical diversity and biochemical relevance, the identification of bioactive compounds is significant to the pharmaceutical drug pipeline for their potential use towards the development of new medicine. In the ongoing search for new bioactive compounds, it is of great interest to identify those that are cytotoxic to cancer cells. The brine shrimp lethality assay is suitable for the preliminary screening of cytotoxic compounds since the brine shrimp's lethality correlates with the cytotoxicity of human lung and colon cancer cells. The aim of this work is to identify bioactive extracts from the brine shrimp assay, and then isolate and elucidate the structure of the bioactive compound. The evaluated extracts came from the University of Oklahoma Schmitz Sponge collection. With the assay, each extract is screened at a low (10.0 ppm), medium (50.0 ppm), and high concentration (100 ppm). Extracts indicating 70% lethality or higher with any concentration are reinvestigated using a confirmation assay. Of 33 extracts tested, 3 are inactive, 6 are moderately active, and 22 are active. Bioactive extracts are fractionated by chromatographic methods, and then the bioactive compound(s) identified using nuclear magnetic resonance spectroscopy, mass spectrometry and infrared spectroscopy.

The Synthesis and Characterization of [Cr(Py3Pyclen)(H2O)] (PF6)

Emily Burgess & Tim Hubin

Abstract

The synthesis of metal-ligand complexes is still a developing area in inorganic chemistry. The development of a stable, pure metal-ligand complex with a high yield is the synthetic goal. The use of $Py_3Pyclen$ with the aim of a hepta-dentate ligand, is a relatively novel area where an exact working sequence with high purity and yield has not yet been determined. This project focused on the synthesis of $Py_3Pyclen$, the development of a chromium-ligand complex with the synthesized ligand, and the characterization of the resulting $[Cr(Py_3Pyclen)(H_2O)]\ (PF_6)$ complex.

Synthesis and Complexation of 15aneN5 using Ni2+

Sierra Long & Tim Hubin

Abstract

Metal-ligand synthesis is still an ongoing adventure in the field of chemistry despite being around for ages. While attempts to synthesize organometallic complexes continue, the development of a stable synthetic process is the main goal. The synthesis of stable pentaazamacrocycle, 15aneN5, and its complexation with metal ions is a new practice in inorganic chemistry and a high yield has not been obtained. The purpose of this project was synthesis of cross-bridged forms of ligand 15aneN5, determining its complexation and the synthesis and complexation of Ni(15aneN5)(OAc)]PF6.

High Temperature Study of the Reactions of Titanium, Silicon, and Yttrium Oxides.

Lizbeth Robles-Fernandez, Fernando Salazar-Salas, & Dwight Myers

Abstract

Reactions of titanium oxide and silicon dioxide are of importance in materials used in high temperature environments. The extent of reaction and temperature range are important questions to answer for this chemical system. Presently we are exploring the reaction of titanium dioxide with silicon dioxide and trace amounts of yttrium oxide added. There are questions concerning the reaction of titanium dioxide (rutile) with silica. Both are important as potential materials or reaction products in thermal barrier coatings or environmental barrier coatings in combustion environments, as for example in gas turbine technologies. Experimental evidence would suggest that a third cation is necessary to have compound formation. Mixtures of the three oxides are being subjected to heatings at various temperatures from ca. 1200-1500°C. Samples are characterized before and after heating by means of X-ray diffraction and diffuse reflectance infrared spectroscopy, transmission infrared spectroscopy, and/or diffuse reflectance, UV/Vis spectroscopy as appropriate. Recent findings have shown that continual hearings and increased amounts of the Yttrium oxide are yielding further interactions between the three compounds. The ternary compound has has not been seen. Results to date will be presented.

Stabilization of Metallo-β;-lactamase using Ionic Liquids

Sung-Kun (Sean) Kim & Deanna Collins

Abstract

Metallo-β;-lactamase from Bacillus anthraces (Bla 2) catalyzes the hydrolysis of β;-lactam ring structure of the β;-lactam antibiotics. This results in the inactivation of β;-lactam antibiotics such as penicillin and cephalosporin. To study this enzyme, long- term storage would be beneficial to future research. Ionic liquids have been thought to be protein stabilizers. Thus, we probed the possibility of stabilizing bla 2 using imidazolium containing ionic liquids, which are suggested to be stabilizers.
Turbidity and enzyme activity tests were performed using Uv-vis spectrophotometry. Turbidity tests at 600 nm indicated that the enzyme was stable whereas enzyme activity tests showed the enzyme was denatured after 15 minutes. The tests at room temperature showed a slight decrease in activity which can be explained by computer analysis. The imidazolium merely bound to the active site of Bla 2 causing the enzyme to become slightly denatured. Imidazolium containing ionic liquids could not be used as a stabilizer of Bla 2, however it may be an inhibitor.

Inhibition of New Delhi metallo-beta-lactamase by hydroxyl(thio)pyrone and hydroxyl(thio)pyridinone compounds

Sung-Kun (Sean) Kim, Ahmed Alkhalifah, & Andrew Huckleby

Abstract

Bacteria has developed naturally to resist antibiotics and this is a major threat for human health. New Delhi metallo-beta-lactamase 1 (NDM-1) is an enzyme that makes bacteria resistant to a broad range of beta-lactam antibiotics. Currently there is no inhibitor of NDM-1 available in clinical therapy, thus making an essential need for research and development of a NDM-1 inhibitor. In this research we collected data using AutoDock to estimate the binding affinity of four potential molecule inhibitors. The molecules were Maltol, Thiomaltol, DMHP, and DMHTP which act as ligands to inhibit the NDM-1 enzyme by binding to the active site and blocking the catalytic enzyme activity and killing the bacteria.

A Molecular Dynamic Study of TAR DNA binding protein 43 Diagnostic Peptides

Sung-Kun (Sean) Kim

Abstract

In human cells, the TAR DNA binding protein, TDP-43, serves multiple functions with regulation of gene expression and mRNA splicing being the primary. An abundant amount of research has linked this protein to neuronal-degeneration in cases of Amyotrophic Lateral Sclerosis (ALS) and Frontotemporal Lobar Degeneration (FTLD), due to its tendency to form stress-induced inclusions. Using a study in which phage display technology was used to select for two peptides that were shown to have a high binding affinity for TDP-43, we performed a computational docking and molecular dynamics simulation to identify theoretical binding sites on the TDP-43 protein that were favored by the two peptides. These results coupled with the experimental data suggests that these peptides function as an effective biomarker in TDP-43 detection.

Theoretical Study of Chlorine Atom Complexation by Chloro-Substituted Methanes: Benchmark Energies and Performance of DFT Methods.

William Kelly

Abstract

Experimental evidence demonstrates that chlorinated solvents CH2Cl2, CHCl3 and CCl4 form stable Cl · solvent complexes during free radical photochlorination reactions. Recent ab initio computations identified stable Cl · CH2Cl2 and Cl · CHCl3 complexes with binding energies determined at the G3 composite method of -3.3 and -6.6 kJ mol-1, respectively. Both complexes have Cs symmetry. A DFT study at M062X/aug-cc-pVTZ model chemistry found a stable Cl · CHCl3 complex of C1 symmetry with a binding energy of -16 kJ mol-1. We probed the potential energy surfaces for Cl atom complexation with CH2Cl2 and CHCl3 employing several recent DFT methods (M062X, M11, WB97X, WB97X-D, B2PLYP, B2PLYPD and B2PLYPD3) and MP2 employing aug-cc-pVXZ (X=2-4). Two Cl atom complex geometries of Cs and C1 symmetry were obtained for each of the chlorinated solvents. Optimizations were carried out both with/without counterpoise corrections. The effect of basis set superposition error (BSSE) on both the potential energy surface and energy was negligible with the aug-cc-pVQZ basis set. Complex stabilization energies were obtained using the supermolecule approach and all electronic energies were corrected by addition of scaled zero point vibrational energies. DFT methods gave stabilization energies for the two complexes obtained for Cl atom interaction with CH2Cl2 ranging from -14.7 to -18.2 kJ mol-1, whereas stabilization energies for the two complexes obtained from CHCl3 ranged from -1

Development of a Microfluidic Device Integrating Solid-Phase Extraction and Microchip Electrophoresis

Mohammad Hossan & Sanjeewa Gamagedara

Abstract

Microfludic devices became popular clinical sample analysis due to small sample size, portability, low cost of fabrication, shorter analysis time and mass productions. In this project, we concentrated on integrating a solid phase extraction (SPE) channel to a microfluidic device. The SPE will help to purify the samples and to preconcentrate the analytes. For this device, PDMS (Polydimethylsiloxane) was used to minimize the cost of fabrication because it is cheaper than the commonly used PMMA (Polymethyl methacrylate) and SU-8. The photolithographic method was used for the fabrication of microfluidic devices using PDMS. The Oasis Hydrophilic-Lipophilic-Balance SPE particles were placed on a segment of the channel for the sample purification and preconcentration. Initially, the particles were carried out during the insertion of the water, but this problem was solved using the small piece of a fritted disk as the barrier on both sides of the segment where the particles were placed. The channel was tested using a syringe pump infusion at a rate of 50µL/ min with 5mL water in the syringe. Further experiments need to be done to have a properly sealed SPE integrated microfluidic device.

Inhibition of Hexokinase II by Fenbendazole

Sung-Kun (Sean) Kim & Hillary Le

Abstract

Fenbendazole (methyl N-(6-phenylsulfanyl-1H-benzimidazol-2-yl) carbamate) (FZ) is a broad spectrum benzimidazole anthelmintic that may disrupt cellular growth in cancer cells by depolymerizing microtubules. FZ may reduce glucose uptake from GLUT4 transporters and expression of glycolytic enzymes, like Hexokinase II. Here, we attempted to identify the binding location of Fenbendazole onto Hexokinase II.The chemical structure of FZ and Hexokinase II was illustrated using cheminformatics and bioinformatics software. We used molecular modeling simulation to find protein-ligand docking to bind the macromolecule with the ligand. The Autogrid parameter file used to pre-calculate maps of the energetics of the specific ligand configuration. This gave us a detailed view of energies and clusters that displayed exact binding site of Hexokinase II to Fenbendazole. In silico studies showed that FZ had altered the microtubule network at the binding site Asparagine D209. Results showed that FZ had 10 dockings with a range of docking energy of -5.5 to 6.75. Identifying the exact location of FZ binding to Hexokinase can have a lot of future implications in its research and possible therapeutic use.

Study of iodine distribution and concentrations in western Oklahoma brine waters

Jason Wickham & Ben Baker

Abstract

In the late 1970's, it was discovered that the brine waters of NW OK contain significant amounts of Iodine (above 60 ppm). However, the exact amounts and distributions of Iodine throughout this region were unknown. Currently, the majority of the world's supply of Iodine comes from mining Iodate minerals in Chile ≈65%), brine water aquifers in NW Oklahoma (≈5%) and Japan (≈25%), and seaweed extraction. With the growing need for Iodine compounds in various fields the demand for Iodine is higher than ever. Thus, Iofina has recruited the aid of NWOSU to quantify the Iodine concentrations and distribution throughout the brine aquifer, as well as, determine the longevity of these iodine concentrations. So far, this study has led to the discovery of new sites within the aquifer that may be of commercial interest and has taken an in-depth look at several possible new plant sites, with one of these sites being built and beginning operation during February 2018 and another currently under construction. Fluctuations in iodine concentrations of up to 100 ppm have been observed throughout this study which is a much larger fluctuation than the expected 10 ppm. We are currently investigating rather these fluctuations are due to the changed from vertical to horizontal wells as a function of the inhomogeneity within the brine aquifer.

A Closer Look At The Chemical Effects Nicotine Has On The Brain

Abul Kasem Rahman

Abstract

Presenting Author : Rahool Barua, Faculty Adviser : A.K.Fazlur Rahman, Ph.D.

Abstract :
Nicotine comes from the tobacco plant and is a stimulant for neural receptors in the nervous system. This stimulation is mediated using several neurotransmitters, such as acetylcholine, serotine, dopamine, etc. The release of dopamine due to stimulation has been cited as the source of addiction and depression due to this neurotransmitter being responsible for happiness. The research done aims to prove the isolation of nicotine in smoking systems such as e-cigarettes and vapes have increased nicotine's addictive properties and has made it more harmful for consumption.

Computational Studies of Structure and Reactivity of Selected Carbenes

Brandon Blankenship & Charles Crittell

Abstract

Carbenes are highly reactive species containing neutral divalent carbon. Carbenes also contain two nonbonding electrons on the carbon center that are either paired, singlet or are unpaired, triplet. While there are some carbenes that are persistant, the overwhelming majority ae short lived and can not be studied directly. The goal of this project is to investigate the nature of several short lived carbenes using theoretical studies. The geometry and relative energy levels of both singlet and triplet carbenes will be explored.

Measuring Thermal Denaturation of Heme Binding Proteins by Differential Scanning Calorimetry

Kyle Moore

Abstract

Protein folding and unfolding is often modeled as an equilibrium between two extreme states, folded and unfolded. Differential Scanning Calorimetry (DSC) is a method by which heat flow between two samples is measured as a function of temperature increasing or decreasing. Proteins thermally denature, and thus transition between folded and unfolded, at a specific temperature known as the melting temperature (TM). A DSC can measure protein unfolding by monitoring the difference in the heat flow between a protein sample dissolved in a buffer and a reference buffer. Heme binding proteins in pathogenic organisms like Listeria monocytogenes are virulence factors when causing infections. In order to investigate the thermal stability of these proteins, we tested two heme binding proteins from L. monocytogenes using a DSC-25. Here we report the change in enthalpy and change in entropy for the thermal denaturation of Hbp1 and Hbp2.

Advances Towards the Utilization of Cucurbut[n]uril and Selected Guests in Molecular Machines and Devices.

Usha Khadka

Abstract

Supramolecular chemistry has found useful application in chemistry, with cucurbit[n]urils (CB[n]) exhibiting unique chemical properties. By the use of primarily hydrophobic interactions, these macrocycles can bind various small molecules with high binding constants in the range of 106 to 1012 M^-1. The potential applications of these host guest systems can include molecular machines, drug delivery, and the purification of water. Our work focused on the synthesis of different viologens and alkynes; and their binding modes were studied by 1H NMR chemical shift data and binding constants by 1H NMR competition with CB[7] and CB[8], which could lead us to strategic incorporation of these molecules into molecular machines and devices. Different mono and di-substituted compounds were synthesized from starting material 4,4-dipyridine and 1,7-octadiyne with varied substituents like methyl, hexyl and 1-ethoxy-2-(2-methoxyethoxy)- groups. These structures have been chosen for their potential for building more complex host-guest systems through organic synthesis.

Isolating Bioactive Compounds from Marine Invertebrates

Michelle Pham & Kendra Brogden

Abstract

Due to natural products' chemical diversity and biochemical relevance, the identification of bioactive compounds is of great interest to the pharmaceutical industry for their potential use towards the development of new medicines especially cancer treatments. The brine shrimp (Artemia spp.) lethality assay is an appropriate preliminary screening of cytotoxic compounds since the brine shrimp's lethality correlates to the cytotoxicity of human cancer cells from the lung and colon lining. The aim of this work was to isolate and identify cytotoxic bioactive compounds for their potential use in pharmaceutical use by fractionating active marine invertebrate extracts. The evaluated extracts were obtained from the University of Oklahoma Schmitz Sponge collection. Each extract was screened utilizing the brine shrimp assay at a low, medium, and high concentration (333 ppm, 1667 ppm, and 3333 ppm). Extracts indicating 70% lethality were considered active and fractioned by normal and reverse phase flash chromatography. The activity was followed in successive brine shrimp lethality assays. Bioactive fractions will be analyzed using nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry, and infrared (IR) spectroscopy to elucidate the structure of the bioactive compound(s) as time allows.

Computational Determination of the Enthalpy of Formation Aluminum Hydroxide Vapor

Dwight Myers & Uendi Pustina

Abstract

Reactivity and compatibility of oxides with other materials and with each other plays a significant role in choice of materials for developing Thermal Barrier Coatings (TBCs) or Environmental Barrier Coatings (EBCs) for use in combustion environments. Aluminum oxide is one material with potential for these applications. However, the oxide coating itself can be eroded away by reaction with hot water vapor in a combustion environment, forming volatile hydroxides. Aluminum oxide can react with water vapor to form a volatile aluminum hydroxide. We are performing a computational study of the gas phase molecule aluminum hydroxide. The ultimate goal of this study is to obtain a reliable value of the enthalpy of formation of aluminum hydroxide. The software we are using is the GAMESS ab initio package. To determine the enthalpy of formation of the aluminum hydroxide molecule, the enthalpy of reaction of the isodesmic, isogyric reaction of aluminum fluoride vapor with water vapor to yield aluminum hydroxide and hydrogen fluoride will be studied. Results at the G3-MP2 level will be compared to higher level computations using the CCSD(T) level of theory. Comparison will be made to other computational results for the aluminum hydroxide vapor species.

Microwave Synthesis of Imidazoles from 1,2-diketones

Peyton Little & Elizabeth Nalley

Abstract

Allowing many chemical reactions to be completed within minutes, microwave technology has revolutionized preparative chemistry. Since it is a green technology, it is becoming widely adopted in both academic and industrial laboratories. Heterocycles are very important functional groups especially in medicinal chemistry. In this research heterocyclic precursors of pharmaceuticals are synthesized using microwave radiation. In this poster we describe the synthesis of a number of 2,4,5-trisubstituted imidazoles from 1,2-diketones and substituted benzaldehydes in the presence of NH4OAc. The imidazoles are purified and characterized using FTIR and NMR. These imidazoles will be tested as possible catalysts in microwave synthesis of esters.

Applications of Magnetite-Glutathionine Based Catalysts in Organic Syntheses

Restituto Paris & Stephen Myers

Abstract

During the past year we have employed microwave radiation and sonication to synthesize a number of heterocyclics which are precursors of a number of medicinal compounds. Both the microwave synthesis and sonichemistry reactions enable us to study the applications of unique catalysts in organic synthesis of these heterocyclics. The synthesis of well-defined nanomaterials and nanocatalysts is an integral part of nanotechnology and catalysis science, because it is imperative to control their size, shape, and compositional engineering for unique deployment in the field of nanocatalysis and organic synthesis. Sustainable nanomaterials and their applications in benign media are an ideal blend for the development of greener methodologies in organic synthesis; MW heating provides superb value to the overall sustainable process development via process intensification. In this study we have synthesized a number of magnetite catalysts using sonication to bond Glutathionine to Magnetite and then bonding the Glutathionine magnetite complex to various transition metals. These catalysts were tested as microwave catalysts in a number of organic syntheses.

Green one-step, one-pot route to cyclic carbonates from soybean, sunflower and corn oils for the synthesis of polyurethanes

Theresa Hinkle

Abstract

As recent literature indicates, microwaves are quickly becoming an accepted tool for investigators in the organic laboratory. Microwave synthesis enables reactions to proceed more rapidly with greater yields than many conventional techniques. In parallel, there is a growing concerned about the isocyanate chemistry used to produce polyurethanes. Indeed, isocyanate are known to be toxic and are synthesized from phosgene an event more toxic gas. An alternative route to the isocyanate/alcohol chemistry is the cyclic carbonate aminolysis. However, the conventional synthesis of cyclic carbonate requires two-step procedure: epoxidation of double bond followed by carbonation.

In this research, we investigated the use of microwaves to synthesize cyclic carbonate from natural products such as soybean, sunflower and corn oils in one-pot, one-step reaction. These monomers can then be converted to polymers, which are produced using derivatized "natural products". We will compare the efficiency of microwave/ conventional synthesis of polymers.

Thermal Degredation of Polystyrene in Lewis Acid Solutions

Alexander Chandler

Abstract

The goal of this project is to determine the effects of Lewis acids in the degradation process of polystyrene, the main component of "styrofoam". Stock solutions of 0.02 M of the Lewis acids and were prepared in DMF. 0.002 g of polystyrene was dissolved in both the lewis acid stock solutions at room temperature. Additionally, these stock solutions were heated to 80 °C. Temperature, as well as the addition of lewis acids, played a major role in the time it takes for the degradation of the polystyrene. Preliminary results have demonstrated a clear link between temperature and the time it takes for the polystyrene to degrade. Further investigations are planned in identifying the products of this degradation, since many are toxic, to optimize degradation while minimizing toxic byproducts. These insights may help provide a viable for disposing of polystyrene wastes.

The Importance of Anti-Psychotics in Mental Health Treatment

Abul Kasem Rahman & Ilana Rozzell

Abstract

Author : Ilana Rozzell, Oklahoma School of Science and Mathematics
Faculty Advisor : A.K.Fazlur Rahman, Chemistry Department

Abstract :

Antipsychotics are a group of extremely vital medications for the improvement of mental health. Both 1st generation and second generation antipsychotic medications are designed to reduce and prevent the return of psychotic symptoms, including hallucinations, delusions and disordered thinking. Modern medications for treating psychosis are known as ‘second-generation’ or ‘atypical’ antipsychotics. In this paper we will investigate the various antipsychotics available in the market. Our main focus will be to understand how these medications function in reducing or eliminating symptoms of psychosis that otherwise can disable a person. We will also describe how antipsychotics work to block dopamine receptors that are thought to be the cause of the psychosis to begin with. A noteworthy example, may include that usage of Thorazine which is believed to block dopamine in the treatment of schizophrenia and manic-depression.

Dihydrodipicolate Synthase and Natural Product Inibitors

Nathan Blythe

Abstract

Lysine is an essential amino acid used in the biosynthesis of proteins. Two main biosynthetic pathways, the diaminopimelate (DAP) pathway and the α-aminoadipate pathway (AAA) synthesize lysine. The targeted pathway of this research is the DAP pathway. Dihydrodipicolinate synthase (DHDPS) is catalyzing condensation reaction of pyruvate and aspartate semialdehyde to form dihydropicolinate. The enzyme is at the committed step of the DAP pathway making it a key target for drug design. Several samples from the National Cancer Institute (NCI) Repository are being investigated for inhibition of the DHDPS. The samples are analyzed with thin-layered chromatography to find the best solvent system. Samples are then analyzed and fractioned using reverse phase and normal phase flash chromatography for partial purification using the High Performance Flash Chromatography system Isolera (Biotage). Active fractions for inhibition of DHDPS are then tested using enzyme kinetic studies.

Photophysical Properties of Fluorescent Texas Red Dyes in Confined Environments

Dr. Rajesh Nayak

Abstract

The photpphysical properties of fluorescent texas red dyes have been investigated in confined reverse micellar environments. The anionic surfactant sodium bis (2-ethylhexyl) sulfosuccinate, also known as Aeresol-OT or AOT and the cationic surfactant Cetyl trimethylammonium bromide, commonly known as CTAB have been used as reverse micelles in these studies. Various steady-state and time-resolved spectroscopic techniques such as UV-Vis absorption, fluorescence emission, Fluorescence Anisotropy, Dynamic Light scattering (DLS) as well as Time Correlated Single Photon Counting (TCSPC) techniques were employed to understand the behavior of the dyes in reverse micelles. The results obtained in confined environments were compared with the results in aqueous environments. Our experimental observation shows that the electronic and hydrodynamic properties of the probe molecules inside crowded reverse micelles can be different as compared to those in aqueous environments. Our present studies have the enormous potential to use fluorescent probe molecules as biomolecule labels and reverse micelle as simple model systems to probe biomolecule dynamics in reverse micelle environment which mimic the crowded biological cell.

Synthesis and Surface Functionalization of Dye Doped Silica Nanoparticles

Tarell Nunley

Abstract

Silica nanoparticles (SiNPs) are highly sought after nanomaterials due to the many applications they offer such as biomarkers, additives in nanocomposites, and optical sensing devices. SiNPs can be synthesized and functionalized through numerous pathways, making them the ideal building block for nano-scale assemblies or nanocomposites. Additionally, their optical transparency allows SiNPS to be applied in nano-scale sensing devices or meta-materials that respond to electromagnetic radiation. Here, we describe the synthesis and surface functionalization of dye-doped SiNPs. The particles were assembled via a modified Stöber method using an aqueous-organic bilayer system. The particles were regrown iteratively to create a core shell motif that allows for further functionalization such as dye incorporation where the dye is trapped in the matrix of silica through an additional layer grown on the surface. The second layer of silica also provides a surface for functionalization, including amine functional groups, providing a pathway for use in an nano-assembly. These dye-doped surface functionalized SiNPs are intended to be used as dye trapping agents in an energy transfer nano-scale assembly with gold nanorods (GNR) with potential contributions to industries such as biomarkers in the medical field to nanocomposites in the aerospace industry. This work addresses the techniques used to synthesize multilayer fluorescent dye dope SiNP with anime surface functionalization.

Biologically Important Compounds: Synthesis and Antitumor Studies of Nicotinic Acid, Thionicotinic Acid, Pryrimidine thiolate and Methionine Complexes of Platinum

Abul Kasem Rahman & Vickie Jean

Abstract

A.K.Fazlur Rahman1, Edwin Ding, Alex Lin, Kevin Thomas, Pedro Lozano-DeAos1, Prabir Chakrabotry2, Pryabratta Mukherjee 2

1. Department of Chemistry, Oklahoma School of Science and mathematics
2. University of Oklahoma Health Science Center, Oklahoma City, OK

Abstract:

In our continuing effort to develop and study anticancer active platinum compounds we have synthesized a series of platinum compounds coordinated to pyridine thiol (I), tetrahydropyrimidine thiol (II) and Amino acids. Some structural features including biological studies will be discussed during the presentation. Preliminary data suggests that some of these compounds have potential antitumor activity. We have screened the efficacy of the synthesized compounds on ovarian cancer (OC) cell lines. Ovarian cancer accounts for high mortality in American women and is attributed to acquired chemoresistance and unavailability of specific targeted therapy. From our initial screen we have identified two compounds showing bolstered cancer cell killing through induction of apoptosis. In conclusion, these compounds hold promise for better therapeutic outcomes in cancer, including OC.

Ab initio calculations of C-C bond activation via protonation or electrophilic methylation in metal complexes

Abul Kasem Rahman

Abstract

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Abstract:

In this study, the reaction profile of metal complexes in the form of M(η5-(C5H5)(η4-bicyclo [2.2.1]-hepta-2,5-diene) was investigated using ab initio density functional theory (DFT) calculations. The calculations were performed following a known reaction route with Co(η5-C5H5)(η4-bicyclo[2.2.1]-hepta-2,5-diene) involving the protonation and activation of a carbon-carbon bond in the 2,5-norbornadiene via agostic M-H-C interactions. Then, the same computational method was used to study the analogous electrophilic methylation of Co(η5-(C5H5)(η4-bicyclo[2.2.1]-hepta-2,5-diene) following a similar reaction mechanism. Additionally, the protonation and electrophilic methylations of analogous metal complexes with central metal Rh and Ir were compared to the Co case. We find that the reaction profiles of both protonation and electrophilic methylation are determined by the type of the transition metal, which thus explains some experimental observations.

Probing Reverse Micelle Environment with Cyanine Dyes using Various Spectroscopic Techniques

Dr. Rajesh Nayak

Abstract

The spectroscopic properties of cyanine dye Cy-5 within water-in-isooctane sodium bis (2-ethyl hexyl) sulfosuccinate (AOT) reverse micellar environment have been investigated as a function of water contents (W0=[H2O]/[AOT]=1-30) in AOT by using steady-state UV-Vis absorption and emission and time-resolved fluorescence as well as Dynamic Light Scattering (DLS) techniques. Our result shows that the Cy-5 dye inside the smallest reverse micelle (W0 =1) environment behaves strangely as compared to bigger reverse micelle sizes. This present investigation shows that the Cy-5 dye probably undergoes aggregation inside the smallest reverse micelle. Furthermore, the spectroscopic properties of the Cy-5 inside micelles were compared with the Cy-5 inside aqueous environment and it was found that the dye behaves differently inside the reverse micelle as compared to the aqueous environment. Further optical spectroscopic and 2D NMR experiments are required to understand the location, electronic and hydrodynamic properties of the dyes.

Preparation and reactions of some novel Phosphorus and Nitriogen heterocyclic compounds

David Esjornson

Abstract

Both phosphorus and nitrogen containing compounds have been used to synthesize a variety of metal complexes. Often the phosphorous atom dominates the coordination of these mixed ligands with metals. The synthesis of nitrogen heterocycles where one or two of the nitrogen atoms has been replaced by phosphorus atoms has been attempted. Some new mixed P,N ligands have been synthesized from Cyclohexylphosphine, Formaldehyde and Aniline. Both a pendant nitrogen compound, CyP(CH2NPh)2 (where Cy = C6H11 and Ph = C6H5), and a heterocyclic six membered ring compound, 5-Cyclohexyl-1,3-diphenyl-1,3,5-diazaphosphinane, have been characterized. This compound has been been reacted with a series of Metal(II) complexes, including Manganese, Iron, Cobalt, Nickel, Copper, and Zinc.

Developing a Green Experiment for an Organic Chemistry Laboratory Course

Hugo Sanchez

Abstract

Oxidation reactions are important because they are sources of energy, both natural and artificial. Unfortunately, many oxidation reactions utilize reagents that are harmful to the environment and may impose safety hazards to the person using them. Such chemical compounds like chromic acid and potassium permanganate pose these kinds of hazards, and as such should be used with the utmost care when handling them in the lab. Green chemistry is an area of chemistry that seeks to prevent the use of harmful chemicals, reduce waste, and prevent harm to human health and the environment. The purpose of this project is to produce a green lab experiment by the conversion of cyclohexanol to cyclohexanone via an oxidation reaction with sodium hypochlorite (bleach) and glacial acetic acid. The goal is to develop a green synthesis that can be purified in good yield and can be analyzed the next day. There have been research articles citing the successful oxidation of cyclohexanol to cyclohexanone, but this work needs to be heavily modified to succeed in a teaching laboratory setting. The current goal of this project is to implement this experiment into a study for undergraduate students who are taking Organic Chemistry II. The final products must be reproduced in good yield and in a timely manner all while analyzing the results using NMR and IR. The study involving undergrads must be taken into utmost consideration which involves getting proper ethical training and IRB approval.

Synthesis, Transport and Recovery of aluminum oxide nanoparticles through limestone and dolomite rock.

Randall Maples

Abstract

Nanomaterials such as metal oxides are finding greater use in industry, for applications such as materials coatings, sensors and even drug delivery. Because of this, there is the increased potential of engineered nanoparticle release into the environment as contaminants when devices and materials containing these are disposed of. It is important to assess the short and long-term fate of these engineered materials and their distribution in groundwater and subsurface. This study looked at the synthesis, characterization, transport and recovery of water dispersible functionalized aluminum oxide nanoparticles through packed stone columns as models for the local groundwater environment in central Oklahoma.

Iron-binding Compound Production in Marine Microorganisms

Jessica Martin, Patrick Huling, & Kyle Brown

Abstract

Iron is the fourth most abundant element on the earth's surface, yet it is only sparingly soluble in the aerobic, near neutral conditions under which most microbes grow. Hence iron limitation is a major factor influencing the growth of microorganisms, from infection of a mammalian host (where iron is tightly controlled by protein complexation) to aquatic and marine environments (where iron is not soluble or is complexed by organic ligands). Many microorganisms produce low-molecular-weight, iron(III)-specific binding compounds called siderophores to compete for iron. Microbes are thought to produce unique siderophore structures to successfully compete for iron against other organisms in their environment. We studied the production of a siderophore by Halomonas cupida ATCC 35135 using low-iron competitive growth environments. Results conclude that Halomonas cupida ATCC 35135 does produce a siderophore. Current studies are on identifying siderophore structure.

The production of siderophores and the methods of testing for new siderophores

Sierra Hinkle & Jessica Martin

Abstract

Iron is a fundamental nutrient in not only human life but also microbial life. While iron is controlled through diet for mammals, microbes have to find other ways to obtain the iron they need for survival. They do so by using siderophores. Siderophores are ferric iron chelating agents, which are typically low in molecular weight. Their job is to seize iron from the environment and make it available to the cell to promote cell growth and survival. This is a necessary process due to the poor solubility of iron in the aerobic conditions in which many microbes cultivate. We report here the production of siderophores by H. pacifica and S. salmonicolor and the methods of testing these compounds for new siderophores.

Siderophore Production and Competition Between Fungi

Jessica Martin & Kylie Whitlock

Abstract

Siderophores are significant to the cellular functions of microorganisms. Microbes produce siderophores to facilitate bringing iron from the environment into the cell. Siderophores are chelating agents which have a high affinity for binding with ferric iron. Without siderophores, microbes would have difficulties competing for iron in certain environments such as the aerobic conditions of marine life. Due to other microorganisms also competing for iron in the same environment, microbes produce siderophores that differ in structure. A look into the competition between fungi and the siderophores they produce can give insight on the importance of siderophore production in microbes. We report here on the production of siderophores by Cunninghamella elegans and Sporidiobolus salmonicolor grown individually as well as the production of siderophores when they are grown together.

Graphene: Its Mass Production and Potential Impact

Lunea Wang & Abul Kasem Rahman

Abstract

Presenting Author : Lunea Wang, Oklahoma School of Science and Mathematics

Abstract
At only one atom thick, graphene, an allotrope of carbon with a hexagonal lattice, has many properties that could lead to significant advancements in fields of engineering, technology, and medicine. After first being isolated from bulk graphite in 2004, it has been discovered that graphene is flexible, durable, transparent, biocompatible, as well as a superconductor of both heat and electricity while also being one of the strongest materials known to man. Traditionally, graphene had been expensive and difficult to make on an industrial scale, hence graphene's potential has remained largely untapped outside of laboratory research. However, researchers recently developed methods to mass produce graphene, creating endless possibilities for the application of graphene. Some of these applications include better transistors and semi-conductors, bendable or wearable electronics, faster charging and longer lasting batteries, better water filtration systems, targeted drug delivery, tissue engineering, and more. Through more research and experimentation, graphene has the potential to bring science-fiction technologies to life and change the world for the better.

Synthesis and Functionalization of DNA Coated Silica Nanoparticles

Tyler Gore

Abstract

Silica nanoparticles are a highly versatile nanomaterial due to their facile preparation and functionalization through surface chemistry. The primary focus of this work is the synthesis of multi-functionalized silica nanoparticles adept for use in highly ordered nanostructures. The synthesis of the silica nanoparticles is accomplished through a modified Stöber method. In this method an aqueous organic bi-layer is used to form highly uniform silica nanoparticles. These nanoparticles are then coated with a fluorophore before being encapsulated by a protective outer layer of siloxane. The outer layer of these nanoparticles is then functionalized with an amine group that can then be linked with a short oligonucleotide sequence. The resulting functionalized silica nanoparticles are then capable of being organized into more complex nanostructures through the hybridization of the DNA sequences found on the surface of the nanoparticles. The application of these methods provides a viable source of silica nanoparticles adept for drug delivery, biomedical imaging, and nano-photonic cell systems.

Synthesis of (3β;,5α,6α)-cholestane-3,6-diol and 5-deutero-(3β;,5α,6α)-cholestane-3,6-diol and their structural investigation using single- and two-dimensional nuclear magnetic resonance techniques

David Martyn

Abstract

Convenient methods for synthesis of (3β;,5α,6α)-cholestane-3,6-diol and 5-deutero-(3β;,5α,6α)-cholestane-3,6-diol from (3β;)-cholest-5-en-3-ol were developed. Hydroboration and oxidation of (3β;)-cholest-5-en-3-ol using deuterated or non-deuterated borane resulted in the formation of the corresponding (3β;,5α,6α)-cholestane-3,6-diol products in good yield. Assignment of the 1H and 13C NMR spectra of cholesterol, (3β;,5α,6α)-cholestane-3,6-diol, and 5-deutero-(3β;,5α,6α)-cholestane-3,6-diol were made by using the following one- and two-dimensional NMR techniques: DEPT, 1D TOCSY, EXSY/NOSEY, 2D COSY, 2D TOCSY, HMQC and HMBC. Analysis of the collected spectra made assignment of all proton and carbon resonance signals of starting material and products possible.

The Impact of Nicotine on Adolescents

Abul Kasem Rahman, Vickie Jean, & Anika Bekkem

Abstract

The impact of nicotine on adolescents is especially prevalent today. Many are attempting to quit their addiction to the harmful substance, and many options are available to help. Some methods of nicotine intake include traditional smoking, e-cigarettes, and dipping. These methods each come with their own effects. One common method of addiction treatment is nicotine replacement therapy. This can be in the form of patches, lozenges, and nasal sprays. There are also several non-nicotine medications that assist in addiction therapy. Each method of nicotine addiction treatment chemically interacts with the body differently. This research will analyze how these chemical interactions occur and the advantages and disadvantages that different methods pose.

Chemical Security Education is needed for Undergraduate and Graduate Students

Chalita Thompson

Abstract

Chemical safety has become a central theme in chemical education, as of late . Recent academic laboratory and industry incidents have led to policy changes in government and academic programs to improve chemical safety. In contrast, not much is known about post-secondary chemical security education. The purpose of this study is to identify why there is such a large gap in the understanding of the need for chemical safety but not much for chemical security, while attempting to identify current practices and attitudes concerning chemical security. For the study, ACS-approved chemistry programs were surveyed to ask questions about their perceived chemical safety and chemical security culture, how chemical safety and chemical security is taught, and how often either were taught at their institution. Nearly all (>99%) of the institutions teach chemical safety to undergraduates at their institutions, 73% to graduate students, while only about one-third of the respondents say that chemical security is taught at any education level. A majority of respondents to the survey (96%) feel that chemical safety should be mandatory while about half (57%) felt that chemical security should be mandatory. The importance of chemical security education must be made a priority by the chemistry community in order for more institutions to commit to chemical security training for faculty and students.

Optimizing an Inorganic Chemistry Lab Experiment for determining the Spectrochemical Series and Magnetic Susceptibility of various Cobalt Complexes

Emily Cowen, Maggie Ward, Alexander Chandler, Kassandra Camua, & Ryan Webb

Abstract

For many inorganic chemistry courses, the spectrochemical series is a classic topic to introduce students to ligand field theory and crystal field theory, as well as providing an entryway to magnetic susceptibility. Our goal was to adapt a lab based off of previously established syntheses for determining the spectrochemical series and number of unpaired electrons. Through this lab, students can compare the different colors and properties of various ligands in cobalt complexes, including glycine, oxalate, water, and ethylenediamine through UV-Vis analysis. The UV-Vis absorption can be used to determine the ligand strength and the d-orbital splitting. We were able to successfully synthesize these four cobalt complexes, perform UV-Vis absorption studies on them, and complete calculations to determine molar absorptivity and d-orbital splitting during a 3-hour lab class. During an additional lab class, magnetic susceptibility and number of unpaired electrons was determined using the Evans method on NMR or an Evans Balance.

The Development and Implementation of a Standard Operating Procedure and Interdisciplinary Applications for the Flame Atomic Absorption Spectrometer in Chemical, Biological, and General Areas of Study

Andreanna Turner

Abstract

Standard operating procedure and interdisciplinary applications for the flame atomic absorption spectrometer were developed for three academic classifications of students. These applications of an underutilized chemical instrument were applied to several academic fields. The chemical application focuses on analysis of lead or other trace metal concentrations in local tap water sources near and around Chickasha, OK. The biological portion utilizes the Flame Atomic Absorption spectrometer to study plant uptake of toxic metals introduced in early developmental stages. Lastly, the general science application investigates the metal content of pond water samples from the University of Science and Arts of Oklahoma. The standard operating procedure was implemented in an instrumental analysis laboratory, a freshman level biology course, and the general education foundations of science laboratory. These standard operation procedures can be broadly applied for use in a range of laboratory and research settings.

Understanding the Value of Good Health: The brain Chemistry and obesity

Abul Kasem Rahman

Abstract

Abstract :
There is a three fold increase of obesity across the globe for the last fifty years. Obesity is one of the leading risk factor linked to 4.7 million adult deaths globally in 2017 which amounts to 8.7%. According to the world health reports 39% of adults in the world are overweight. Among the children the ratio is about 25%, which is alarming.

Obesity is attributed to the imbalance of energy intake and lack of efficient utilization in our physiological system.

Many metabolic related disease such as high blood pressure, diabetes, cardiovascular are also attributed to obesity. Studies tells us that differences in brain chemistry could explain why obese people may be more tempted to eat than people of normal weight. Published data suggests that environmental factors also triggers to eat, such as food smells, were found to cause different reactions in the brain in obese people, compelling them to eat more often.This presentation will attempt to illustrate this paramount public health problem by presenting some relevant data to bring awareness thereby.

Increasing Student Preparedness Using Demonstration Videos in a General Chemistry Laboratory

Emily Falcon

Abstract

The use of interactive educational models is increasing in the new technological age. As shown in the Spring 2019 semester by two senior Chemistry students, undergraduates in General Chemistry 1 Laboratory classes would appreciate having demonstration videos to aid in their learning. These senior students made six videos and showed them to the students at the end of the Spring 2019 semester. This new project extends to showing the undergraduate students videos while learning the corresponding topic in recitation. The students' confidence in the material and perception of the helpfulness of the video was surveyed and evaluated one week later. Additionally, two new videos were made for the class (Making Tables in Microsoft Word and Equation Editor in Microsoft Word) and evaluated as before. These videos were made by taking screenshots of the process, inserting them into the website Explain Everything, and adding voiceovers and live drawings. A control class was used as a comparison for all the surveys conducted. Some of the videos had no effect on the students' ability to perform the given task, and others were significantly beneficial. This indicated that videos were as effective or more so than a traditional lecture-based recitation. Therefore, more demonstration and explanatory videos should be made for the chemistry laboratories so students can have an additional learning resource and some faculty could move toward teaching recitation in a flipped-classroom styl