Mar 8th, 9:59 AM

04. Chemistry

Southwestern Oklahoma State University

FaithOkorocha, TimothyHubin

Southwestern Oklahoma State University

Primary amine pendant arms useful for conjugation of cross-bridged tetraazamacrocycles to other bioactive groups

Cross-bridged tetraazamacrocycles have made important contributions as ligands that strongly bind transition metal ions. This property is very useful when the metal complex is intended for use under harsh conditions. One application that has benefited from such complexes is medical imaging, where radioactive transition metal ions can be stably bound to the cross-bridge ligand, injected into patients, and used to identify diseased tissues, such as cancerous tumors. Pendant arms can be added to the cross-bridged tetraazamacrocycle to allow conjugation to other biologically active compounds, or biomolecules such as proteins and nucleic acids themselves. The conjugated bioactive compound might perform various therapeutic activities, while the cross-bridged tetraazamacrocyle metal complex attached serves as an imaging agent to help illuminate the biological effect of its conjugated partner. In this project, we are developing the synthesis of a primary amine pendant arm to the known ethylene cross-bridged tetraazamacrocycles. This functional group is well-known for its ability to be conjugated to biomolecules. Synthetic and characterization methods and results for these novel compounds will be presented.

Mathematics and Science.Chemistry.02

TannerTadlock, TimothyHubin

Southwestern Oklahoma State University

Pyridine linked bis cross-bridged tetraazamacrocycles

Bis cross-bridged tetraazamacrocycles, and their transition metal complexes, have become one of the most effective classes of CXCR4 chemokine receptor antagonists. These cell surface receptors are important to a number of disease states, including HIV, cardiovascular disease, and cancer. Our group has continued to produce new analogues of these compounds in an effort to improve further the efficacy, specificity, and drug-like properties of this class of compounds. In this presentation, we will describe the synthesis, chemical characterization, and biological activity of a new series of bis cross-bridged tetraazamacrocyles in which the unit linking the two macrocyclic units is a nitrogen-containing pyridine, rather than the typical all carbon aromatic linking units of our previous compounds. Results include the apparent production of a 2+2 cyclic version of our typical ligands apparently driven by the change to the pyridine linker.

Mathematics and Science.Chemistry.03

AbnerNimsey, TimothyHubin

Southwestern Oklahoma State University

Mono- and bis-cross-bridged tetraazamacrocycles with thiol pendant arms for biomolecule conjugation

Cross-bridged tetraazamacrocycles have made important contributions as ligands when their metal complex is intended for use under harsh conditions. Applications that have benefited from such complexes are: oxidation catalysis, medical imaging, and protein-binding drug molecules. Bis cross-bridged tetraazamacrocycles, and their transition metal complexes, have become one of the most effective classes of CXCR4 chemokine receptor antagonists. These cell surface receptors are important to a number of disease states, including HIV, cardiovascular disease, and cancer. Our group has continued to produce new analogues of these compounds in an effort to improve further the efficacy, specificity, and drug-like properties of this class of compounds. In this presentation, we will describe the synthesis, chemical characterization, and biological activity of a new series of bis cross-bridged tetraazamacrocyles in which the cross-bridged macrocycle is appended with either a thiol or primary amine pendant arm. These pendant arms are intended to allow conjugation to biologically active compounds, or biomolecules such as proteins and nucleic acids themselves. Once conjugated, the bis cross-bridged tetraazamacrocycle unit would serve as the targeting unit which would bind specifically to cells expressing high concentrations of CXCR4 on their surfaces, such as certain cancer cells. Synthetic and characterization methods and results for these novel compounds will be presented.

Mathematics and Science.Chemistry.04

TimothyHubin

Southwestern Oklahoma State University

Sterically hindered cross-bridged tetraazamacrocyles

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.

Mathematics and Science.Chemistry.05

TimothyHubin

Southwestern Oklahoma State University

Novel ethylene cross-bridged tetra- and penta- azamacrocycles

Ethylene cross-bridged tetraazamacrocyclic ligands have gained common use in applications where transition metal complexes must withstand harsh aqueous conditions, such as oxidation catalysis, biomedical imaging, and bioinorganic medicinal compounds. We wish to add additional members to this ligand family by (1) using sterically-hindered parent tetraazamacrocyles; and (2) expanding the macrocyclic parent to pentaazamacrocycles. Here, we present strategies for producing both new kinds of ethylene cross-bridged azamacrocycles and their transition metal complexes.

Mathematics and Science.Chemistry.06

DanielMcInnes

East Central University

Polycyclic Aromatic Hydrocarbons: Photoionization Efficiencies vs. HOMO-LUMO Gaps

Polycyclic aromatic hydrocarbons (PAH’s) are relevant in many fields. Johansson and coworkers measured the photoionization-efficiency (PIE) curves for various PAH’s. PIE curves can be used to determine photoionization cross-section curves of compounds, which are useful for identification purposes. Photoionization cross-section curves were determined for the PAH’s pyrene, fluoranthene, chrysene, perylene, and coronene. Our study involves determining HOMO-LUMO gaps of PAH’s, and comparing them with the corresponding photoionization cross-section curves.

Mathematics and Science.Chemistry.07

Jia XuanMak, SanjeewaGamagedara

University of Central Oklahoma

HPLC Method Development and Validation for Quantitative Determination of Lung Cancer Biomarkers in Urine

Lung cancer is the most common cause of cancer-related death in men and second most common in women. There are no good clinical markers that can be used to diagnose lung cancer at an early stage and predict its prognosis have been found. A recent study analyzed metabolites in plasma and serum blood samples from lung cancer patients and individuals without cancer using GC/MS and identified a set of metabolites differently expressed in cancer patients. Based on this study, we developed an high performance liquid chromatography (HPLC) diode array detection (DAD) method to detect fumaric acid, L-glutamic acid, pyruvic acid, inosine, and creatinine simultaneously in urine. Creatinine was included to account for the renal dilution. Baseline resolutions for all five biomarkers were obtained in synthetic urine matrix by using a 5% methanol and 95% of 0.6% acetic acid, using a C18 column. The developed HPLC method was validated in synthetic urine matrix using analytical method validation parameters such as linearity, accuracy, reproducibility, robustness, limits of detection and quantitation 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.

Mathematics and Science.Chemistry.08

RandallMaples

East Central University

Transport and Recovery of Fe3O4 nanoparticles through limestone and dolomite rock.

Nanomaterials are used in an increasing number of applications, thus potentially leading to a wide variety of engineered nanoparticles being released into the environment at some point as devices and materials are disposed of. Thus, it is important to be able to assess the fate of these engineered materials and their distribution in groundwater and the subsurface. This study continues the examination of the movement and recovery of engineered Fe3O4 nanoparticles through environmental matrices, using locally sourced water and sedimentary rocks.

Mathematics and Science.Chemistry.09

CassandraWeeks

Northeastern State University

Synthesis of trans-Vitamin D2

The synthesis of the trans-vitamin D2, via its sulfur dioxide adduct, is presented here. The trans isomer of vitamin D2 will be used as a model molecule, for the study of the photo-sensitized photoisomerization of vitamin D2 from its trans isomer to the naturally occurring, biologically active, cis isomer. The photoisomerization study will help advance the synthesis of a cis-vitamin D5 intermediate, subject to a different, multistep synthesis of 1-hydroxyvitamin D5, a cancer chemopreventive agent. The synthesized trans-vitamin D2 was purified by column chromatography and characterized by 1H-NMR spectrometry. The overall chemical yield was of 71%.

Mathematics and Science.Chemistry.10

RachelHoffmeister, Sung-Kun (Sean)Kim

Northeastern State University

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

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 a couple of 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 with only the use of BNAs and a Tm value measurement.

Mathematics and Science.Chemistry.11

MichellePham

University of Central Oklahoma

Isolating Bioactive Marine Invertebrate Extracts Using Brine Shrimp Lethality Assay Screening

Natural products are defined as small molecules extracted and 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 well with the cytotoxicity of human cancer cells from the lung and colon lining. The aim of this work is to identify cytotoxic bioactive compounds for their potential use in pharmacology from screening marine invertebrate extracts. The evaluated extracts are derived from the University of Oklahoma Schmitz Sponge collection, which contains over 300 marine invertebrate samples. Each extract is screened utilizing the brine shrimp assay at a low, medium, and high concentration – 10.0 ppm, 50.0 ppm, and 100 ppm. Extracts indicating 70% lethality or greater are reinvestigated using a confirmation assay. Promising extracts will be fractionated by chromatographic methods, and then the bioactive compound identified using nuclear magnetic resonance spectroscopy, mass spectrometry and infrared spectroscopy.

Mathematics and Science.Chemistry.12

JordanStaggs, CortneySchartz

University of Central Oklahoma

Kinetic and Structural Studies of Histidine-tagged Tetrahydrodipicolinate N-succinyltransferase

Tetrahydrodipicolinate N-succinyltransferase (THDP succinyltransferase) catalyzes the reaction of tetrahydrodipicolinate (THDP) and succinyl-CoA to form L-2-succinylamino-6-oxopimelate and coenzyme A (CoASH) in the succinylase branch of lysine biosynthesis. Because lysine is an essential amino acid to humans, THDP succinyltransferase is a potential target for designed antibiotics. The DapD gene encodes the enzyme. While DapD from a number of sources has been characterized, no data exists for the enzyme from Serratia marcescens, a pathogen known to frequently cause hospital-acquired infections. In our lab, the crystal structure of THDP in Apo form and in complex with an activator is under investigation.

The protein was expressed and purified. Based upon SDS/PAGE, the expressed protein is 95% pure and 3 liters of culture produced 50-80 mg of protein.

Initially, the PEG/ION screen was used to find the crystallization condition. Using this screen, several conditions produced crystals. A solution containing ammonium acetate and polyethylene glycol 4000 produced small crystals. Therefore, this crystallization condition is being modified to produce diffraction-quality crystals.

*This research is funded by Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103447 and P20GM103640 (OCAST).

Mathematics and Science.Chemistry.13

CharlesCrittell

East Central University

Papain is an enzyme found in papaya plants. It is a thiol protease and contains a sulfhydryl group in the active site. The substrate, Nσ-benzoyl-arginine-p-nitroanilide (BAPNA), is used, which is hydrolyzed by papain to form a bright yellow product, p-nitroaniline. The reaction is monitored spectrophotometrically by measuring the rate of formation of the p-nitroaniline product as a function of the increase in absorbance of the solution at the lambda max of p-nitroaniline (400 nm) over time at various substrate concentrations. Lineweaver-Burke double reciprocal plots are used to determine Vmax and Km of the enzyme. The effect of pH on enzyme activity will also be explored.

Mathematics and Science.Chemistry.14

KatrinaBetz, MaxwellArcher, jasonwickham

Northwestern State University

Study of an Iodine Distribution in Western Oklahoma Brine Waters

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 the 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. Currently, 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 four of these possible sites, as well as, measuring iodine fluctuations up to 100 ppm which is a much larger fluctuation than the expected 10 ppm. Currently, we are investigating rather these fluctuations are due to the changed from vertical to horizontal wells or inhomogeneity within the brine aquifer.

Mathematics and Science.Chemistry.15

VivekSwami, VinaySwami

University of Central Oklahoma

The Synthesis of Aluminum Clusters via Basic Dissolution of Aluminum Hydroxide Gel to Mimic High pH in an Aqueous Environment.

Aluminum clusters have previously been synthesized in acidic aqueous environments. Some are naturally occurring and have various uses in industries like materials science and water purification technologies. These previous clusters were synthesizes, isolated, and characterized, notably by single crystal X-ray diffraction. Using basic starting materials, we are attempting to synthesize these clusters in aqueous systems and isolate them using a similar process to these previously isolated aluminum clusters. An aluminum hydroxide solution was created from Al(OH) 3 dried gel with the addition of various bases. Like previous work, we attempted to crystalize aluminum clusters from these aqueous solutions. As we move forward, we will include additives that may aid in the crystallization of anionic aluminum clusters in the high pH ranges.

Mathematics and Science.Chemistry.16

ChalitaThompson

University of Central Oklahoma

Training Undergraduate Research Students in Cluster Synthesis and Crystallization Techniques for Single-Crystal X-ray Diffraction

The University of Central Oklahoma (UCO) has participated in a program called “Summer Bridge” that brings STEM students that have just graduated from high school to UCO’s campus to do research for the summer before their first year of college. These students have little chemistry experience, yet are expected to participate in research projects on campus. We have recently developed a useful system for training these students in crystallization techniques along with the accompanying chemistry skills needed for routine inorganic cluster synthesis. This training utilized skills like using a micropipette, using molar ratios, making solutions, and using a microscope. The calculations needed for this research are especially common in numerous areas of chemistry and provide a valuable starting point for training research students with little previous chemistry experience. We will review the system that we are using for the training of undergraduate research students for techniques in co-crystallization, cluster synthesis, and numerous other laboratory techniques commonly utilized in aqueous inorganic chemistry.

Mathematics and Science.Chemistry.17

JoanneAdams

University of Central Oklahoma

Collaboration Between Chemists and Artists in Academic Settings

Scientific innovation thrives off a collaboration of diverse ideas. To encourage more diversity in science we, as academics, must make our subjects more accessible to a variety of learning styles. As a visual learner, and interdisciplinary student of art and science, I had difficulty wrapping my mind around chemistry. Chemistry as a subject is often taught verbally, through lecture and reading. It is difficult to teach visually because we can’t see chemicals at the atomic level. Researching with my mentor Dr. Montes, I use my artistic experience to make chemistry concepts more accessible to people who learn visually. I build off the efforts of my mentor, reviewing his lesson plan and use of figures. After my review on what can be improved upon, I illustrate the figures, being careful to use font and colors that are accessible to as many people as possible. The General Chemistry II class of Fall 2018 will review these efforts and offer their input as students. Although people cannot see at the atomic level, people understand chemical properties. Chemical concepts can be represented symbolically for students. This collaboration between chemistry and art makes the sciences more accessible to a diverse student body, ensuring a bright future of scientific discovery.

Mathematics and Science.Chemistry.18

JessicaMartin, AndrewJenison

Northeastern State University

The Isolation and Purification of Siderophores From Marine Halomonas Strains

The isolation of iron(III)-specific chelators also known as siderophores could have many beneficial properties including antimicrobial or antineoplastic functions. Three different strains of Halomonas bacteria were tested for siderophore production. All three strains were tested using ferric Chrome Azurol Sulfonate (Fe-CAS) in an agar plate. One strain tested positive for siderophore production and was grown in a low iron artificial seawater broth. The broth was centrifuged to collect the supernatant and a polystyrene resin was added to bind to the siderophores in the supernatant. Column chromatography was used to elute the siderophores from the polystyrene resin. The mobile phase was collected and then purified using reversed-phase high-performance liquid chromatography (RP-HPLC).

Mathematics and Science.Chemistry.19

NhuDang, DanaRundle

University of Central Oklahoma

Synthesis of a Biotin-Conjugated Linker on a Flexible Heteroarotinoid

The objective of this study is to synthesize E15 with a biotin-conjugated linker on a methyl moiety in order to isolate specific Flexible Heteroarotinoid (Flex-Het) binding partners in Staphylococcus aureus (ATCC 43300). Flex-Hets are compounds composed of a 4-nitrophenyl group, a linker region, and an aryl ring containing an R group. E15, a Flex-Het containing a methyl R group and a thiourea linker region, has been shown to significantly inhibit the growth of Staphylococcus aureus (ATCC 43300). The reagents used to synthesize E15 are m-toluidine and 4-nitrophenyl isothiocyanate. The amino component on m-toluidine is converted to an amide to protect it while a leaving group is attached to the methyl moiety. Following this, the amide is converted back to an amino group. E15 is synthesized at room temperature by reacting m-toluidine with 4-nitrophenyl isothiocyanate for 24 hours, followed by recrystallization. The biotin-conjugated linker replaces the leaving group on E15, and the product is recrystallized and evaluated by nuclear magnetic resonance.

Mathematics and Science.Chemistry.20

KatherineDang, CortneySchartz

University of Central Oklahoma

Kinetic and Structural Studies of E. coli Dihydrodipicolinate Synthase and Meso-diaminopimelate

Lysine is a member of the aspartate family of amino acids. In general, there are two different pathways for the biosynthesis of lysine; the diaminopimelate (DAP) pathway is found in all bacteria, algae, and plants, and the α-aminoadipic acid pathway seen in fungi and euglenoids. Neither pathway is found in mammals.

Dihydrodipicolinate synthase catalyzes the first step in the DAP pathway for the biosynthesis of L-lysine. The enzyme is feedback inhibited allosterically by L-lysine which reduces enzyme activity by ninety percent compared to the uninhibited activity. The kinetic mechanism for DHDPS is ping pong with pyruvate binding first to apo-enzyme followed by generation of a Schiff’s base between pyruvate and K161. Subsequent loss of a proton from the β-methyl group of the bound pyruvate leads to formation of an enamine intermediate.

Based on protein docking studies several substrate and transition analogues of DHDPS have been designed. Kinetic and structural studies was performed on meso-diaminopimelate (meso-DAP). Meso-DAP is a weak activator of DHDPS, increasing the rate of the reaction by 20%.

Crystals of dihydrodipicolinate synthase co-complexed with meso-DAP formed in PEG 3350, sodium tartrate, and HEPES at pH 7.5. The diffraction data will be collected at the OU X-ray facility. Structural studies elucidate the binding site for meso-DAP.

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Mathematics and Science.Chemistry.21

KaylinShackelford, TristenUnruh-Cone, Sung-Kun (Sean)Kim

Northeastern State University

HYPEREXPRESSION OF BIOFILM-BREAKING ENZYMES AND DISTURBANCE OF BIOFILM FROM STAPHYLOCOCCUS AUREUS AND STAPHYLOCOCCUS EPIDERMIDIS

The formation of biofilm by bacteria poses serious challenges in the treatment of many infectious diseases. To address this issue, an assay of biofilm from Staphylococcus aureus and Staphylococcus epidermidis were used with dispersin B (DspB) and lysostaphin (LSS), enzymes that are known to play a role in impeding biofilm and peptidoglycan formation. Dsp B catalyzes the hydrolysis of linear polymers of N-acetyl-D-glucosamines, which are part of the biofilm matrices. LSS is capable of cleaving the crosslinking pentaglycine bridges found in the cell wall peptidoglycan of certain Staphylococci. We successfully cloned and purified the two enzymes. We added various concentrations of glucose to bacterial media to determine the optimal growing conditions for the bacteria before adding the two enzymes. We found that each enzyme, Dsp B and LSS manifested, statistically, no significant impedance of biofilm formation in either bacteria, and yet the combination of Dsp B and LSS was shown to be much effective in cleaving the biofilm in S. aureus. These observations may support the notion that there is a synergistic effect to impede the formation of biofilm in certain strains of bacteria. The purified Dsp B, in fact, showed the hydrolysis of a polymer of N-acetyl-D-glucosamines present in the biofilm matrix, suggesting that the polymer is a major factor for breaking biofilms and may be useful for further research concerning medical conditions related to antibiotic resistance

Mathematics and Science.Chemistry.22

AndrewHuckleby, Sung-Kun (Sean)Kim

Northeastern State University

INTERACTION BETWEEN CD19 AND ANTIBODY B43

CD19 is a transmembrane protein found on the surface of, and unique to, all B cell lineages. This property allows it to function as the primary antigen for B cell specific antibodies, such as antibody B43. Functioning as the primary antibody for targeting CD19, B43 is currently utilized in genetically engineered T cells for the treatment of acute lymphoblastic leukemia. To learn more and improve upon this binding, we utilized the crystal structure of B43 complexed with CD19 to understand the interactions between the two proteins. This structure showed that it would be reasonable to state that the binding between the epitope and the antigen recognition sites follows a lock and key fashion. Plus, the complexed structure revealed a unique molecular orientation for the extracellular domain of CD19 showing an elongated Beta sandwich. A better understanding of the binding would provide the way to design a more efficient antibody.

Mathematics and Science.Chemistry.23

RajeshNayak

Cameron University

Understanding Spectral Properties of Fluorescent Dyes in Aqueous and Micellar Environment

Photophysical properties of fluorescent probe molecules in aqueous and in confined media have been the subjects of extensive investigation. Among the most widely studied of confined media is the environment of the reverse micelle. Reverse micelle can be used as a simple model system to understand dynamic properties of dye molecules. We will present electronic and hydrodynamic properties of fluorescent dyes in aqueous and confined environment using various steady state spectroscopic techniques

Mathematics and Science.Chemistry.24

FernandoSalazar-Salas, LizbethRobles-Fernandez, DwightMyers

East Central University

High Temperature Study of the Reaction of Silicon, Titanium and Yttrium Oxides

Reactions of titanium oxide and silicon dioxide are of importance in materials used in high temperature environments. 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. The extent of reaction and temperature range are important questions to answer for this chemical system. Experimental evidence would suggest that a third cation is necessary to have compound formation. Presently we are exploring the reaction of titanium dioxide with silicon dioxide with small amounts of yttrium oxide being added. Mixtures of the three oxides are being subjected to heatings at various temperatures from ca. 1200-1500ᵒC. 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. Results to date will be presented.

Mathematics and Science.Chemistry.25

UendiPustina, DwightMyers

East Central University

Computational Study of Volatile Aluminum Hydroxide

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. Presently we are to the stage of optimizing the geometry of the molecule. Results to date will be presented.

OladayoSeweje

Cameron University

Synthesis of cyclic Imides using Microwave Radiation

Allowing many chemical reactions to be completed within minutes, microwave heating has revolutionized preparative chemistry. This is a green technology and is becoming widely adopted in both academic and industrial laboratories. Heterocycles are very important functional groups especially in medicinal chemistry. Not only are they pivotal in the synthesis of drugs but also form part of the structure of a diversity of drugs, vitamins, natural products and biomolecules. In this research a clean green method was implemented for the preparation of different cyclic imides from acid anhydrides using aniline or N-substituted anilines with microwave radiation as the energy source. The unsubstituted imides were synthesized by reacting the acid anhydrides with urea using imidazole as a catalyst. These compounds will be evaluated against antibacterial and antifungal species.

GeraldWard, MaggieWard, EmilyCowen, AlexanderChandler

University of Central Oklahoma

The synthesis of Aluminum Clusters using Naphthalene Based Crystallization Agents

Oxy-Hydroxy-Aluminum clusters have various industrial uses, including waste water treatment and materials science. There may also be use for these clusters to remove contaminants from aqueous environmental systems. It is important to synthesize, then isolate these clusters to observe how they will behave and bind in environmental systems to contaminants or surfaces. Using basic starting materials, we are attempting to synthesize these clusters in aqueous systems for study. An aluminum hydroxide solution was created from Al(OH)3 dried gel with the addition of selenic acid. Then we attempted to isolate the clusters by slow evaporation or by using different naphthalene-based crystallization agents from previous work. Once the clusters were crystallized and observed under a microscope, we planned to characterize them using single x-ray diffraction. Our goal was to synthesize the Al8 selenate cluster, based on a previously synthesized Al8 sulfate cluster, using this dissolution method with selenic acid. It is unclear if this cluster is naturally occurring, though the conditions of synthesis are similar to acidic environmental systems including acid mine drainage or acid rain systems.

Mathematics and Science.Chemistry.28

LindsayMaez, VictoriaBrown

Cameron University

Investigation of Microwave Energy in the Synthesis of Heterocycles Related to Medicinal Chemistry

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. An important class of heterocyclics, derivatives of isatin (indole-2,3-dione), as well as its Schiff and Mannich bases, have already been reported to show a variety of biological activities,

such as antibacterial, antifungal and anti-HIV activities. The wide spectrum of isatin derivatives and their various chemical properties has led to their increasingly expanded use as precursors for the preparation of many biologically active compounds. Hydrazine derivatives of isatin have been found to be active

against Walker carcinosarcoma. In this research isatin derivatives were synthesized using microwave technology. Their antimicrobial activity will be tested.

MicahFoale, Brooke Lizotte, MadisonDuckwall, LoriGwyn

Southwestern Oklahoma State University

Determination of the Sensitivity of an Arsenic Biosensor

Arsenic (As) is of concern locally and globally in drinking water. Commercial As test kits are available; they are time-consuming, involve multiple steps, and create more toxic waste. We utilized synthetic biology to develop a simple and sensitive As biosensor. Previously, we constructed the biosensor using the Biobrick parts J33201 (an As sensitive promoter); E1010 (red fluorescent protein); and pSB1A3 (an ampicillin resistant destination plasmid). Current efforts focused on testing the viability of the bacterial cells in varied arsenite and arsenate media. Moreover, we wanted to determine the levels of “pinkness” based on the amount of arsenite/arsenate present in the media. Growth conditions were quantified measuring the OD-600 of cell cultures grown up to 20 hours. Results showed the growth of the bacteria containing the different BioBrick plasmids did not grow well under any arsenite and arsenate concentrations used. We also noted that the bacteria was not turning pink in the presence of arsenate/arsenite as had been shown in the past. It was concluded that the effective concentration of ampicillin in the growth medium was lower than expected. The quality of cell lines was also suspect. These issues most likely resulted in reduced growth and protein production. These experiments will be reproduced using a higher concentration of ampicillin and re-tested for As sensitivity. Biological systems are a relatively inexpensive approach to creating easy to

Mathematics and Science.Chemistry.30

JonHenrikson

Southwestern Oklahoma State University

Developing NMR and Visible Spectroscopy Methods to Determine pKa’s of Glycine Metal Complexes

Peptidomimetics offers the potential of drug design using small peptide sequences designed to mimic the tertiary structure of a large protein to act as a pharmacophore in the active site. Unnatural amino acids are often used to create tertiary structural features in small peptide mimetics, yet, synthesizing unnatural amino acids still remains a challenge. The use of electron withdrawing groups is a well-known approach to change the chemical properties of a molecule, including the acidity. Our project's goal is to quantify the changes in pKa of previously synthesized ligands with the presence or absence of electron withdrawing groups attached to the molecule in organic solvents. Challenges in determining the pKa’s of these ligands include monitoring the equilibrium of a weak acid-weak base chemical reaction and the use of different methods in determining the acidity of a proton in organic solvent conditions, since common aqueous methods do not apply in organic solvent. Therefore, we are applying proton nuclear magnetic resonance (1H-NMR) and visible spectroscopy as means to monitoring the weak acid-weak base interaction and to quantify the pKa by proton integration and wavelength absorbance changes, respectively.

Mathematics and Science.Chemistry.31

SindhuBharathi

University of Central Oklahoma

Physio-chemical and Functional Characteristics of Raffinose-oligosaccharide Fortified Yogurt

Yogurt is known for its nutraceutical properties. Beans are a healthy and easily affordable pulse containing good amount of raffinose which has been proven to possess prebiotic properties. The objective of this research is to isolate, characterize raffinose from soybeans and demonstrate practical utility of raffinose by studying its effect on the quality of yogurt. We hypothesize that this research will result in developing a soybean based prebiotic powder and a synbiotic yogurt. Raffinose was prepared from soybeans by soaking, incubation and freeze drying. Raffinose was then quantified using enzyme assay and UV spectrophotometer. 2% milk was fortified with starter culture and raffinose at varying concentrations (2%, 4%, 6% and 8%), studied for changes in physiochemical, fermentation and microbiological properties. These changes will be compared with the effects of commercially available prebiotic powder, inulin (2%). Based on the research work done so far, it has been found that the actual concentration of raffinose in the freeze-dried powder is 1.75 ± 0.03 g/L and that 2% raffinose-yogurt (4 hours) takes lesser time to ferment when compared to 2% inulin-yogurt (6 hours). In the coming days, raffinose-yogurt will be analyzed for changes in microbiological and physiochemical properties.

Mathematics and Science.Chemistry.32

SanjeewaGamagedara

University of Central Oklahoma

Separation and Enrichment of Low Abundant Proteins in a Microchannel using Isotachophoresis

Low abundance of circulating proteins in blood is one of the major challenges in on-chip purification and extraction from highly abundant proteins like Albumins. In this presentation, we will demonstrate the separation of low abundant proteins from highly abundant albumin in a microchannel using isotachophoresis (ITP), non-linear electrophoresis. A PMMA (poly-methylemethacrylate) microchannel with a change in cross-sectional area was made using photolithographic processes and solvent assisted thermal bonding. The bonding strength of the microchannel was tested using a universal testing machine and pressurized flow through the channel. The leading electrolyte (LE) was prepared from KOH, Urea, Triton X-100, PVP by adjusting pH to 4.0 with acetic acid. The terminating electrolyte (TE) was 20 mM Acetic Acid, PVP, and Triton X-100. PVP suppresses electroosmotic flow while the urea and Triton X-100 remove precipitates that form during ITP. The ITP experiments were conducted by applying an electric potential of 200 V across the channel and images of sample migrations were taken using a fluorescent microscope.

Mathematics and Science.Chemistry.33

AaronXue, Abul KasemRahman, JefferyLiu

Oklahoma School of Science and Mathematics

The Fight between Antioxidants and Free Radicals

Abstract

Antioxidants are molecules that commonly interact with the free radicals to terminate the chain reaction in biological system in such a way that the vital molecules are not damaged. It is known that there are several enzyme systems within the body that disarm free radicals. This review describes the behavior of antioxidants in battling excessive oxidative stress in the human body. Although free radical creation is essential to cells, the propagation of radicals may grow beyond a healthy limit and damage tissue. Excessive free radicals harmfully oxidize essential biomolecules such as DNA, proteins, and lipids, which causes a breakdown of proper cellular function. For example, radical-induced damage to DNA may cause chromosomal defects that lead to cancer initiation and propagation. While the diseases associated with free radical damage are extensive, they can be grouped based on the type of cell that is oxidized. In this presentation, we will discuss the different kinds of radicals that cause oxidative stress in the body, analyze the common symptoms that result from these radicals, and evaluate antioxidants that impede these reactions from occurring.

Mathematics and Science.Chemistry.34

LeviClements, AmyBrooks, Abul KasemRahman

Oklahoma School of Science and Mathematics

Implications of Aspirin in the Agricultural Field

Aspirin (acetylsalicylic acid) is commonly known as a pain relief and anti-inflammatory agent, however it is less well known that aspirin benefits plants in various ways. Aspirin promotes growth, lengthens lifespan, and strengthens the immune system of plants. In this study, the structure of aspirin and its reactions within plants will be analyzed. Aspirin is the product of acetic anhydride and salicylic acid, which is a substance that is naturally formed in plants in small dosages and protects the plants from diseases. The artificial synthesis of aspirin could potentially be used in large-scale farming to produce healthier crops. Further study on the application and implication of aspirin in the agricultural industry could potentially save money and replace harmful fertilizers.

Mathematics and Science.Chemistry.35

Julia Hua, Abul KasemRahman, A.K.Fazlur Rahman

Oklahoma School of Science and Mathematics

Types of Hallucinogens as Drugs and Its Effects on the Human Body

Abstract:

Hallucination drugs posses a catastrophic challenge for the society and the medical community. Various studies suggest that the usage of hallucinogens causes many devastating health problems including mental illnesses and the irreversible damage of the nervous system. Hallucinating effect involves the altering of one’s senses, where one, for instance, may see or feel something that is not truly there. Common drugs of these type include Dimethyltryptamine (DMT) is an intense naturally-occurring psychedelic that’s also found endogenously in the human body. Dextromethorphan (DXM or DM) is a medication most often used believed to be a naturally occurring substance in certain foods or can be chemically synthesized. This presentation will describe the types and chemical structures of hallucinogens and its effects on the human body, including physical and mental illnesses and benefits.

Mathematics and Science.Chemistry.36

GraceWu, SophiePatrock, Ruth AnneDunn, Abul KasemRahman

Oklahoma School of Science and Mathematics

Medicinal Applications of Radioisotopes

In the medical field, radioisotopes are used for two distinct functions: diagnosis and therapy. The four main diagnostic radioisotopes are technietium-99m, thallium-201, iodine-123, and gallium-67, which are used to figure out which areas of the body have accumulated ions that indicate sickness. Doctors combine radioisotopes with other chemicals and activate them on the afflicted part of the patient’s body. They also use Single Photon Emission Computer Tomography (SPECT) imaging to emit a single gamma ray into the patient’s body. These tests are used to discover bone tumors. After surgery, these medicines can be used to prevent malignancies from growing again. Even though radioisotopes have many medical advantages, they can also cause cancer themselves. These presentations will provide an overview the many drugs made from radioisotopes examining the long term costs and benefits to human health.

Mathematics and Science.Chemistry.37

AubryStomprud, Sung-Kun (Sean)Kim

Northeastern State University

Using Solvate Ionic Liquids to Address Polymorphism in Pharmaceuticals

Polymorphism is the recrystallization of the solid phase of a substance. This recrystallization has posed a problem in the pharmaceutical industry leading to problems of patent litigation. To address this problem, we employed the idea of ionic liquids. By using ionic liquids, the drugs would be potent and since they would be in the liquid form, the solid phase recrystallization would no longer pose a problem. Our research explores the system of Penicillin G and three glycols, Triethylene glycol, Tetraethylene Glycol, and Pentaethylene glycol. We looked at the stability of the solutions by tracking their rates of degradation through IR and UV-vis spectroscopy. We also used tests with Escherichia coli BL21 (DE3) to see if the solutions remained biologically active once the penicillin was wrapped by the glycol. Our results showed that the most effective glycol was the pentaethylene glycol and that it remained biologically effective for longer amounts of time than the traditional solution penicillin in water. This establishes the validity of the idea and therefore further research can be conducted to create a nontoxic glycol with similar properties of pentaethylene glycol.

Mathematics and Science.Chemistry.38

UshaKhadka, ShawnaEllis

University of Central Oklahoma

Advances Toward the Utilization of Cucurbit[n]uril and Selected Viologens in Molecular Machines and Devices

Rotaxanes composed of a cyclic host molecule coordinating with an axle of one or more binding sites are key to creating molecular machines and devices. In this study, pseudorotaxanes of cucurbit[n]urils and a series of viologens are created in varying concentrations. After synthesis and characterization, the equilibrium binding constants and binding modes were determined by NMR. These studies will lead to the design of more complicated host guest systems.

Mathematics and Science.Chemistry.39

StephenMyers

Cameron University

Investigation of Microwave and Ultrasonic Energy in the Synthesis of Heterocycles Related to Medicinal Chemistry

Allowing many chemical reactions to be completed within minutes, microwave heating and ultrasonic energy have revolutionized preparative chemistry. Both are green technologies and as a result, are becoming widely adopted in both academic and industrial laboratories. This is especially true for microwave synthesis but not many applications of ultrasonic energy in organic synthesis have been reported. Heterocycles are very important functional groups especially in medicinal chemistry. Not only are they pivotal in the synthesis of drugs but also form part of the structure of a diversity of drugs, vitamins, natural products and biomolecules. In this poster we will present the results of syntheses of imidazoles and azolines by both microwave and ultrasonic energy. Derivatives of these two classes of compounds are known for analgesic, antifungal, antihypertensive, antiobesity, anticancer and other biological activity.

Mathematics and Science.Chemistry.40

TheresaHinkle

Cameron University

Microwave Synthesis of Novel Esters Using Sulfuric Acid and Imidazole as Catalysts

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 this research we have investigated the synthesis of several esters using a conventional microwave oven and a new method of purification. We compared these syntheses using both sulfuric acid and imidazole as catalysts, as well as a comparison of acid and acid anhydride products. It was hypothesized originally that the esters could be synthesized using the imidazole as a catalyst with any acid. However, we found that we were not able to obtain product without using anhydride acids. Also, for purification, we found it more efficient for the Sulfuric catalyzed esters to first be mixed with ether and then to wash the mixture with sodium bicarbonate then sodium hydroxide, draining and discarding the lower layer each time. When this is done sodium bicarbonate removes any excess sulfuric and the sodium hydroxide removes excess acid.

Mathematics and Science.Chemistry.41

TrevorEllis

Southwestern Oklahoma State University

Synthesis and Competitive of Reaction Rate Experiments for a Series of Ni(II) Complexed Nucleophilic Glycine Equivalents

The preparation of two Ni(II) complexed Schiff’s Base derived nucleophilic glycine equivalents will be described including the synthesis of the required ligands and 2-aminobenzophenones. Additionally, these complexes will be evaluated regarding their utility for the preparation of non-proteinogenic -amino acids. Two methods of homologation, alkyl halide alkylation and Michael Addition Reactions, will be utilized to evaluate the reactivity of these Ni(II) complexed glycine equivalents compared to previous generations that have been introduced through competitive reaction approaches.

Mathematics and Science.Chemistry.42

ElizabethHicks, TrevorEllis

Southwestern Oklahoma State University

The Design, Synthesis of Novel Ligands for the Optical Purification of -Amino Acids

Research associated with the application of a-amino acids has been a topic of interest in various scientific fields ranging from agriculture to pharmacy due to the versatility of these relatively simple compounds. One of the hurdles that has slowed progress in these areas has been the access to these compounds in enantiomerically pure form. Therefore the focus of the investigations to be presented will be the development of efficient methods for increasing access to these materials. Specifically, the rational design and preparation of an optically active ligand system will be presented. Additionally, the application of this system for the preparation of a-amino acids will be demonstrated through a dynamic resolution process.

Mathematics and Science.Chemistry.43

Abul KasemRahman

Oklahoma School of Science and Mathematics

The Chemistry of Medical Marijuana

Abstract

Marijuana is a psychoactive drug from the plant genus Cannabis that is used for medical or recreational purposes. Medical marijuana refers to the use of marijuana’s chemical compounds to treat diseases, pain, and symptoms. Some of these chemical compounds are called cannabinoid that act on certain receptors to alter neurotransmitter release in the brain. Two of the most prevalent active ingredients of marijuana are Cannabidiol (CBD) and Tetrahydrocannabinol (THC).

Due to previous associations with other illegal narcotics, it has a stigmatism. This stigmatism has played a huge role in the legalization of the drug for medical and recreational uses and has required the industry to show its uses and prove its harmlessness. There has also been concern about the distribution and possible addictions. Governmental agencies have labeled the drug as addictive with no medical use and proving that the drug does have use will be the prerequisite for legalization throughout the United States.

However, medically, Marijuana has been shown to have positive impacts on people suffering from diseases such as Alzheimer’s Disease, Multiple Sclerosis, and Post-Traumatic Stress Disorder. Though the physiology of these cures has not yet been proven, the numerous anecdotal evidence combined with the benefit of finding a possible cure for such widespread diseases warrants an in-depth investigation into how marijuana works and how it can be used.

Mathematics and Science.Chemistry.44

StephenMcBride

Cameron University

Photocatalytic Degradation of Acesulfame Potassium Using TiO2/UVA, S2O82-/Fe2+/UVA, and H2O2/Fe2+/UVA Processes

Acesulfame potassium (ACE) is a ubiquitous artificial sweetener that has recently been shown to be toxic to the environment and damaging to DNA in both mice and humans. Photocatalytic degradation of ACE using TiO2/UVA, S2O82-/Fe2+/UVA, and H2O2/Fe2+/UVA processes show promising results with complete degradation and 57-80% mineralization of ACE and their resulting products have been shown to be non-toxic to the environment. The reaction kinetics of these two processes are examined.