Jan 4th, 12:00 AM

05. Chemistry

Northeastern State University

Abstracts from the 2016 Oklahoma Research Day

Held at Northeastern State University

05. Mathematics and Science

05. Chemistry

05.05.01 Analysis of dibutyl phthalate, a possible endocrine disruptor, in infant formula.

Bowen,John *University of Central Oklahoma*

Lewis,Dalton *Other*

We will discuss the quantitation of dibutyl phthalate, a suspected endocrine disruptor and common plasticizer, using Solid Phase Microextraction (SPME) and Gas Chromatography Mass Spectrometry (GC MS). Though this compound is apparently banned in the US, we were able to identify and quantitate it in infant formula using an internal standard.

05.05.02 Synthesis and use of reduced graphing oxide to sparge low level contaminants from drinking water.

Bowen,John *University of Central Oklahoma*

Chapman,Tye *University of Central Oklahoma*

The synthesis and use of reduced graphine oxide, a particle of graphing oxide with the surface reduced to graphing, is known as a high capacity adsorbent of chemicals in water. The ability of this compound to extract dibutyl phthalate from drinking water will be addressed using solid phase micro extraction (SPME) analyzed by gas chromatography-mass spectroscopy (GCMS).

05.05.04 Analysis of bacterial odors from several strains of methicillin resistant S. aureus (MRSA) and non resistant S. aureus and other bacteria using solid phase micro extraction (SPME) and GCMS

Bowen,John *University of Central Oklahoma*

Dressler,Garrett *University of Central Oklahoma*

Odors from the selected strains of S. aureus from methicillin resistant strains and non resistant strains are presented as well as those of other genera will be presented.

05.05.05 Development of an analytical method and quantitation of glyphosate in Oklahoma surface waters.

Bowen,John *University of Central Oklahoma*

Colby,Devon *Other*

A method for the extraction and derivitization of glyphosate for its quantitation using gas chromatography mass spectrometry (GC MS) will be discussed.

05.05.06 Analytical method for the determination of stress in university students using the analysis of zinc in hair and cortisol in saliva.

Bowen,John *University of Central Oklahoma*

Olsen,Dr. Jacilyn *University of Central Oklahoma*

Lavine,Barry *Oklahoma State University*

Liu,Jianguo *University of Central Oklahoma*

Montalvo,Daniel *University of Central Oklahoma*

Shaffer,Nicolas *University of Central Oklahoma*

Gamagedawara,Sanjeewa *University of Central Oklahoma*

An analytical method was developed for the analysis of zinc in hair using Flame Atomic Absorption and the analysis of cortisol in saliva using LCMS was developed to determine if the stress of major exams could be detected in university students.

05.05.07 Synthesis and Biological Studies of Nicotinic and Thio-Nicotinic acid complexes of Platinum

Rahman,A.K. Fazlur *Oklahoma School of Science and Mathematics*

Lozano-DeAos,Pedro *Oklahoma School of Science and Mathematics*

We have synthesized a series of Platinum complexes coordinated to organic acids such as nicotinic acid, thionicotinic acid and thio-salicylic acid. Infrared, mass spectroscopic data along with solubility, melting point properties of these complexes will be presented during the presentation.

05.05.08 Investigating the Origin of GTP Inhibition within E. coli CTP Synthetase

Johnson,Jason *Southwestern Oklahoma State University*

Pickens,Ashley *Southwestern Oklahoma State University*

CTP synthetase (CTPS) is responsible for the de novo synthesis of CTP from UTP, using activated glutamine as the amino donor molecule. Since the enzyme supports DNA replication and concomitant cell division, cancers have been found to be sensitive to drugs that competitively bind within either the pyrimidine pocket or the glutamine active site of CTPS. Recent observations that the allosteric ligand GTP not only activates glutamine hydrolysis activity at low concentrations, but also inhibits CTP synthesis activity at higher concentrations also suggest the GTP analogs might serve as antineoplastic agents. However, earlier research groups report, and our own studies agree, that GTP and its analogs act only as potent activators of CTPS activity, showing no evidence for GTP-mediated inhibition. Certainly, a prerequisite for the rational design of GTP analog drugs is a clear reconciliation of the ligand's impact on CTPS activity. Therefore, we are investigating the origin of reported discrepancies in the mechanism whereby the allosteric effector GTP impacts CTP synthetase activity. Methods include site-directed mutagenesis of CTPS residues highlighted from structural and sequence analysis to potentially mediate the GTP-induced allosteric change, and the expression, purification, and kinetic analysis of the resultant protein variants.

05.05.09 Computational Study of Hydrogen Bonding in Alkanes

McInnes,Daniel *East Central University*

Russell,Charles *East Central University*

Hydrogen bonding as conventionally described by Pauling, is an electrostatic bond that forms between the most electronegative atoms in the form D---H•••A (D being electronegative atoms such as O or N, and D and A both having at least one lone pair). Hydrogen bonding has also been found occurring between a larger range of donors and acceptors, which implies that hydrogen bonding can nearly always be described as an incipient proton transfer. Further implications are that all molecules that are capable of undergoing Bronsted acid base reactions may also form hydrogen bonds. We are interested in alkanes, which are weakly basic molecules.

05.05.10 Detection and Quantification of Single-Walled Carbon Nanotubes by Chemically Conjugating With Fluorescein Isothiocyanate

Lam,Ahn *University of Central Oklahoma*

Zhou,Feifan *University of Central Oklahoma*

Chen,Wei *University of Central Oklahoma*

Fluorescein Isothiocyanate (FITC) is a derivative of the bright green fluorescein. With unique properties such as high light absorption, excellent water solubility, and good fluorescein quantum yield, it is commonly used as a functional dye in a wide-range of scientific research. Single-walled carbon nanotubes (SWNTs) are promising materials for biomedical applications. Having the ability to cross cellular membranes without eliciting cytotoxicity, SWNTs have been studied to deliver many drugs or proteins to target cells. Moreover, with a high optical absorbance in the near-infrared region, SWNTs also play a novel role in photothermal therapy for cancer treatment. To determine the appropriate amount of SWNTs needed in biomedical applications, SWNTs were conjugated with FITC to form a nanocomplex that could be detected by fluorescein microscope or fluorescein spectroscopy in our laboratory. Because the fluorescence intensity is proportional to the radiant power and the concentration of the emitting substances, we also developed a standard FITC calibration curve to determine the amount of SWNTs in the nanocomplex. Our research could lead to the development of new applications of SWNTs in the biomedical fields, particularly in cancer detection and treatment.
Keywords: Single-walled carbon nanotube (SWNT), Fluorescein Isothiocyanate (FITC), Photothermal therapy, Cancer treatment

05.05.11 Inhibition Testing of the Metallo-beta-lactamase (Bla2) found in Antibiotic Resistant Bacillus anthracis

Demuth,Mara *Northeastern State University*

Kim,Sung-Kun *Northeastern State University*

Antibiotic resistance has emerged as a serious threat to public health. Much of the resistance is found in the widely used beta-lactam antibiotic groups and is due to genetic mutations that cause the development of an enzyme called metallo-beta-lactamase (MBL). Unavailability of therapeutic inhibitors has led to a search for novel inhibitors. The MBL from Bacillus anthracis (Bla2) was chosen for this study. Successful purification for Bla2 was confirmed by SDS-PAGE analysis, and attempts were made to inhibit this enzyme using hydroxamate-group-containing molecules. Initial kinetic studies suggest significant inhibition in the molecule containing two hydroxamate functional groups with a promising IC50 value but no significant inhibition in the single hydroxamate containing molecule. Later kinetic analysis reveals the significant inhibition to be competitive with an extraordinary Ki value. Dimethyl sulfoxide was used to increase inhibitor solubility, and further enzyme assay revealed enzyme stability up to approximately 2% dimethyl sulfoxide. In silico analysis showed inhibitor docking to the active site of Bla2 which provides a link between experimental and theoretical work. These findings offer new avenues for designing better inhibitors against MBLs.

05.05.12 Inhibition of Thermus aquaticus DNA Polymerase by Bridged Nucleosides using Real-Time qPCR

Dinkel,Austin *Northeastern State University*

Kim,Sung-Kun *Northeastern State University*

The inhibition of DNA replication is a vital strategy for combatting cancers and viruses. The long-term use of current agents leads to adverse side affects and the development of resistance. Nucleosides with modifications to the sugar moiety have proved dominant in research to develop new potential drug candidates to inhibit DNA replication. The modification of the 2'4' position of the ribose with inclusion of a bridge was tested on its inhibition of Taq DNA Polymerase using real-time quantitative PCR. This revealed the significant inhibitory action of 2',4'-bridged thymidine. A deeper look into the mechanics revealed the competitive mechanism by which 2',4'-bridged thymidine operates. With a Ki value of 9.7 ± 1.1 μM, the 2',4'-bridged thymidine proved to be a very promising inhibitor. Further analysis shows all nucleosides tested bind in the active site, proving the substrate analogs are structurally complementary to the active site. Evidence shows the importance of Asp610 in the active site when binding with 2',4'-bridged thymidine. Overall, the active site inhibition of 2',4'-bridged thymidine shows the potential of bridged nucleosides as drug candidates.

05.05.13 Purification and Characterization of the IMP-1 Metallo-Beta-Lactamase From Pseudomonas aeruginosa

Schmidt,Alexander *Northeastern State University*

Kim,Sung-Kun *Northeastern State University*

Beta-lactam antibiotics are among the most important drugs to fight bacterial infection, but due to misuse, some bacteria have become resistant to these antibiotics. Metallo-beta-lactamase is a resistant enzyme that catalyzes the hydrolysis of beta-lactam antibiotics. Unlike metal-independent beta-lactamases, no clinically useful inhibitors of metallo-beta-lactamases have been found. To further characterize metallo-beta-lactamases, the metallo-beta-lactamase IMP-1 from Pseudomonas aeruginosa has been overexpressed and purified to homogeneity by Ni2+ affinity chromatography. Homogeneity was confirmed by SDS-PAGE. An enzyme assay was performed on IMP-1 with penicillin G as a substrate. The results showed that the Km, Vmax, kcat, and catalytic efficiency of the IMP-1 tested were in accordance with previous IMP-1 studies. The effects of temperature on IMP-1 was tested with various temperatures ranging from 20 oC to 70 oC. The results showed that IMP-1 was able to maintain high levels of activity with temperatures up to 60 oC. In silico, pH-dependent assay analyses are underway in order to further investigate the inhibition by chelators and completely understand the mechanism of IMP-1.

05.05.14 Quantitative Determination of Calcium Content in Commercially Available Cereal Samples Using Flame Atomic Absorption Spectroscopy

Gamagedara,Dr. Sanjeewa *University of Central Oklahoma*

Ellis,Tanara *University of Central Oklahoma*

Collins,Leslie *University of Central Oklahoma*

The purpose of this project was to utilize the tools and knowledge in studied Quantitative Chemical Analysis class to quantify calcium in multiple brands of popular cereal. Also to determine if it is a sufficient source of calcium to meet the daily dietary recommendations for ages 19-50. The calcium content was measured using Flame Atomic Absorption (FAA) Spectroscopy. Standard Addition calibration method was used to prevent the suppression or enhancement of the signal by the matrix of the aqueous solution. Approximately 5 grams of each sample of cereal was crushed, then placed in a muffle furnace to dry to weight constant. After heating and cooling, a 5-mL of 12 M HCl was used to dissolve the cereal, then diluted to 100-mL and filtrated. For each sample, a 5-mL aliquot was pipetted into 50-mL volumetric flask, along with 5-mL of Lanthanum Matrix Modifier solution, and diluted with deionized water. For the Standard Addition solutions, a 1-mL aliquot was pipetted into a 50-mL volumetric flask, along with 5-mL of La Matrix Modifier solution and 1-5 mL of CaCl2 standard solution, and diluted with deionized water. The absorbance for each solution was measured using FAA. Overall, our determined calcium content matched the percentage of calcium on each box, for each brand of cereal. The percent recoveries of Ca were calculated based on the label values. The percentage recovery of Lucky Charms, Cinnamon Toast Crunch, Cheerio's, Golden Graham's, and Hershey Kisses were 59

05.05.14 Quantitative Determination of Calcium Content in Commercially Available Cereal Samples Using Flame Atomic Absorption Spectroscopy

Dinh,Phuong *University of Central Oklahoma*

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05.05.15 Quantitative Determination of Caffeine in Popular Energy Drinks using High Performance Liquid Chromatography

Gamagedara,Dr. Sanjeewa *University of Central Oklahoma*

Collins,Leslie *University of Central Oklahoma*

Craig,Cole *University of Central Oklahoma*

Caffeine has become a globally consumed food constituent for its physiological effects. While coffee has historically been the most popular way to consume caffeine, energy drinks have been gaining popularity among teens and young adults. The current recommendation for caffeine consumption is 5.7 mg/kg of body weight. High pressure liquid chromatography was employed in order to estimate the amount of caffeine contained in commercially available popular energy drinks. The five energy drinks that were used in this study were: Rockstar, Full Throttle, Monster, Nos, and Redbull. The commercial energy drinks were obtained from a local retail store in Edmond, OK. Caffeine was separated using C18 column with 60:40 ratio of methanol and NaH2PO4 as the mobile phase. Each energy drink sampled was ran in triplicates to assure statistical significance. The results from this study indicated that all five of the energy drinks examined displayed a higher caffeine content than what was represented on the nutritional facts label.

05.05.16 Stereoselective Hydroxylation of Vitamin D Core System

Albinescu,Dragos *Northeastern State University*

This research project presents the 1alpha-hydroxylation sequence of vitamin D core fragment, as part of a multistep synthesis of 1alpha-hydroxyvitamin D5, a potent anticancer agent and an inhibitor of the renin gene expression. The 1alpha-hydroxylation of vitamin D is the final metabolic step that occurs in kidney and fully activates vitamin D to its most potent metabolite. In the chemical synthesis of the 1alpha-hydroxyvitamin D5, the 1alpha-hydroxylation step was accomplished by using selenium dioxide/ N-methylmorpholine-N-oxide (MNO) oxidation system, that produced the desired 1alpha-hydroxylated derivative in an excess of 4:1 to the 1beta-hydroxylated, inactive derivative.

05.05.17 Using Microwaves for Organic Syntheses in Undergraduate Organic Labs

Rivas,Alexander *Cameron University*

Nalley,Elizabeth *Cameron University*

Allowing many chemical reactions to be completed within minutes, microwave heating has revolutionized preparative chemistry. As a result, this technology has been widely adopted in both academic and industrial laboratories. Integrating microwave-assisted chemistry into undergraduate laboratory courses enables students to perform a broader range of reactions in the allotted lab period. As a result, they can be introduced to chemistry that would otherwise have been inaccessible due to time constraints (for example, the need for an overnight reflux). A number of the chemical transformations use water as a solvent in lieu of classical organic solvents. This contributes to greener, more sustainable teaching strategies for faculty and students, while maintaining high reaction yields. The advantages inherent in microwave use make it ideal for the undergraduate laboratory. Although students are exposed to many different reactions in the classroom, many important organic reactions described in undergraduate textbooks are presently not included in the laboratory course owing to long reaction times, high temperatures, or sensitive reagents that present a potential danger to the students. In this poster, five syntheses using microwave heating will be described.

05.05.18 PCBP2 Knockdown Leads to Iron Overload in Mouse Liver Tissue

Rivas,Alexander *Cameron University*

Li,Fengmin *Other*

Philpott,Caroline *Other*

Iron is an essential co-factor for many proteins involved in central cellular processes and is toxic at high concentrations. Therefore, iron storage, uptake and utilization are tightly regulated. Ferritin, the ubiquitous iron storage protein, Hepcidin a liver hormone that controls cellular iron release, Iron Regulatory Protein 2 (IRP2) and the Transferrin receptor, a protein and transmembrane iron importer respond to fluctuations in iron concentration and function to bring iron to stable levels. Poly (rC)–binding proteins 1 and 2 (PCBP1 and PCBP2) are multifunctional adaptor proteins that bind cytosolic iron for delivery to target apoproteins. We studied the regulation of iron related proteins in a mouse model of PCBP2 knockdown mice. We hypothesized that PCBP2 knockdown leads to iron overload in liver tissue. We used western blots to measure protein expression in response to PCBP2 is knocked down, Real-Time PCR to quantify the gene expression levels of iron related proteins. Compared to the wild type Heterozygous PCBP2 Knockdown mice showed significant elevation in liver Hepcidin levels along with decreased transferrin, and IRP2 levels. PCBP1 remained constant and PCBP2 expression was reduced by half. This shows that PCBP2 has a role in cellular iron regulation.

05.05.19 Microwave Synthesis of Tetraphenylporphyrins and Tetraphenylporphyrin Derivatives

Hyolmo,Pasang *Cameron University*

Nalley,Elizabeth *Cameron University*

Rupakheti,Sujana *Cameron University*

Allowing many chemical reactions to be completed within minutes, microwave heating has revolutionized preparative chemistry. As a result, this technology has been widely adopted in both academic and industrial laboratories. Integrating microwave-assisted chemistry into undergraduate laboratory courses enables students to perform a broader range of reactions in the allotted lab period. As a result, they can be introduced to chemistry that would otherwise have been inaccessible due to time constraints (for example, the need for an overnight reflux). A number of the chemical transformations use water as a solvent in lieu of classical organic solvents. This contributes to greener, more sustainable teaching strategies for faculty and students, while maintaining high reaction yields. Tetraphenylporphyrins can be synthesized from pyrrole and benzaldehyde using a conventional microwave oven. This synthesis and other synthesis of other derivatives of tetraphenylporphyrins will be described.

05.05.21 Malaria, A Parasitic Disease : An Educational Study of its Cause and Cure

Rahman,A.K.Fazlur *Oklahoma School of Science and Mathematics*

Pan,Amanda *Oklahoma School of Science and Mathematics*

Gattani,Mansi *Oklahoma School of Science and Mathematics*

Zhangs,Maggie *Oklahoma School of Science and Mathematics*

Title : Malaria, a Parasitic Disease : Cause and Cure Authors : Mansi Gattani, Amanda Pan, and Maggie Zhang's Oklahoma School of Science and Mathematics Advisor : A.K.Fazlur Rahman, Ph.D. Abstract: An estimated 2 billion people are infected with at least one parasite. Malaria causes about 2.5 million deaths annually. Malaria and other parasitic diseases have ravaged mankind, presenting a health crisis throughout the world. This year's Nobel Prize in Medicine provided a possible solution to combat this debilitating disease. Two compounds, Ivermectin and Artemisinin are the two key compounds discovered independently by two different groups. These compounds have fundamentally also changed treatment of parasitic diseases such as River Blindness and Lymphatic Filariasis. This presentation aims to provide an overview of the cause and cure of the 2015 noble winning parasitic diseases, Malaria. In particular, the authors will examine the source, extraction, structure and the application chemistry of Artemisinin and Ivermectin.

05.05.22 Nonsteroidal anti-inflammatory drug (NSAID) : Understanding How Does it Work ?

Rahman,A.K.Fazlur *Oklahoma School of Science and Mathematics*

Nuguri,Sona *Oklahoma School of Science and Mathematics*

Lee,Michael *Oklahoma School of Science and Mathematics*

Nonsteroidal anti-inflammatory drug (NSAID) : How Does it Work ? Authors : Sona Nuguri and Michael Lee Oklahoma School of Science and Mathematics 1141 N Lincoln Blvd, OKC, OK 73104 Faculty Advisor: A.K.Fazlur Rahman, Ph.D Abstract : Non-Steroidal anti-inflammatory agents such as aspirin and naproxenes act by inhibiting the biosynthesis of prostaglandins (PGs from arachidonic acid (AA). There are two human enzymes that catalyze the first step in the biosynthesis of PG’s cyclooxygenase 1- and 2 (COX-1 and COX-2). NSAIDS are usually used for the treatment of acute or chronic conditions where pain and inflammation are present. Since most NSAIDS inhibit the activity of COX-1 and COX-2, It is believed that inflammatory function is a part of the human healing process as it resolves in pain and fever. In this presentation we discuss an overview of inflammation and how do the anti-inflammatory drugs works?

05.05.23 Chemistry Explains the Spiciness in Chilli Papers : Capsicinoids

Rahman,A.K.Fazlur *Oklahoma School of Science and Mathematics*

Abstract : Chemists have long been seeking to understand and explain the hotness in chillies. Literature study suggests that there are two compounds namely Capsaicin and Dihydro-capsaicin are responsible for the hotness in chilli. The authors will explain Scovile heat index in this presentation

05.05.24 Characterization of the Slow-Binding Inhibition by Acetopyruvate of the Dihydrodipicolinate Synthase from E. coli

Fleming,Christian *University of Central Oklahoma*

Mesiya,Sidra *University of Central Oklahoma*

Karsten,William *Other*

Thomas,Lenorad *Other*

Chooback,Lilian *University of Central Oklahoma*

Dihydrodipicolinate synthase (DHDPS) catalyzes the first step in the biosynthetic pathway for production of L-lysine in bacteria and plants. DHDPS reaction is the rate limiting step in lysine biosynthesis and involves the condensation of aspartate-β-semialdehyde (ASA) and pyruvate to form 2, 3-dihydropicolinate. The kinetic mechanism is ping pong with pyruvate initially forming a Schiff base with K161 followed by loss of a proton to generate an enamine intermediate followed by binding of ASA. The enzyme has received interest as a potential drug target owing to the absence of the enzyme in mammals. Acetopyruvate (ACP) is a slow-binding inhibitor of DHDPS that is competitive versus pyruvate with an initial Ki of about 250 μM and a final inhibition constant of about 2 μM. The enzyme:ACP complex displays an absorbance spectrum with a λmax at 303 nm and a longer wavelength shoulder. The rate constant for formation of the complex is 0.03 s-1. The enzyme forms a covalent enamine complex with the first substrate pyruvate and can be observed spectrally with a λmax at 275 nm. The spectra of the enzyme in the presence of pyruvate and ACP shows the initial formation of the enamine intermediate followed by the slower appearance of the E:ACP spectra with a rate constant of 0.005 s-1. The crystal structure of the enzyme:ACP complex confirms the formation of the Schiff base.

05.05.25 The Effect of Macromolecular Architecture on Functional Group Accessibility: Hydrogen Bonding in Blends Containing Linear Homopolymers and Linear Copolymers.

Dunn,Tia *Northeastern State University*

An investigation of phenolic functional group accessibility in poly(2-vinyl pyridine-co-styrene) (P2VPS) and poly(2-vinyl pyridine) (P2VP) with hyper branched poly(4-hyroxystyrene) (PHS-B) is presented. The extent of hydrogen bonding and phase behavior in blends of P2VP/PHS-B and P2VPS/PHS-B with the corresponding Lewis base were measured using differential scanning calorimetry and calculated by the increase is glass transition temperature (Tg). Evaluated with respect to the weighted average for the 2VP polymers and PHS-B, both P2VP/PHS-B and P2VPS/PHS-B blends observed at least one glass transition. Two Tg's were observed in heating at some compositions for the PHS-B/ co-polymer system only of which were significantly higher than the weight average for P2VPS and PHS-B. The Kwei q parameter was higher for P2VP homo-polymer compared to P2VPS co-polymer. Incorporating styrene simply decreased the number of sites available for inter-molecular interactions.

05.05.26 Organic Synthesis of a Novel Compound for Inhibition Studies on Dihydrodipicolinate Synthase

Evans,Russell *University of Central Oklahoma*

Fleming,Christian *University of Central Oklahoma*

Chooback,Lilian *University of Central Oklahoma*

The molecule 2-hydroxy-4-oxobutanic acid is similar to pyruvate, the natural substrate for DHDPS, and is believed to have strong inhibitory properties and could lead to a model for drug design. The enzymes, DHDPS and the coupling enzyme, dihydrodipicoliante reductase (DHDPR), were purified from E. coli. Protein purification was completed using nickel affinity chromatography. Inhibition studies will be carried out with the synthesized product and DHDPS.

05.05.27 A Computational Study of Product Distribution in Free Radical Halogenations

Crittell,Charles *East Central University*

Clark,Mark *East Central University*

This project will measure the activation energy of several free radical chlorination reactions by empirically determining the energy levels of the different transition states. These calculations will be performed using the program WebMo on the super computer at the University of Oklahoma. The transition state energies will then be used to estimate the distribution of the monochlorinated products. These ratios will be compared to those determined experimentally.

05.05.28 A Kinetic Study of the Enzyme Papain.

Crittell,Charles *East Central University*

The enzyme papain is a thiol protease containing a sulfhydryl group in the active site of the enzyme. Papain is found in papaya. This enzyme has many industrial and commercial uses. The kinetic parameters including Vmax and KM were measured at different pH using the chromogenic substrate N-benzoyl-arginine-p-nitroanilide (BAPNA). It was determined the KM had a minimum value at pH of 6.5 indicating tight binding to the substrate.

05.05.29 High Performance Liquid Chromatography Method Development and Validation for the Quantification of 4-hydroxybenzoate and Related Biomarkers in Urine

Gamagedara,Dr. Sanjeewa *University of Central Oklahoma*

Hassan,Zayed *University of Central Oklahoma*

Yen,Ting-An *University of Central Oklahoma*

Urine analysis to detect biomarkers associated with diseases, especially cancer is getting much attention because of its noninvasiveness. In an effort to identify useful biomarkers for kidney cancer, recent studies have shown that 4-hydroxybenzoate, related metabolites can be potentially used for the diagnosis process. High Performance Liquid Chromatography (HPLC) coupled with Diode Array Detection (DAD) provides an ideal tool for urine analysis of these biomarkers due to its availability most analytical laboratories. In this study, we developed a noninvasive method to separate and quantify 4-hydroxybenzoate, 2,3-pyridine carboxylic acid, 2,5-dihydroxy benzoic acid in synthetic urine using reverse phase HPLC, with creatinine as an indicator for renal dilution. After getting the optimum separation in HPLC, a thorough analytical method validation was conducted to optimize the method validation parameters such as LOD, LOQ, linearity, accuracy, robustness and precision. The detailed experimental conditions and the results will be presented at the conference.

05.05.30 The Effect of Compatible Solutes on the Melting Temperature of Halorhodospira Halochloris DNA

Deole,Ratnakar *Northeastern State University*

Rojo,Lindsey *Northeastern State University*

Behdad,Layli *Northeastern State University*

Aquatic saline environments compose approximately 97% of water on earth and salt deposits may be found in over one fourth of the land. Organisms living in these hypersaline conditions are classified as Halophiles. Halophiles have adapted survival strategies that allow for growth, metabolism and reproduction in hypersaline conditions. One of these adaptations includes de novo synthesis of intracellular compatible solutes. These compatible solutes, called osmolytes, balance the osmotic pressure inside the cell with the pressure surrounding the cell allowing the organism to maintain cell turgor and reduce osmotic stress. Furthermore, compatible solutes also play a role in protein stabilization, protecting against denaturation at high temperatures and in hypersaline conditions. Extensive research has been conducted to investigate the stabilizing mechanisms and effects of compatible solutes on proteins, however, limited research has been conducted on the effects of compatible solutes on DNA. Halorhodospira halochloris, an extreme halophile, accumulates ectoine, proline and trehalose as compatible solutes. H. halochloris was grown in media supplemented with NaCl ranging from 5 – 35%. DNA was extracted from the cells growing at each of the listed concentrations and was treated with ectoine, proline and trehalose at range of concentrations going from 100mM to 1M. DNA melting curves were obtained using a UV/Visible Spectrophotometer, equipped with a Peltier temperature control

05.05.31 Synthesis, Mass Spectroscopic and Cell Culture Studies of Platinum complexes of Carboxylic acid Complexes

Hillis,Nathan *Oklahoma School of Science and Mathematics*

Rahman,A.K.Fazlur *Oklahoma School of Science and Mathematics*

Cis-Platin, (NH3)2PtC2 and Carbo-platin (C2O4)PtCl2 are well established therapeutic metal complexes for various form of cancer. In this project we have conducted reactions with platinum moiety with various carboxylic acids such as Nicotinic acid, salicylic acid and amino acids. In this presentation we will discuss how we have synthesized and spectroscopically characterized some of these complexes. Biological study of these complexes such as antitumor activity of these complexes are underway.

05.05.32 Determination of dibutyl phthalate in infant formula

Bowen,John *University of Central Oklahoma*

Lewis,Dalton *Other*

Phthalate ester plasticizers, including dibutyl phthalate have been implicated as endrocrine disruptors. These compounds leach from plastics into liquids and many were banned from toys and baby products in 1996, but is commonly found in water in contact with PVC piping. For this study, an analytical method was adapted to detect and quantitate phthalate esters in infant formulas and baby food sold in plastic containers for the head space analysis using gas chromatograph mass spectroscopy with concentration by solid phase microextraction (HS SPME GC-MS). Results from various products will be discussed.

05.05.33 Utilizing Volatile Organic Compounds to differentiate between Methicillin Resistant and Sensitive Strains of Staphylococcus Aureus using Solid Phase Micro Extraction (SPME) and Gas Chromatography-Mass

Bowen,John *University of Central Oklahoma*

Dressler,Garrett *University of Central Oklahoma*

Brennan,Robert *University of Central Oklahoma*

It is well known that microorganisms can and do give off distinct odors such as body odor or the characteristic odor of yeast. In light of that knowledge, pure strains of Staphylococcus Aureus, both methicillin resistant and methicillin sensitive, were sampled during this study. The motivation behind this was to attempt to identify the different volatile organic compounds (VOC) given off by both the resistant and sensitive strains. The end goal of the study was to be able to establish that the resistant strains give off unique VOC's apart from the sensitive strains. Solid Phase Micro Extraction (SPME) is a very useful technique for the analysis of VOC's. Therefore, for this study, headspace samples were collected using SPME with subsequent analysis using Gas Chromatography/Mass Spectrometry (GC-MS). Data and results to be presented.

05.05.34 Analysis of Quercetin and Resveratrol in red wines and grapes using HPLC

Bowen,John *University of Central Oklahoma*

Jin,Quanxiu *University of Central Oklahoma*

Liu,Jianguo *University of Central Oklahoma*

An analytical method for high performance liquid chromatography (HPLC) was developed for the analysis of the antioxidents resveratrol and quercetin in goji berry. Quantitative results will be presented for these compounds.

05.05.35 Synthesis of Malachite Green and Its Application In Solar Cells

Lutz,James *Cameron University*

Hillis,Nathan *Cameron University*

In this research a new synthesis of Malachite Green has been developed using microwave technology to prepare the dye. The procedure for synthesizing the dye and its application in dye-sensitized solar cells will be discussed. These cells consist of titanium dioxide nanocrystals that are coated with light-absorbing dye molecules and immersed in an electrolyte solution, which is sandwiched between two glass plate Light striking the dye frees electrons and creates "holes"--the areas of positive charge that result when electrons are lost. The semiconducting titanium dioxide particles collect the electrons and transfer them to an external circuit, producing an electric current. The cells can be connected in series to produce cells with voltages as high as five volts which can be used to power a small motor.

05.05.36 Solid State Reactions of Titanium Dioxide with Silicon Dioxide

Myers,Dwight *East Central University*

Brown,Chundira *East Central University*

There are questions as to the reaction or extent of reaction of titanium dioxide (rutile) with silica. Conflicting reports have been made as to whether they are reactive or not, and at what temperatures. Both are important as potential 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. Solid state reactions of titanium dioxide with silicon dioxide are being attempted. Mixtures of the two oxides have been subjected to heatings at various temperatures from ca. 1200 - 1500°C. Samples are being characerized before and after heatings 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.

05.05.37 Synthesis of Azo Dyes Prepared from Diazonium Salts and Their Applications in Dye Sensitized Solar Cells

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Nalley,Elizabeth *Cameron University*

Cameron University, Lawton, OK 73505 Arenediazonium salts are generated by the reaction of a primary amine with nitrous acid (produced from sodium nitrite) as shown below. The aromatic amines (anilines) are generated by the reduction of the corresponding nitro compound, which is easily prepared via electrophilic nitration of the ring (see nitration of methyl benzoate). The diazonium salts are unstable at temperatures above 5 - 10°C and some explode if allowed to dry. The aliphatic counterpart can be prepared in the same way; however, even at low temperature it is more unstable and can spontaneously decompose by loss of nitrogen to produce carbocation. A useful reaction of diazonium ions is their use as electrophiles in electrophilic aromatic substitution reactions. They will react with highly activated aromatic systems (phenols, arylamines) to yield azo compounds (diazo coupling reaction). Due to the extended system of delocalized pi electrons, azo compounds are usually colored and therefore have found use as dyes. In this presentation, the synthesis of several dyes will be described. These dyes were tested as possible photoreceptors in dye sensitized solar cells. The results of these tests will be discussed.

05.05.38 Isolation and Structure Elucidation of Siderophores Produced by Marine Bacteria

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Martin,Jessica *Northeastern State University*

In low-iron environments, many bacteria utilize iron (III) chelators to solubilize and transport iron into the cell. These iron (III) chelators, called siderophores, can have many different structures. The objective of this project is to identify novel siderophores produced by marine bacteria. Before determining the structure, siderophores were first grown in cultures of low-iron artificial seawater and purified using RP-HPLC. To test for the presence of siderophores before purification, Fe(III)-CAS Assay was used. Purified siderophores were then analyzed using mass spectrometry and tandem mass spectrometry. Structure determination was done using amino acid analysis and NMR.

05.05.39 Production of Siderophores by Marine Fungi to Determine Known and Unknown Structures

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Some marine fungi have developed mechanisms for the uptake of iron in marine environments. These fungi produce siderophores, which are secreted into the environment and bind iron. They are then brought back into the cell. Siderophores have many different identified structures with potential for new unidentified structures to be discovered. In this experiment two marine fungi, C. eleans and another fungi labeled 05-001, were grown in artificial seawater separately and were later isolated. HPLC was run with mass spec to determine structures. The two fungi were then grown together, allowing competition to produce more known structure siderophores and new unidentified siderophores.

05.05.40 A Study of Iodine Gas Scrubber Efficiency and Iodine Distribution in Northwestern Oklahoma Brine Waters

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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 to the discovery of new sites within the aquifer that may be of commercial interest and has taken an in-depth look at three 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. We also studied iodine gas scrubber efficiencies, which captures Iodine gas during the crystallization process. A balance between fluid recirculation rate, air flow, internal surface area, and a chemical balance without disrupting other plant operations is needed, which will result in improved overall iodine