Abstracts

Undergraduate Research in Chemistry Regional Poster Competition

Jacobs Science Building
April 27, 2018
11:30am - 3:30pm

Department of Chemistry
University of Kentucky
Lexington, KY 40506

Author Index of Abstracts

#	Name	Group*	#	Name	Group*
1	Alyson Ackerman	A	21	Jumanah (Jay) Mahmoud	A
2	Cassandra Almasri	B	22	Nicole Martin	B
3	Corbin Arrasmith	A	23	Mayte Murillo	A
4	John Attelah	B	24	Alexander Newmark	B
5	Jenna Bingham	A	25	Christine Phipps	A
6	Alexandra Davis	B	26	Meranda Quijas	B
7	Brady Ekman	A	27	Evan Reeder	A
8	Kate Fraser	B	28	Jacquelyn Rhinehart	B
9	MacKenzie Freeman	A	29	Gregory Rummel	A
10	Emily Fryman	B	30	Brad Seahorn	B
11	Sara Garner	A	31	Chia-Hsuan Shen	A
12	Kimberly Gleason, Ryan Sanders, and Jacqueline Smith	B	32	Janice Sikon	B
13	Ellen Gouws	A	33	William Smith	A
14	Madisyn Hayes	B	34	Kristen Sportiello	B
15	Collan Henderson	A	35	Nicholas Stafford and Phong Thai	A
16	Angela Hinchie	B	36	Kyle Starkey	B
17	William Jackson III	A	37	Brandyn Thompson	A
18	Katherine Kloska	B	38	Darin Vaughan	B
19	Regan Lee	A	39	Anna Verlander	A
20	Amber Lewis	B	40	Eric Vogt	B

*Group A presents from 11:30am to 1:00pm.
*Group B presents from 1:00pm to 2:30pm.

1 CHARACTERIZATION OF BSN175: A SUGAR SUBSTITUTE DRUG

Alyson Ackerman, Senior, Chemistry, University of Kentucky
Robert Lodder, Pharmacy, University of Kentucky

Abstract:
BSN175 is a novel sugar substitute drug intended to treat Prader-Willi syndrome, a condition that affects thousands of children worldwide. Characterized by weakness in infancy and obesity, behavioral issues, and an insatiable appetite from the age of two onwards, this condition is all-consuming and can be devastating to those experiencing it and their families. Type II diabetes frequently accompanies this obesity. While there is no cure for Prader-Willi, there are ways to manage the symptoms. Sugar substitutes are used to reduce caloric intake and sate those who cannot control their appetites. BSN175 is one such sugar substitute drug that has been investigated for use in treatment of type II diabetes. To provide quantifiable, reproducible analysis of BSN175, the active pharmaceutical ingredient, D-tagatose, needs to be easily identified and differentiated from its decomposed form and other possible impurities. Infrared and proton NMR spectroscopy will be applied to the drug to build a package that can be used to determine the identity and purity of D-tagatose to meet FDA regulations for quality and safety.

2 THE DESIGN AND FABRICATION OF COMPONENTS FOR A STAGE-TOP HIGH-THROUGHPUT TIRF MICROSCOPY MODULE

Cassandra Almasri, Senior, Chemistry, University of Kentucky
Chris Richards, Chemistry, University of Kentucky
Jason DeRouchey, Chemistry, University of Kentucky

Abstract:
Total Internal Reflection Fluorescence Microscopy (TIRFM) is a technique used to directly visualize the fluorophores on the surface of a given sample. TIRFM is best known for its applications used to visualize processes occurring in the plasma membranes of cells; however, it has a wide variety of applications beyond the visualization of biomolecules. TIRFM works by using fiber optics to project a laser beam of desired wavelength onto the surface of the sample at an incident angle. By shining light at an incident angle greater than the critical angle, light will be reflected from the sample and only the surface of the sample will be illuminated and analyzed.

Current methods for analyzing samples using TIRFM are directed towards single sample analysis. This becomes particularly challenging in fields that are interested in carrying out reliable studies with different samples and/or different timepoints. The purpose of this research is to propose and develop a system that allows for widespread analysis of samples using high-throughput TIRF. In this project we suggest HT-TIRF would employ a prism-based stage top design compatible with a 96 well plate. This design will allow for HT-TIRF on a fluorescent microscope by shining a laser onto a prism located directly under the wells and allowing a propagated evanescent illumination to extend onto the wells that will be analyzed. The efficiency and reliability of the device and corresponding fiber optic system will be further investigated by imaging several test samples.

3 QUANTIFYING DIFFUSION OF A MODEL ANALYTE SET VIA CAPILLARY ELECTROPHORESIS

Corbin Arrasmith, Junior, Chemistry, Northern Kentucky University
Charlisa Daniels, Chemistry, Northern Kentucky University

Abstract:
The goal of this project was to further understand the relationships between the temperature, analyte, and concentration of the analyte within a capillary. This was investigated using Capillary Electrophoresis (CE) on the PAH series (Naphthalene through Chrysene). This series was selected based on their use in previous studies. In addition further analysis's on the GMA:EDMA polymers was completed along with Scanning Electron Microscope (SEM) images to show the pores size of the polymer and how they change based of GMA:EDMA ratios and porogen size.

4 SEPARATION AND ANALYSIS OF HEPARAN SULFATE TETRASSACHARIDE MIXTURES USING CAPILLARY ELECTROPHORESIS, AND ORBITRAP MASS SPECTROME

John Attelah, Junior, Chemistry, Berea College
Patience Sanderson, Chemistry, University of Georgia
Morgan Stickeney, Chemistry, University of Georgia
Jonathan Amster, Chemistry, University of Georgia

Abstract:
Glycosaminoglycans (GAGs) are complex polysaccharides, expressed at the cell surface and in the extra-cellular matrix, which comprise the carbohydrates portion of proteoglycans and are found in a variety of organisms ranging from bacteria to humans. GAGs participate in a number of significant biological processes, such as cell-cell and cell-matrix signaling at the origin of a variety of physiological and pathological functions such as embryonic development, cell adhesion, the regulation of biochemical pathways, cell growth and differentiation, homeostasis, and the mediation of inflammatory reactions. They have also been implicated in the initial step of some pathogenic infections and have been observed to undergo some alteration in some tumor growth. There are different types of GAGs which include Chondroitin Sulfates(CS), Dermatan Sulfates (DS), Keratan Sulfates(KS), Heparin and Heparan Sulfates(HS). This research focused on separation and analysis of heparan sulfate tetrassacharide mixture using Capillary Electrophoresis and Orbitrap Mass Spectrometry.

5 FLUOROAMIDE-DIRECTED FLUORINATION OF UNACTIVATED C–H BONDS

Jenna Bingham, Senior, Chemistry, Indiana University
Brian Groendyke, Chemistry, Indiana University
Silas Cook, Chemistry, Indiana University

Abstract:
Organofluorine compounds possess unique and desirable properties with applications spanning the pharmaceutical, agricultural, and materials industries. Despite being ideal transformations, methods to selectively fluorinate Csp3-H bonds are still scarce and in need of development. Previous work in the Cook Group demonstrated that N-fluoro-2-methylbenzamides selectively transfer fluorine upon reaction with iron (II) triflate to provide the benzyl fluoride in yields up to 93%. Attempts to change from the rigid 2-methylbenzamide class to linear alkyl systems caused the yields to plummet. This work presents our latest efforts in the optimization of the fluorine transfer reaction for open-chain, unactivated systems.

6 SYNTHESIS OF MULTICOLOR FLUORESCENT LIGANDS FOR NICOTINIC ACETYLCHOLINE RECEPTORS

Alexandra Davis, Senior, Chemistry, Indiana State University
Richard Fitch, Chemistry, Indiana State University

Abstract:
Nicotinic acetylcholine receptors (nAChR) are ligand gated ion channels sensitive to the neurotransmitter acetylcholine and serve critical roles in pre- and postsynaptic neurotransmission in the central and peripheral nervous systems. Fluorescent ligands for nAChR can be used to locate nicotinic receptors in isolated tissues and cultured cells. Our design of fluorescent ligands include a ligand motif (A-84543), a hydrophilic linker, and terminal fluorophore. We are examining a variety of fluorophores for multilabeling applications in fluorescent microscopy, flow cytometry and binding/functional assays for nAChR. Our results to date will be described.

7

COMPARING DNA CONDENSATION BY PISCINE PROTAMINES

Brady Ekman, Junior, Chemistry, University of Kentucky
Daniel Kirchhoff, Chemistry, University of Kentucky
Jason DeRouchey, Chemistry, University of Kentucky

Abstract:
Protamines are short arginine-rich proteins that mediate the near crystalline DNA packaging in sperm chromatin. Protamines are synthesized during spermiogenesis and condense the DNA in spermatocytes into a transcriptionally inactive state. The purpose of this study is to compare the condensation of protamine from different piscine sources, including commercial protamine chlorides and protamine sulfates from salmon and herring as well as protamine chloride extracted from salmon sperm nuclei. The purity and quality of the protamines were analyzed using polyacrylamide gel electrophoresis. The DNA-binding efficiency of the different protamines was quantified by DNA precipitation assays using UV-Vis spectroscopy. Lastly, the resulting DNA packaging density and structure was determined using small-angle X-ray scattering. Our results show that despite being widely used for DNA condensation studies, commercial salmon protamine chloride shows signs of degradation when compared to commercial salmon and herring protamine sulfates and isolated salmon protamine from salmon sperm nuclei. Interestingly, protamine-induced precipitation of DNA and the internal DNA packaging structures are not significantly altered for the partially degraded salmon protamine chlorides compared to non-degraded salmon protamines.

8 STERIC MANIPULATION AS A MECHANISM TO TUNE THE REDUCTION POTENTIALS OF SMALL MOLECULES

Kate Fraser, Junior, Chemistry, University of Kentucky
Chad Risko, Chemistry, University of Kentucky

Abstract:
Phenothiazines are of interest as redox-active materials for energy storage applications. Here, for a series of five N-substituted phenothiazine derivatives, we study the impact of strain- and electronic-induced substituent effects on the reduction potential. Using density functional theory (DFT), the vertical and adiabatic electron affinities (VEA and AEA, respectively) and ion relaxation energies are determined for N-phenothiazines with either donor or acceptor substituents in four configurations – substitution at either the 1,9-, 2,8-, 3,7-, or 4,6-positions. While the 2,8-, 3,7-, and 4,6-substitution patterns result in mainly electronic control of the electron affinities, substitution at the 1 and 9 positions results in considerable steric interactions with N-alkyl substituents, resulting in smaller relaxation energies. Even when the substituents are electron withdrawing, the steric effects make it more difficult to reduce the phenothiazines. Coupled with like effects for the oxidation potentials, these results demonstrate an intriguing means to control the redox activity.

9 LEAD CONCENTRATIONS IN AVIAN EGGSHELLS AND EGG CONTENTS

MacKenzie Freeman, Senior, Chemistry, University of Kentucky

Abstract:
Heavy metal pollution in the environment continues to be a significant issue. Lead in particular has been of high interest due to the high levels expelled into the environment during the era of leaded gasoline and paints. Children aged six years and younger are the most vulnerable to lead poisoning, and pregnant women should be wary because it can cause premature births, low birth weight, and even slowed growth of a newborn. Chicken eggs are a possible source of lead consumption in the American diet. Hence, the amount of lead in chicken eggs and egg contents was measured (by atomic absorption spectroscopy) to investigate the correlation between lead content in eggs and the proximity of chickens to traffic-heavy roads or highways. No lead concentrations over the FDA daily limit for children six years or younger (6 μg) were observed. Locally-sourced chicken eggshells (from Yellow Springs, OH) had a lead concentration of over 3 μg, while supermarket eggshells had only 0.75 μg of lead, on average. Therefore, the environment in this area was either not significantly polluted with lead to begin with, or it has been able to recover from any contamination that may have occurred in the past.

10 UNDERSTANDING DIFFUSION IN POLYMER GELS WITH ELECTROSTATIC INTERACTIONS

Emily Fryman, Senior, Chemistry, University of Kentucky
Jason DeRouchey, Chemistry, University of Kentucky
Joseph Duke III, Chemistry, University of Kentucky
Kanthi Nuti, Chemistry, University of Kentucky

Abstract:
Biological hydrogels are heterogeneous polymer networks with complex biophysical properties. Biogels are known to fulfill a number of important physiological functions including the filtering and regulation of nutrients, pathogens, and other small molecules in vivo. Alongside volume exclusion and hydrodynamic effects, it is knownthat nonsteric interactions, such as electrostatic or hydrophobicity, are major factors that govern the mobility of particles in biogels.
Translational diffusion coefficients are determined by fluorescence correlation spectroscopy measurements for charged probe molecules (Alexa and ATTO dyes) in uncharged as well as cationic, anionic and mixed charge dextran and chitosan polymer solutions. We show that particle transport in the charged hydrogels is highly asymmetric, with diffusion slowed down much more by electrostatic attraction than by repulsion, and that the filtering capability of the gel is sensitive to the solution ionic strength. Furthermore, even small fractions of oppositely charged interaction sites lead to strong trapping of the particle. Quantitative agreement is found between experiment and theoretical predictions.

11 MEASUREMENT OF CHEMICAL SHIFT TENSORS AND J-COUPLING IN SODIUM/LEAD MIXED PRYOPHOSPHATE GLASSES

Sara Garner, Senior, Chemistry, Berea College
Dr. Jay Baltisberger, Chemistry, Berea College
Tomas Flores, Chemistry, Berea College
Shay Steele, Chemistry, Berea College

Abstract:
In pyrophosphate, the J-coupling distribution is strongly correlated with P–O–P bond-angle distribution. By using solid state Nuclear Magnetic Resonance (NMR) J-coupling patterns can be viewed and help determine structural information. The hypothesis that was proposed was that the mixed glasses would have two regions of J-coupling patterns. Rich regions of Pb2+ and another region with both Na+ and Pb2+ patterns. The pyrophosphate samples were synthesized by mixing solid compounds of varying Pb2+ and Na+ ions. The mixed solids was then placed in a muffle furnace and heated to 1100°C. The molten glass was poured onto a copper plate and quenched. The samples were ground to a fine powder and packed into rotors. The samples were analyzed using solid state NMR experiments. PASS (Phase Adjusted Spinning Sidebands) and TE-PIETA (Total-Echo Phase Incremented Echo Train Acquisition). The raw data was then placed into a specialized program to view J-coupling of the PASS and PIETA. Many of the mixed samples displayed as two types of J-coupling. When compared to a pure lead sample the J-coupling was close to 23 Hz; however, the mixed samples seemed to lower the J-coupling to about 14 Hz. We also looked at the chemical shift anisotropy (CSA) of the samples and appears that there is not much variability within them.

12 A CATION EXCHANGE-SOLID PHASE EXTRACTION PROTOCOL FOR THE ISOLATION AND ANALYSIS OF ALKALOIDS IN POISON FROGS

Kimberly Gleason, Junior, Chemistry, University of Kentucky
Ryan Sanders, Chemistry, Indiana State University
Nicholas Andreasen, Chemistry, Indiana State University
Kameron Bell, Chemistry, Indiana State University
Jacqueline Smith, Chemistry, Indiana State University
Richard Fitch, Chemistry, Indiana State University

Abstract:
Tropical poison frogs are well-known for their conspicuous bright coloration and toxic secretions. We use Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid Chromatography-Mass Spectrometry (LC-MS) for qualitative and quantitative analysis of secretions from poison frogs which contain acids, bases, polars, and neutrals. The goal of the current work is to develop a protocol for Cation Exchange-Solid Phase Extraction (CA-SPE) for the purpose of separating basic alkaloids from nonbasic compounds in a single process for easier identification. Prior to analysis of field extracts, a standard mixture of 20 known alkaloids was analyzed to test the efficiency, reproducibility, and robustness of the process. Preliminary results are thus far promising, providing near quantitative recoveries, and demonstrating reusabilility of the media, a potentially valuable cost-saving measure when using 96-well CA-SPE plates. We are currently evaluating the method as applied to field extracts from Madagascar and South America. Our results to date will be presented.

13 ANALYSIS OF AROMA COMPOUNDS IN KENTUCKY BOURBONS

Ellen Gouws, Senior, Chemistry, University of Kentucky
Bert Lynn, Chemistry, University of Kentucky

Abstract:
Kentucky bourbon is well known for its unique aroma, with its smoky, spicy, and vanilla-like flavor notes. Bourbons from three different Kentucky distilleries were analyzed to determine if the quantity of aroma producing compounds differed from bourbon to bourbon. Although most bourbons undergo similar fermentation and distillation processes, products can differ in grain bill and aging time in the barrel. To characterize compound variation of bourbon whiskey, we first used dispersive liquid-liquid micro-extraction with chloroform as the solvent to extract the aroma compounds. Then, the aroma compounds from the bourbons were analyzed by gas chromatography-mass spectrometry (GC/MS). These data were input into Automated Mass Spectral Deconvolution and Identification System (AMDIS) software package to generate feature lists (co-eluting mass/charge ratios) and their total signal counts. In order to identify the features, mass spectra were searched against the NIST database of organic compounds. Based on available literature, we expected to observe differences in the quantity of common bourbon aroma compounds such as vanillin, whiskey lactones, decanoic acid, butanoic acid, hexanoic acid, syringaldehyde and carboxylic acid ethyl esters resulting in unique aroma profiles for each bourbon. The signal counts for each identified compound were compared to an internal standard (anthracene) and then cross analyzed with one another to find differences and similarities. Results from this study will help illuminate how unique aromatic profiles are created in Kentucky bourbons despite similar production processes.

14 AN INVESTIGATION INTO THE FACTORS THAT AFFECT POLYMERIZATION OF AN EXTERNAL STIMULI RESPONSIVE MATERIAL

Madisyn Hayes, Freshman, Chemistry, Northern Kentucky University
Megan Lang, Biology, Northern Kentucky University
Charlisa Daniels, Chemistry, Northern Kentucky University

Abstract:
The goal of this investigation was to develop an understanding of how different cross-linkers and porogens affect the structure and behavior of poly(2-dimethylaminoethyl methacrylate) (DMAEMA) polymers. To do this, factors such as the identity and ratio of cross-linker used, the identity of porogen, the heating method, and the temperature and duration of the polymerization were manipulated to find the best composition and conditions. This was done by incorporating cross-linkers such as styrene, 1,3 BDDA, and 1,4 BDDA with the DMAEMA at different concentrations, then adding casting solutions of various porogens, such as propanol, hexanol, octanol, or dodecanal. The mixture was then placed in either a water bath or an oven at temperatures ranging from 70-90 degrees Celsius and left for either twenty-four or forty-eight hours. The results showed that the cross-linker styrene, at concentrations ranging from 50-75%, produced the most ideal results when combined with the porogens hexanol or propanol and baked at 90 degrees Celsius in a water bath. With this discovery, further experimentation, including polymerization within fused silica capillaries for investigation through capillary electrochromatography, to monitor how pore size inhibits environmentally relevant analytes. This will contribute to studies of the mobility of the analytes in an external stimuli responsive material, which could potentially lend itself to water remediation research.

15 SIZE-DEPENDENT OPTICAL PROPERTIES OF CADMIUM SELENIDE QUANTUM DOTS

Collan Henderson, Junior, Chemistry, Transylvania University
Megan Quackenbush, , Transylvania University
Kyle Schnitzenbaumer, Chemistry, Transylvania

Abstract:
The optical properties of Cadmium Selenide quantum dots were explored in relation to their size and concentration. Quantum dots have a wide range of potential applications such as photovoltaics, optical displays and photocatalysts. UV-Vis, Atomic Absorption spectroscopy and electron microscopy were used to characterize the peak wavelength of absorbance, concentration and size, with smaller diameter crystals absorbing shorter wavelengths due to the effects of quantum confinement. The results were analyzed and used to determine the relationship between size, molar absorptivity and peak wavelengths absorbed. The procedure used could be applied to characterize other species of quantum dots in the future.

16 IMPACT OF PARKINSON DISEASE ON THE MTOR PATHWAY USING A PINK1 KNOCKOUT RAT MODEL

Angela Hinchie, Senior, Chemistry, University of Kentucky
D. Allan Butterfield, Chemistry, University of Kentucky

Abstract:
Parkinson disease is a neurodegenerative disorder that affects movement and, in late stages, also causes cognitive deficits. The PINK1 gene is one of several genes whose mutation causes familial Parkinson disease. The PINK1 gene codes for a mitochondrial kinase protein that accumulates on damaged mitochondria, a process which signals the damaged mitochondria for mitophagy. This project explored the impact of knocking out the PINK1 gene on the activation of the mTOR pathway. The mTOR pathway is an important cell signaling pathway that is heavily impacted in another neurodegenerative disorder, Alzheimer disease, and influences both autophagy and insulin resistance among others targets. For this project, rats with a knocked-out PINK1 gene were used, with brain samples collected at two, four, six, and eight months of age. Using western blotting, the activation of several key proteins in the mTOR pathway was measured for all collected months. These proteins included PI3K, Akt, mTOR, and p70S6k. Akt showed decreased activation at six months compared to the four and eight month rats, which is consistent with other results on autophagy markers and insulin activation. The mTOR and p70S6K proteins showed a decrease in activation at eight months, with a modest decrease in activation at six months for p70S6K. The results for PI3K are still in progress. These results help to illuminate the changes with age on the mTOR pathway in a novel rat model of Parkinson disease, and will open new avenues of research into this devastating age-related, neurodegenerative disorder.

17

ANTI-TES-ADT: IMPROVING THE SYNTHESIS

William Jackson III, Senior, Chemistry, University of Kentucky
John Anthony, Chemistry, University of Kentucky

Abstract:
5,12-bis(triethylsilylethynyl) anthradithiophene, TES-ADT for short, is an organic semiconductor with many applications, namely high-performance electronics. It has been shown that the *anti* isomer performs significantly more efficiently than its *syn* counterpart as pertains to charge carrier transport. The effort was to find a more quicker and more efficient method to isolate the *anti* isomer whilst not compromising yield. It was discovered that the introduction of triethylsilylchloride (TES-CL) increased the solubility of the isomer, allowing for it to separate much easier in Column Chromatography. The poster associated with this research will present the synthesis of the anti-TES-ADT and its applications with collaborators.

18 GAS-PHASE SPECTRA OF MGO MOLECULES: A POSSIBLE CONNECTION FROM GAS-PHASE MOLECULES TO PLANET FORMATION

Katherine Kloska, Junior, Chemistry, University of Kentucky
Ryan Fortenberry, Chemistry, University of Mississippi

Abstract:
A more fine-tuned method for probing planet-forming regions, such as protoplanetary discs, could be rovibrational molecular spectroscopy observation of particular premineral molecules instead of more common but ultimately less related volatile organic compounds. Planets are created when grains aggregate, but how molecules form grains is an ongoing topic of discussion in astrophysics and planetary science. Using the spectroscopic data of molecules specifically involved in mineral formation could help to map regions where planet formation is believed to be occurring in order to examine the interplay between gas and dust. Four atoms are frequently associated with planetary formation: Fe, Si, Mg, and O. Magnesium, in particular, has been shown to be in higher relative abundance in planet-hosting stars. Magnesium oxide crystals comprise the mineral periclase making it the chemically simplest magnesium-bearing mineral and a natural choice for analysis. The monomer, dimer, and trimer forms of (MgO)_n with n = 1 - 3 are analyzed in this work using high-level quantum chemical computations known to produce accurate results. Strong vibrational transitions at 12.5 {\mu}m, 15.0 {\mu}m, and 16.5 {\mu}m are indicative of magnesium oxide monomer, dimer, and trimer making these wavelengths of particular interest for the observation of protoplanetary discs and even potentially planet-forming regions around stars. If such transitions are observed in emission from the accretion discs or absorptions from stellar spectra, the beginning stages of mineral and, subsequently, rocky body formation could be indicated.

19 FORMATION OF INTRAMOLECULAR DITYROSINE LINKAGES VIA PEROXIDASE-CATALYZED OXIDATION OF POLYPEPTIDE TAGS

Regan Lee, Senior, Chemistry, University of Kentucky
Yinan Wei, Chemistry, University of Kentucky

Abstract:
Certain oxidizing agents can remove one electron from the phenol group of a tyrosine residue within a protein molecule, forming a tyrosyl radical. If two tyrosine residues are in close proximity during such a reaction, the tyrosyl radical products may cross-link to form a dityrosine moiety. The strong fluorescent signal of dityrosine allows it to be used as a probe for detection of proteins as well as analysis of their properties. In this study, cyan fluorescent protein (CFP) was genetically tagged at its carboxy-terminus with one of two different amino acid sequences containing two tyrosine residues separated by a short spacer (CYSDPRCAFRY and YSDPRSAFRY). Each tagged protein was subjected to an oxidation reaction in the presence of horseradish peroxidase (HRP) and hydrogen peroxide. Such treatment has been proven to induce site-specific dityrosine linkages between different molecules of the same protein to form homoconjugates (Minamihata, et al., 2010), as well as between molecules of different proteins to form heteroconjugates (Minamihata, et al., 2011). The purpose of this project is to find if the method is useful to induce such linkages between the two tyrosines in the short sequence to create a fluorescent tag. SDS-PAGE analysis was used to determine purity and concentration of protein, as well as extent of reaction completion via concentration of any remaining enzyme. The reacted protein was analyzed via fluorescence spectroscopy and compared to unreacted protein to determine success of the oxidation reaction. The reaction was repeated under different conditions with varying concentrations of reagents, and these results analyzed similarly to those of the first condition. Spectroscopic analysis showed the signature fluorescence signal of dityrosine. The intrinsic fluorescence of CFP was partially affected by the oxidation condition. These results indicate that a dityrosine tag is useful in protein labeling, and the usefulness of such a tag in more proteins needs to be tested.

20 THIOLATE COMPOUNDS WITH CADMIUM, MERCURY AND LEAD

Amber Lewis, Senior, Chemistry, University of Kentucky
David Atwood, Chemistry, University of Kentucky

Abstract:
MEAB9 (3-Mercapto-2-[3-(2-mercapto-1-methoxycarbonyl-ethylcarbamoyl)- benzoylamino]-propionic acid methyl ester) (1) was created as an alternative solution to BDTH2 (N,N′-bis(2-mercaptoethyl)isophthalamide) to bind with toxic metals including cadmium, mercury and lead that can be found in polluted water. The principle was to create metal thiolates in hopes of being able to dissolve in water after binding for further testing using X-Ray crystallography. Using X-Ray crystallography would give better insight to the structure and bonding properties of metal thiolates. MEAB9 metal complexes were found to be very stable, most likely due to their strong covalent bonding with the sulfur atom and were not soluble in water. X-Ray crystallography was tested and the results showed the compound was amorphous, but was still useful for metal precipitation.

21 SYNTHESIS OF CHELATING BIS-N-HETEROCYCLIC CARBENE COMPLEXES OF RU(II) AS POTENTIAL ANTI-CANCER AGENTS

Jumanah (Jay) Mahmoud, Senior, Chemistry, University of Kentucky

Abstract:
N-heterocyclic carbenes, (NHCs) are ubiquitous in organometallic chemistry due to their electron-donating properties. Glazer and coworkers corroborated the effects of strained ruthenium bipyridyl complexes to be light-activated anticancer agents in a method known as photodynamic therapy (PDT). [Ru(bpy)2]2+ (bpy = 2,2'-bipyridyl) is released upon irradiation of the appropriate wavelength of light, in which it exhibits DNA crosslinking abilities. By taking advantage of the well knownwell-known trans-labilizing effects of NHCs, it will be possible to generate ruthenium complexes with N-heterocyclic carbenes (NHC's) as co ligands in order to increase ligand-loss selectivity upon visible light irradiation. The reaction of [RuCl(η6-p-cymene)(κ2Ck2C,C-diNHCme)][PF6][1] with $AgPF_6$ and 2,2'- bipyridyl in DMF leads to [Ru(η6-p-cymene)(kκ2C,C-diNHCme)(bpy)2]2+[1]. This ruthenium complex demonstrated dark toxicity with an increase activity with visible light. Structure of [1] was determined by X-ray crystallography.

22

THE ROLE OF ALPHA-ENOLASE DYSFUNCTION IN ALZHEIMER'S DISEASE

Nicole Martin, Senior, Chemistry, University of Kentucky
D. Allan Butterfield, Chemistry, University of Kentucky
Elizabeth Head, Sanders Brown Center on Aging, University of Kentucky

Abstract:
Millions of Americans today live with Alzheimer's disease (AD)—the most common cause of dementia in the elderly. Numbers of cases continue to rise, and it has become the 6th leading cause of death. For this reason, identifying novel molecular pathways that may lead to AD have become of great importance. Alpha-enolase, a glyclolytic enzyme that plays a key role in metabolism, has been thought to, when HNE modified, be associated with a higher risk of AD. The study of this metabolic process can provide a connection between brain vascular pathology, oxidation, and AD. In people with Down Syndrome (DS) the effects of alpha-enolase could be even exacerbated as they have significant oxidative stress from birth. The current study tested the hypothesis that alpha-enolase dysfunction will be correlated with severe AD and also with age, in DS autopsy cases. An anti alpha-enolase antibody was used with immunohistochemistry on a control case of 24 years old with DS without AD and in a group of cases with DS/AD ranging of ages 40-66 years old. Results suggest differences in alpha-enolase levels in the white matter of the frontal cortex that will be quantified using an Aperio Scan Scope. Alpha-enolase is observed in the cell bodies and processes of the glial cells, which will be confirmed with double labeling immunohistochemistry. These results could further knowledge on the causes of AD in DS and in the general population and could serve as a target for intervention.

23 A COMPARISON OF ANALYTICAL TECHNIQUES USING B-CYCLODEXTRIN

Mayte Murillo, Senior, Chemistry, University of Kentucky
Robert Lodder, Chemistry, University of Kentucky

Abstract:
Each NDA filed at the Food and Drug Administration (FDA) must include the analytical procedures necessary to ensure the identity, strength, quality, purity, and potency of a drug substance and drug product. The BSN389 drug product (being developed to treat Ebola virus infections) includes beta cyclodextrin. Data must be available to establish that the analytical procedures used in testing BSN389 meet proper standards of accuracy, sensitivity, specificity, and reproducibility and are suitable for their intended purpose. (When an analytical procedure is approved/licensed as part of the NDA, it becomes the FDA-approved analytical procedure for the approved product.) Early in the development of a new analytical procedure, the choice of analytical instrumentation and methodology is made based on the intended purpose and scope of the analytical method. During early stages of method development, the robustness of methods should be evaluated because this characteristic can help decide which method will be submitted for approval. Analytical procedures in the early stages of development are initially developed based on a combination of mechanistic understanding of the basic methodology and prior experience. Experimental data from early procedures are used to guide further development. The most commonly used method for analyzing compounds is high-performance liquid chromatography (HPLC). However, each sample is known to take 10-20 minutes to run, and is time consuming for pharmaceutical companies. Spectroscopic methods have the potential to be faster. The BEST software will be used to measure the quantitative and qualitative power differentiate of IR and 1H NMR for beta cyclodextrin, and the best one will go into the analytical package in the IND submitted to FDA.

24 SOLVOTHERMALLY PRODUCED FE-DOPED CARBON NANODOTS SHOW BIO-IMAGING POTENTIAL WITH TEMPERATURE-DEPENDENT PHOTOLUMINESCENCE

Alexander Newmark, Senior, Chemistry, University of Kentucky
Tim Pillar-Little, Chemistry, University of Kentucky
Doo Young Kim, Corresponding Author, Department of Chemistry, University of Kentucky

Abstract:
The emergence of carbon nanodots (CNDs) as a new class of carbon nanomaterial has generated excitement as CNDs have advantageous physicochemical and optical properties. Particularly, CNDs are attractive as alternatives to inorganic quantum dots in bio-imaging, photocatalysis, solar cells, and sensory applications. In addition these CNDs have low production cost, chemical inertness, and are highly bio-compatible which makes them a promising material in nanotechnology and nanomedicine. It was recently reported that hydrothermal treatment of porphyrins in the presence of ethylenediamine produced fluorescent CNDs in high yield. The present study aims to explore the optical properties of CNDs produced from bovine hemin and ethylenediamine through a temperature-dependent solvothermal treatment. Optical properties of the heme-CND were probed through UV-visible spectrophotometry and fluorescence spectroscopy. The chemical nature of the principal elements of the CND (Fe, C, N, and O) were characterized by Fourier-transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS). The resulting products showed weak emission in the short wavelength region at high treatment temperatures, but more desirable results were obtained as the temperature of pyrolysis was lowered. Additionally, a distinct red-shift coupled with an increase in emission intensity was observed as the reaction temperature was lowered. The observed change in optical properties is attributed to hydrothermal cutting effects and the chemical state of the heme-group on the CND. In summary, temperature-dependent solvothermal processes provided a simple route to investigate the structural motifs of heme-CNDs on optical properties.

25 SYSTEMATIC INVESTIGATION INTO THE BONDING, ELECTRONIC STRUCTURE, AND REACTIVITY OF METAL/ SOFT-DONOR COMPLEXES

Christine Phipps, Junior, Chemistry, Transylvania University
Jessie Brown, Chemistry, Transylvania University

Abstract:
Some unusual transition metal centers (e.g. vanadium, molydebnum, and tungsten) are surprisingly crucial for metalloenzymatic activity found in certain extremophiles. Structural studies of the active sites indicate that they typically contain soft-donor atoms (e.g. S, Se) bonded to the metal centers, which has been hypothesized to facilitate activation of small molecules. Our guiding objective is to prepare a series of transition metal complexes in order to investigate systematic studies regarding trends and differences within the family of complexes.This presentation will provide our latest results and developments in this pursuit.

26 DETERMINATION OF THE EFFICACY OF GAMMA-GLUTAMYLCYSTEINE ETHYL ESTER (GCEE) AS A TREATMENT STRATEGY FOR MODERATELY TRAUMATIC BRAIN INJURED RATS

Meranda Quijas, Senior, Chemistry, Eastern Kentucky University
Tanea Reed, Chemistry, Eastern Kentucky University

Abstract:
Traumatic brain injury (TBI) is damage that occurs suddenly to the brain that can become permanent. During the primary injury, the initial external force encountering the brain and secondary injury, the biochemical cascade that can occur up to months after the primary injury. Oxidative damage is a result of TBI that is referred to as an imbalance of reactive oxygen species (ROS) and antioxidants. Protein carbonyls can be used as a biological marker for oxidative damage to the brain. As the levels of ROS increase during oxidative stress, apoptosis occurs in excess, cell communication is inhibited, and proteins and lipids are altered from their native conformations. Gamma-glutamylcysteine ethyl ester (GCEE), a glutathione (GSH) mimetic, is an antioxidant that occurs naturally in the brain. Glutathione can counteract the increased levels of ROS in brain. GCEE may be used as a potential therapy for TBI due to its ability to upregulate GSH in brain. This work investigates protein carbonylation levels after administration of GCEE 30 minutes post injury in moderate TBI rats. Slot blot and 2D gel electrophoresis were used to obtain results. Slot blot analysis, an immunochemical tool, yielded overall protein carbonylation while 2D gel electrophoresis identified specific protein spots. Our findings showed a significant difference in the number of proteins expressed between all three groups (sham, saline, and GCEE treatment). These results provide evidence that GCEE treatment reduces protein carbonylation to create a more homeostatic state in the brain and prevent further oxidative damage.

27 EFFICIENT DEACTIVATION OF ELECTRONICALLY EXCITED SINGLET OXYGEN BY POTENT ANTI-CANCER AU (I) AND AU(III) COMPLEXES BEARING CHIRAL PHOSPHINE LIGANDS

Evan Reeder, Senior, Chemistry, University of Kentucky
Jong Kim, Chemistry, University of Kentucky
Rosemary Calabro, Chemistry, University of Kentucky
Sean Parkin, Chemistry, University of Kentucky
Doo-Young Kim, Chemistry, University of Kentucky
Samuel Awuah, Chemistry, University of Kentucky

Abstract:
We describe the synthesis of novel distorted Au(I) and cyclometalated Au(III) bearing chiral phosphine ligands. Luminescent studies reveal direct quenching of singlet oxygen (O21Dg) in solution by the Au(I) or high-valent Au(III) reagents. The complexes evoke potent anti-proliferating cellular responses with IC50s in the nanomolar range. Complexes 1 - 3 induce predominant G1 cell cycle arrest with no evidence for direct DNA interaction and DNA damage response. In an apoptosis study, OVCAR8 cells were found to be largely necrotic after incubation with the compounds 1 or 3 compared to auranofin or cisplatin treated cells. Predominantly, the compounds accumulated in the cytoplasm as measured by ICP-OES. These compounds represent a new class of anticancer agents with a distinct mechanism of action from cisplatin or auranofin.

28

UNDERSTANDING THE ROLE OF PROTAMINE DISULFIDE BONDS ON DNA CONDENSATION IN MAMMALIAN SPERM NUCLEI

Jacquelyn Rhinehart, Senior, Chemistry, University of Kentucky
Daniel Kirchhoff, Chemistry, University of Kentucky
Jason DeRouchey, Chemistry, University of Kentucky

Abstract:
Short arginine-rich proteins called protamines mediate the near crystalline DNA packaging in most vertebrate sperm cells. Protamines are synthesized during spermiogenesis and condense the paternal genome into a transcriptionally inactive state in late-stage spermatids. Protamines from eutherian mammals, including bulls and humans, also contain multiple cysteine residues that form intra- and interprotamine sulfur-sulfur bonds during the final stages of sperm maturation. In bull, it has been shown that seven cysteine residues form inter- and intramolecular disulfide bonds to form a unique hairpin structure. These cysteine residues are missing in other species such as fish. Recent work by the DeRouchey lab showed that complete reduction of the disulfide bonds ultimately leads to decondensation in bull sperm suggesting that disulfide-mediated secondary structure is also critical for proper protamine function. In this study, we have further examined the role of protamine disulfide bonds in bull and horse sperm chromatin through fluorescent microscopy studies. Microscopy studies confirm that the disruption of intra-protamine bonds in mammalian sperm results in decondensation, despite the high cationic charge of mammalian protamine. Decondensation in the isolated nuclei is reminiscent of nuclear vacuoles that are known to correlate negatively with male fertility. Piscine sperm chromatin is unaffected by the presence of a reducing agent. Poorly formed protamine intramolecular disulfide bonds have implications in assessing male fertility potential and could play a role in increased DNA damage to spermatic DNA.

29

SYNTHESIS OF AMMONIUM SUBSTITUTED ACENCE'S: TOWARD ACENE CONTAINING LEAD HALIDE PEROVSKITES

Gregory Rummel, Senior, Chemistry, University of Kentucky
John Anthony, Chemistry, University of Kentucky

Abstract:
Since Prof. Henry Snaith's discovery of solution processable methylammonium lead halide perovskite solar cells in 2012, scientists have been attempting to increase the efficiency of these cells to meet or exceed that of tradition silicon solar cells. However, very little work has been done on the modification of the ammonium salt, though if it contained a conjugated pendant group it could expand the absorption range and in turn increase the efficiency of the cell. The incorporation of a naphthalene or anthracene derivative could create a layered packing which could also lead to improved charge transport. This poster will describe the synthesis and characterization of various anthracene and naphthalene chromophores bearing different ammonium side chains, as well as preliminary data on blends of these compounds with PbI_2.

30 CHEMOTHERAPY INDUCED COGNITIVE IMPAIRMENT: MECHANISMS OF OXIDATIVE STRESS CAUSED BY DOXORUBICIN

Brad Seahorn, Senior, Chemistry, University of Kentucky

Abstract:
Advancements in medicine and cancer detection techniques has allowed cancer survival rates to steadily rise. However, up to 70% of these cancer survivors experience symptoms of memory loss, increased distractibility, and inability to perform multiple tasks, resulting in decreased quality of life. These symptoms have been attributed to chemotherapy induced cognitive impairment (CICI), which involves oxidative damage to the brain. Many chemotherapeutic agents used for cancer treatment do not cross the blood-brain barrier, however, oxidative damage is still observed. This research focused on how the chemotherapy drug Doxorubicin generates large amounts of reactive oxygen and nitrogen species in the blood, which causes a rise in the levels circulating tumor necrosis factor (TNF)-□, which can cross the blood-brain barrier and inevitably result in oxidative damage to neurons, mitochondrial dysfunction, and cell death.

31 IMPACT OF SIMULTANEOUS DRUG USE ON CYTOCHROME P450 METABOLISM AND STABILITY

Chia-Hsuan Shen, Junior, Chemistry, University of Kentucky
Catherine Denning, Chemistry, University of Kentucky
David Heidary, Chemistry, University of Kentucky
Edith Glazer, Chemistry, University of Kentucky

Abstract:
Prescription opioid use has become a major epidemic in the United States, resulting in 64,000 deaths per year from accidental overdose. A majority of drug overdoses result from the simultaneous use of multiple drugs (National Institute on Drug Abuse, 2018).
Cytochrome P450s (CYPs) are enzymes mostly present in the liver and are responsible for xenobiotic degradation, as approximately 75% of medications on the market rely on CYPs for metabolism. Therefore, the study of CYPs is essential for drug development and understanding multidrug interactions. In our lab, we are using P450BM3 as a model for human CYP metabolism of nicotine and dextromethorphan. Unlike other CYP's, P450BM3 is soluble, easily purified, and does not require a reductase partner for electron transfer making catalysis more efficient. We hypothesize that when CYPs are confronted with combinations of substrates, a change in products may occur. We believe that when nicotine is metabolized in the presence of dextromethorphan, the product profile will be modified. Therefore, we will be determining the product profile of nicotine and dextromethorphan. We will then test them in combination by using high-pressure liquid chromatography (HPLC) and gas chromatography mass spectroscopy (GCMS). We will also be testing if these drugs impact enzyme stability by examining degradation of the global structure with pulse proteolysis. Preliminary results have shown that in combination with dextromethorphan, nicotine metabolism is drastically decreased.

32 RAMAN-BASED IMAGING FOR CHARACTERIZING SILVER NANOPARTICLE-MINERAL INTERACTIONS

Janice Sikon, Senior, Chemistry, Wright State University
Seth Brittle, Chemistry, Wright State University
Daniel Foose, Chemistry, Wright State University
Kevin O'Neil, Chemistry, Wright State University
Jasmine Johnson, Chemistry, Wright State University
Adam Stahler, Chemistry, Wright State University
John Ryan, Chemistry, Wright State University
Steven Higgins, Chemistry, Wright State University
Ioana Sizemore, Chemistry, Wright State University

Abstract:
Silver nanoparticles (AgNPs) currently represent over 54% of the total number of consumer products containing nanomaterials, mostly exploiting their unique antimicrobial properties. However, little is known about AgNPs released into the environment through irrigation and rainfall and their interactions with one of the major components of soil (~45%), minerals. The main goal of this study was to develop a label-free or label-enhanced micro-Raman-based mapping method for imaging the distribution of AgNPs on various mineral surfaces and their potential molecular interaction mechanisms. This new methodology was successfully tested on a) two macro- and micro-sized mineral models, muscovite [KAl2(AlSi3O10)-(OH)2] and corundum (α-Al2O3), and b) two positively and negatively charged AgNPs models, under key environmental conditions (ionic strength and pH). Collected Raman maps (n = 625-961 spectra each) were rapidly analyzed using well-established chemometric methods in Vespucci, a free open-source software developed by our group, and the Raman results were confirmed by ICP-OES, AFM, and SEM-EDX. Covalent interactions through the formation of Ag-O-Al- bonds were detected in a label-free manner for both AgNPs+ and AgNPs-, when exposed to corundum minerals (pHpzc = 9.1), thereby potentially reducing the environmental mobility of these AgNPs. No molecular interactions were identified in between AgNPs- and muscovite in the label-free Raman approach; thus, label-free Raman imaging was developed for mapping the scarce spatial distribution of AgNPs- on such mineral surfaces. The proposed Raman-based imaging requires minimum to no sample preparation; is sensitive, noninvasive, cost-effective; and might be extended to other environmentally relevant systems or other metallic nanoparticles.

33 DENSITY FUNCTIONAL THEORY INVESTIGATIONS OF THE OPTOELECTRONIC PROPERTIES OF ORGANIC CHROMOPHORES FOR LIGHT-EMITTING APPLICATION

William Smith, Senior, Chemistry, University of Kentucky
Sean Ryno, Chemistry, University of Kentucky
Chad Risko, Chemistry, University of Kentucky

Abstract:
Organic electronic materials have been of academic and industrial research interest given their compatibility with technologies where traditional inorganic semiconductors cannot be used. Here, we make use of density functional theory (DFT) and it's time-dependent (TDDFT) analog to explore the electronic and optical characteristics of π-conjugated chromophores that are of interest for light-emitting applications. Specifically, we have focused on two chromophore classes: 1) carbazole-based molecular materials that are of interest as hosts in light-emitting diodes, and 2) extended acene-like structures that demonstrate liquid-crystal behavior. The DFT and TDDFT results provide atomistic-scale details behind the materials electronic, redox, and optical response. This project is providing key details that, in collaboration with synthetic chemists, is leading to new design platforms for molecular materials.

34

REACTIVITY OF REDOX-ACTIVE CP*IR(TSDPEN) CATALYST: O–H BOND ACTIVATION OF CARBOXYLIC ACIDS

Kristen Sportiello, Sophomore, Chemistry, University of Evansville
Todsapon Thananatthanachon, Chemistry, University of Evansville

Abstract:
Metal complexes containing redox-active ligands such as Cp*Ir(TsDPEN) (TsDPEN = Tosylated-diphenylethylenediamine) have been demonstrated as active catalysts for transfer hydrogenation reactions where hydrogen donor alcohol undergoes O–H bond activation to yield a metal hydride via a formation of metallacycle intermediate. To prove this mechanism, we study the reactivity of the redox-active Cp*Ir (TsDPEN) catalyst with various carboxylic acids such as benzoic acid. As anticipated, carboxylic acids undergo O-H bond activation across the Ir center and the TsDPEN ligand to yield novel Cp*Ir(carboxylato) (TsDPEN-H) products. which have been characterized by NMR spectroscopy as well as single crystal X-ray diffraction.

35 TRANSFER HYDROGENATION OF UNSATURATED COMPOUNDS WITH NOVEL COBALT (PNP) AND NICKEL (PNP) PINCER CATALYSTS

Nicholas Stafford, Junior, Chemistry, University of Evansville
Phong Thai, Sophomore, Chemistry, University of Evansville
Todsapon Thananatthanachon, Chemistry, University of Evansville

Abstract:
Hydrogenation, a crucial process in many industries, is mainly relied on the use of explosive hydrogen gas. Therefore, alternative hydrogen sources that are less dangerous such as alcohols have been employed. This study utilizes six different earth-abundant Co and Ni metal-pyrrole (PNP) pincer catalysts in the transfer hydrogenation of various unsaturated compounds containing a C=O bond using isopropanol as the hydrogen donor. The synthesis of the catalyst and insights toward catalytic cycles will be presented.

36 COMPARING DNA CONDENSATION AND RELEASE BY ACETYLATED AND SUCCINYLATED POLYETHYLENEIMINE (PEI) DERIVATIVES

Kyle Starkey, Senior, Chemistry, University of Kentucky
Joseph Duke III, Chemistry, University of Kentucky
Jason DeRouchey, Chemistry, University of Kentucky

Abstract:
Polymeric materials provide attractive scaffolds for the creation of supramolecular bioconjugates for the delivery of nucleic acids, but typically lack the efficiency and biocompatibility to be clinically relevant. To address both issues, derivatives of branched polyethylenimine (bPEI) via acetylation or succinylation of primary and secondary amines were synthesized. Acetylated PEI (acPEI), reduces the protonation properties of the polymer by neutralizing some of the amine charge while succinylated PEI (zPEI) introduces zwitterionic character to the polymer. Characterization of polymer/DNA interactions revealed that the presence of acetyl and succinyl groups decreased buffering capacity in both systems and polyplexes dissociated in the presence of lower amounts of a competing counter-anion compared to unmodified PEI. Packing density was also investigated for acPEI/DNA and zPEI/DNA using small-angle X-ray scattering (SAXS). Overall, the data suggest that the increased gene delivery activity may be attributable to an appropriate balance between polymer buffering capacity and strength of polymer/DNA interactions. At comparable degrees of amine modification, zPEI shows amplified effects for both buffering and modified interactions with DNA than acPEI. These polymers are currently under investigation for their abilities to transfect cells both out of and in serum.

37 COMPUTATIONAL STUDY OF SINGLET FISSION MECHANISM IN SOLID STATE ACENES USING CASSCF

Brandyn Thompson, Senior, Chemistry, University of Kentucky
Chad Risko, Chemistry, University of Kentucky
Sean Ryno, Chemistry, University of Kentucky

Abstract:
Singlet fission is the process by which a singlet excited state transforms into two, uncorrelated triplet states. This process is important in solar cell materials because one photon can yield double the amount of charge carriers. In this computational study, materials known to exhibit singlet fission are examined to study the singlet fission mechanism. The ground states and singlet and triplet excited states for monomers and dimer and trimer complexes of pentacene, TES-pentacene, and TIPS-pentacene were explored using the CASSCF method. Natural orbital analyses were carried out to study the frontier orbitals of each system and MP2 calculations were run to find energies of each system. In addition, the influence of the packing of these materials on the electronic coupling in the solid state was studied as a function of orbital overlaps in two theoretically constructed dimer systems. This study can provide atomic scale intuition for the design of new singlet fission materials.

38 THE ROLE OF NUCLEAR CALCIUM-MEDIATED TRANSCRIPTION IN DYSREGULATION IN CARDIAC MYOCYTES

Darin Vaughan, Senior, Chemistry, Morehead State University
Dr. Pete Kekenes-Huskey, Chemistry, University of Kentucky

Abstract:
Disorganization of the normally highly-regular transverse tubule network in cardiac ventricular myocytes is among the most apparent morphological changes in many models of cardiomyopathy.
Frequently, this disorganization correlates with impaired Ca2+ homeostasis, which motivates inquiry into relationships between TT (transverse-tubule) configuration and regulation of Ca2+ -mediated excitation-contraction coupling.
In this study, we characterize the extent and manner by which TT remodeling develops in hyperamylinemic (HIP) rats.
Second, we investigate the extent to which calcineurin, a protein implicated in the activation of pro-remodeling genes, co-distributes with the TT network and moreover, whether this distribution influences calcineurin Ca2+ -dependent activity.
Our data suggest that TT remodeling may present in HIP rats, that calcineurin aligns with the TT network and higher diastolic Ca2+ load predicted in HIP rats may prime IP3 receptor-mediated Ca2+ release.
Altogether, these findings support relationships between myocyte intracellular structure and the propensity to activate remodeling pathways implicated in cardiac failure.

39 THIOBARBITURIC ACID TEST FOR RATES AND LEVELS OF SATURATED, MONOUNSATURATED, AND POLYUNSATURATED DIETARY TRIGLYCERIDE OXIDATION

Anna Verlander, Senior, Chemistry, Transylvania University

Abstract:
The structure and saturation of fatty acids determines function within the body, as well as readiness and rate of oxidation. Oils were oxidized under controlled conditions to compare oxidation rates of saturated lauric acid from coconut oil, monounsaturated oleic acid from olive oil, omega-3 polyunsaturated EPA and DHA from fish oil, and omega-6 polyunsaturated linoleic acid from soybean oil. Whole oils were used rather than isolated acids in order to observe oxidation rates in whole food sources, rather than as a fatty acid isolate. The desired fatty acids made up approximately 50% or more of the total fat composition of the respective oils. Vitamin E (a common fat soluble antioxidant which prevents the formation of reactive oxygen species when fatty acids undergo oxidation (8)) was added to one treatment to observe whether or not this would slow rates of oxidation. After periods of one week, and two weeks with an hour of heating; malonaldehyde (a secondary oxidation product of fatty acids) concentrations were measured for all samples with the use of a thiobarbituric acid test. Polyunsaturated fatty acids showed the greatest oxidation rates, followed by saturated lauric acid, and finally monounsaturated oleic acid. While these rate differences were significant, different oils started with different oxidation levels (drastically different in the case of fish oil), and oxidation rate did not necessarily determine highest levels of oxidation after the full experimental period. Vitamin E effectively lowered rates of oxidation for all oils, but effectiveness varied with different fatty acids.

40 ACTIVATION LEVELS OF MTOR PATHWAY OVER TIME IN PINK1 KO RAT MODEL OF PARKINSON DISEASE

Eric Vogt, Senior, Chemistry, University of Kentucky
D. Allan Butterfield, Chemistry, University of Kentucky

Abstract:
Parkinson disease is neurodegenerative disease that is characterized by the death of dopaminergic neurons in the substantia nigra. The loss of these cells leads to problems controlling movement and balance and can eventually cause cognitive problems. The PINK1 knockout model is used as a rat model for Parkinson disease. The PINK1 gene codes for a protein kinase that primarily serves to mark damaged or dysfunctional mitochondria for degradation. This gene is knocked out to test its effect on the levels of activation of specific proteins in the mTOR pathway. The mTOR pathway is extremely important due to the role the proteins play in autophagy and insulin resistance. The activation levels of the proteins in this pathway were found using the ratio of phosphorylated to non-phosphorylated proteins. This was determined by the intensity of the bands on the Western Blots, which was the primary method utilized. In order to find out how the levels of activation vary at differing ages the PINK1 KO rats were sacrificed at two, four, six and eight months of age. Beclin 1, MAPLC3B, and IRS-1 were the three proteins that were investigated. All three of these proteins showed an increase in activation between the two and four month samples. Both Beclin 1 and MAPLC3B are involved in autophagy, so it makes sense that they follow the same general trend. These two proteins showed a significant decrease in the activation levels between the four and six month samples, followed by an increase in activation levels between the six and eight month samples. IRS 1 is deactivated by phosphorylation, so it follows the same trend as the other two proteins, but it is reversed. This means that there is a significant increase in activation levels between the four and six month samples, and then a decrease between the six and eight month samples. These results help give insight into how the activation levels of the proteins in the mTOR pathway vary with age in the PINK1 KO rat model of Parkinson disease. The mTOR pathway has been shown to be over activated in Alzheimer disease, so the hypothesis is this will also be the case in Parkinson disease. It is also hypothesized that there will be a correlation between age and activation levels. If this is the case it will further the knowledge of the disease and hopefully lead to a better treatment.