



NCUR 2021 Proceedings

A Brief Synopsis of the Synthesis and Characterization of Rhodium-Aluminum and Iridium-Aluminum Heterobimetallic Complexes Bridged by 5-Hydroxyquinoline

Chemistry - Time: Tue 3:30pm-4:30pm - Session Number: 711

Michael Chaney, Natalie Taylor, Ray Charles, and Dr. Timothy Brewster, Department of Chemistry, University of Memphis, 3720 Alumni Avenue, Memphis TN 38152

Michael Chaney Jr.

This project is aimed to serve as an intermediate step towards the final goal of creating a heterobimetallic complex capable of tunable catalysis. We aim to determine if the reactivity of the transition metal of interest can be modulated by adjusting the electrochemical activity, or oxidation state, of an attached redox active aluminum complex.

The molecule to be used towards either proving or disproving this theory will be a heterobimetallic complex consisting of Vaska's Complex and Graves' Complex, graciously provided by the Graves' Group of Swarthmore College, bridged by 5-Hydroxyquinoline. Vaska's Complex does not possess any noteworthy characteristics as a catalyst, but the complex serves as an excellent placeholder due to its consisting of either Rhodium or Iridium as its transition metal center, and its Carbonyl group. The carbonyl group is especially of interest due to its ability to be utilized as a measurement of electrochemical activity by method of Infrared Spectroscopy. If changes can be observed regarding the relative placement of the IR Spectra peak associated with the Vaska's Complex Carbonyl, a change in electrochemical activity can be inferred. The Graves' Complex will serve as the site of oxidation in this instance, with the Vaska's Complex serving as a placeholder for the catalyst portion of the complex. The heterobimetallic complex of interest has been synthesized, but further research will be necessary for testing to commence. The first method of synthesis had poor yields, with an excess of starting materials being noted in the mass spectra. As a result, new methods are being explored to bring about the synthesis of the desired heterobimetallic complex. This presentation will explore the first methodology utilized towards the Synthesis of the complex of interest, the current methods being explored, and the future of this project.

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Aerosols and Particulates Emitted while Speaking and Singing

Mechanical & Industrial Engineering - Time: Tue 3:30pm-4:30pm - Session Number: 737

Eric Alan Pillow, Dr. Jeff Marchetta, Department of Mechanical Engineering, University of Memphis - Herff College of Engineering, 3720 Alumni Ave., Memphis TN 38152

Eric Pillow

The COVID-19 pandemic is significantly impacting professional practices such as dentistry, speech pathology, and music education as well as avocational practices such as athletics and other extracurricular activities because they typically involve close, face-to-face contact. A major obstacle these activities face is the transmission of disease due to aerosolized particles emitted from the oral cavity while breathing, speaking, and singing. Modifications to the basic procedures for these activities must be made such that they follow new, safe practices if they are to continue in the future. A lack of data exists concerning the extent of exposure to aerosolized particles in relevant scenarios. This data is necessary to inform the new, safe practices that will enable many activities, from professional to amateur, to resume operation. This research aims to meet this need by investigating the quantity, concentration, and distribution of particles exhaled while speaking, singing, and breathing. To accomplish this, specific vocal exercises and activities will be performed in the laboratory to generate the airborne droplets associated with each activity. Images of these particles will be captured using a 1200 frame-per-second optical camera and a high-power laser, then analyzed numerically using computer software. The resulting data sets will be compared to draw conclusions about the volume and behavior of aerosolized particles associated with various vocal activities. Before data collection with participants, initial findings support the hypotheses that the number and distribution of particles emitted vary based on the vocal exercise being performed and the person who is performing it. Once more data is collected, correlations can be drawn between vocal activities, an individual's physiology, and the inherent exposure risk of specific scenarios. This could prompt future investigations into suggestive patterns that are uncovered and the effectiveness of risk mitigation in light of new knowledge.

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Assessing Cortical Dopamine Transmission in a Genetic Rat Model of ADHD

Psychology - Time: Wed 1:30pm-2:30pm - Session Number: 6551

Author: Carina Hicks Faculty: Dr. Deranda Lester and Dr. Helen Sable Department: Psychology

Institution: The University of Memphis, 3720 Alumni Ave, Memphis, TN 38152

Carina Hicks

Attention-Deficit Hyperactivity Disorder (ADHD) is characterized by symptoms such as inattention, hyperactivity, and compulsive behavior. ADHD has a strong genetic basis, as heritability is associated with 70-80% of child ADHD cases and 30-40% of adult cases. Identifying specific genetic causes can help identify genetic risk and vulnerable populations while also shedding light on neural alterations underlying ADHD symptoms. Recent clinical studies have identified the LPHN3 gene as a candidate, and rats with this gene knocked out have shown to be more impulsive. Given that dopamine transmission in the PFC is often altered in ADHD, the proposed study aims to assess the neurochemical functioning in the PFC of LPHN3 knockout rats. Specifically, we will use in vivo fixed potential amperometry to quantify PFC dopamine release before and after administration of the dopamine agonist nomifensine, which functions similarly to commonly prescribed ADHD medications. We hypothesize that LPHN3 KO rats will exhibit hypodopaminergic transmission, with lower percent changes following nomifensine administration, relative to wildtype control rats. The results of the proposed study will improve understanding of the role the LPHN3 gene plays in neural development, particularly related to pathologies associated with ADHD.

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Assessment of Methacrylated Chitosan Hydrogels for Local Delivery of Simvastatin

Engineering - Time: Tue 5:00pm-6:00pm - Session Number: 822

Emily Coleman, Hengjie Su, Karla Cisneros, Naisha Chowdhury, Dr. Tomoko Fujiwara, Dr. Joel D. Bumgardner, Dr. J. Amber Jennings, Departments of Biomedical Engineering and Chemistry, The University of Memphis, 201 Engineering Administration Building, Memphis, TN 38152
Emily Coleman

Local delivery systems are considered useful for tissue regeneration after musculoskeletal trauma. The anti-cholesterol drug simvastatin (SMV) has been shown to promote bone healing, but it needs a delivery system for optimal activity. Hydrogels are a potentially effective option for tissue regeneration scaffolds because they can resemble the chemical properties of the natural cell environment. Taking this into consideration, we tested 3D-printed chitosan (CS)-based and polylactide (PLA)-based hydrogels, with varying ratios and concentrations, to determine their capabilities in delivering substances promoting tissue regeneration, while being biodegradable and providing support for cell ingrowth. These studies included tests to assess mechanical compressive load, SMV release through HPLC testing, and cell viability through cell staining and imaging of NIH3T3 fibroblasts in direct contact. The mechanical testing showed a range of strength for the different types of hydrogels with the group that contained the least amount of water having the highest compressive load (PLA: 6.22 N, CS: 5.72 N) and the group containing the most water having the lowest compressive load (PLA: 1.82 N, CS: 1.93 N). The HPLC testing produced similar releases between groups, with an initial 5% release of SMV followed by a slow linear release that was assessed for 3 weeks, with total release over 3 weeks being less than 15% of the loaded amount. The cell viability tests were performed and revealed that the hydrogels are biocompatible and promote cell growth. This research supports the claim that 3D-printed hydrogels are effective options for local delivery systems.

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Evaluating the Effect of Flavonoids on Neutrophil NETosis

Engineering - Time: Tue 5:00pm-6:00pm - Session Number: 822

Author: Kian Ziai Faculty Mentor: Dr. Gary Bowlin Department: Biomedical Engineering Institution: University of Memphis Institutional Address: 3817 Central Ave, Memphis, TN 38111
Kian Ziai

Honey is a natural product that has been used from ancient times to assist with improving human health and contains an important component flavonoids. Research has demonstrated the anti-inflammatory effects of honey on neutrophil behavior. As noted, the flavonoid component of honey contributes to its anti-inflammatory effects. This component serves an important role in which it neutralizes free radicals, I.e. reactive oxygen species (ROS) created during inflammation and implicated in tissue damage. Neutrophils constitute the first line of defense of innate cellular immunity. At the formation of a wound or implantation of a tissue engineering template, neutrophils flood the wound site and carry out several inflammatory activities. including NETosis. Excessive NETosis on the template surface is non-ideal because it is correlated with fibrosis around a tissue engineering implant site which is considered a foreign item and is not desirable. The purpose of this study was to investigate the ability of several flavonoids commonly found in honey to reduce the degree of neutrophil. Previous data collected demonstrates that Manuka honey reduces neutrophil NETosis within a therapeutic window. I investigated whether this reduction in NETosis is due to the honey's flavonoid component, and, if so, intended to find the ideal concentration and combination of flavonoids for reducing this NETosis response. We also investigated the ability of these flavonoids along with a MPO-inhibitor also found in Manuka honey, methyl syringate, to reduce neutrophil NETosis on tissue culture plastic. Based on several experiments using dHL-60's and neutrophils, Chrysin was the flavonoid that resulted in the greatest reduction of NETosis. This work is a promising step on the path towards the goal of regulating excessive neutrophil inflammation and its many downstream pathologies throughout the body.

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Evaluation of G Protein Coupled Receptor Interaction Fingerprints in Docking Protocols

Chemistry - Time: Tue 3:30pm-4:30pm - Session Number: 711

Lindsey N. Baker, Makenzie C. Griffing, Dr. Daniel L. Baker, and Dr. Abby L. Parrill, Department of Chemistry, University of Memphis, 3744 Walker Avenue, Memphis, TN 38152

Lindsey Baker

G Protein coupled receptors (GPCR) are important drug targets for many diseases. Computational modelling is an important tool for studying GPCR, though current software and protocols have limitations. To investigate the accuracy of current docking protocols, known ligand-GPCR crystal structure pairs were docked (self-docking) or ligands crystallized in a protein were docked into other crystal structures of the same protein (cross-docking). When GPCR have a known crystal structure, a root mean square deviation (RMSD) can be calculated to quantify how docking poses differ from the known crystal structure. This research investigated whether GPCR family-derived interaction fingerprints could be used to define a binding site for ligand docking to improve docking approaches. The purpose of optimizing RMSD in docking trials with known crystal structures is to apply the optimized protocols to identify potential ligands for GPCR (including those that lack known crystal structures). Fingerprints were compiled of residues often found to be involved in ligand binding across the GPCR family, one frequency based (fingerprint A) and one with an additional energy cut-off (fingerprint B). Docking of each crystal structure-ligand pair was done three times, each allocating the docking site differently, using the Molecular Operating Environment (MOE) Site Finder, fingerprint A, or fingerprint B. Following docking, RMSD values were calculated comparing the top 400 poses for each docking job to the associated crystal structure in RCSB PDB. Analysis between site allocations focused on the lowest RMSD pose within the top 400, or the top 5 scoring poses, or those within 0.5 kcal of the top scoring pose. Using GPCR family-derived interaction fingerprints to define binding sites produced lower RMSD values within the top 400 poses, however certain GPCRs still lack acceptable poses (RMSD less than 3Å), suggesting that fingerprints for GPCR subfamilies may be necessary to allow for more accurate docking.

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Examining the Effect of Kratom on Dopamine Transmission Related to Abuse Liability

Psychology - Time: Wed 12:00pm-1:00pm - Session Number: 947

Lindsay Ringer, Paul Manus, Dr. Deranda Lester - Department of Psychology The University of Memphis Department of Psvchology 400 Innovation Drive Memphis. TN 38152

Lindsay Ringer

Mitragyna speciosa Korth (*M. speciosa*) is a tree primarily found in regions of southeast Asia, Philippines, and New Guinea. *M. speciosa* is commonly referred to as kratom and is currently legally available for purchase over the counter in most of the US. In other countries such as Thailand and Malaya, Kratom has been used traditionally to treat intestinal infections, diarrhea, fever, pain, morphine dependence, and opium substitute. Mitragynine (MG) is the main psychoactive alkaloid accounting for 66% of the total alkaloid contents extracted from kratom leaves. Clinical reports have shown that lower doses of kratom result in stimulant-like effects, while higher doses result in opioid-like effects. However, little is known about the abuse liability of kratom. Drugs with a high abuse liability either directly or indirectly increase extracellular dopamine in the mesolimbic pathway, specifically in the nucleus accumbens (NAc). To determine the potential abuse liability of kratom, we used in vivo fixed potential amperometry to measure real time dopamine release in anesthetized mice before and after administration of MG (1, 15, or 30 mg/kg, i.p.) or vehicle (control). Results suggest that MG administration did alter dopamine release patterns over the 90 min recording period, with low dose MG resulting in more dopamine release over time compared to vehicle and the other MG groups (medium and high doses). However, analyses at specific time points revealed no significant dopamine release differences between any groups. The findings indicate that MG does not alter dopamine release in the same way that is observed with typical drugs of abuse, suggesting kratom may not have the abuse liability problems that are associated with dopamine agonists. These findings could have major impacts on public health if kratom proves to be a useful substitute for opioid medications with little risk of addiction.

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Experimental Validation of Structure-Based Pharmacophores: Toward a High-Throughput Screening Tool for GPCR Ligand Discovery

Biochemistry - Time: Tue 2:00pm-3:00pm - Session Number: 602

Martin Guerrero, Gregory L. Szwabowski, Kristie R. Ruddick, Daniel L. Baker, and Abby L. Parrill,
Department of Chemistry, University of Memphis, 101 Wilder Tower, Memphis TN 38152
Martin Guerrero

A powerful tool in drug discovery is the pharmacophore; a model that approximates key steric and electronic features necessary for optimal ligand-target interaction and hence drug-induced biological response. Using molecular modeling techniques, our group has developed a protocol for generating structure-based pharmacophores via feature annotation of energetically optimized chemical functional group fragments. Generated pharmacophores can then be used to search compound databases containing millions of drugs to elucidate candidate active ligands for a target, the results from which can be further analyzed to identify a set of potential novel therapeutic drugs for experimental validation. This work will include background and rationale for the cell-based assay systems; we will use to validate the model and test the druglike features of computationally predicted hit list compounds. We will first test the model using the well-known dopamine D2 receptor as proof-of-principle. The D2 receptor is a well-studied G protein-coupled receptor (GPCR) that signals via the interaction between the receptor in the cell membrane and the G α i G-protein subunit to inhibit adenylate cyclase and trigger a cellular response involving downstream effectors (2nd messengers) such as cyclic AMP (cAMP), calcium ions (Ca $^{2+}$), and ERK (MAP kinase). We have found cell-based assays designed to monitor various 2nd messengers problematic due to the complex nature of engineered mammalian cell line-based host cells which contain thousands of endogenous GPCR and other receptors; thus, no true null live cell-line exists. For this reason, we will screen drug candidates for the D2 receptor using the NanoLuc-based complementation assay (Promega) which is independent of cellular interference. NanoLuc is an engineered luciferase from the deep-sea shrimp, *Oplophorus gracilirostris*, and this technology can monitor the interaction of the receptor with specific G-proteins and has been proven effective as a high-throughput screening tool.

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Exploring Undergraduate Biology and Chemistry Students' Understanding of Enzymes

Education - Time: Tue 2:00pm-3:00pm - Session Number: 4517

Emma Micer, Nathan DeYonker, and Jaime L. Sabel, Department of Biological Sciences and Department of Chemistry, University of Memphis, 3720 Alumni Ave, Memphis, TN 38152.

Emma Grace Micer

Student understanding of enzymes in introductory biology and chemistry courses tends to be superficial, and students often lack the ability to visualize enzyme interactions. When students begin taking bioorganic chemistry, they are often blindsided by the level of detail regarding enzymes. Using Dr. Nathan DeYonker's NSF CAREER grant funded web interface, the Residue Interaction Network-based Residue Selector (RINRUS) software, we created an assignment to enhance student understanding of enzyme structure and substrate interactions to address our goal of increasing long-term retention. In this assignment, students find enzymes within the Protein Data Bank and read the associated literature for information about substrate interactions. Students are then tasked with inserting the 3D structure file into the RINRUS website, which allows students to view this complex in many forms.

We conducted a pilot study in a graduate chemistry class to test the effectiveness of the assignment. Following completion of the assignment, we conducted interviews to view their experiences and to evaluate what changes should be made to adapt the assignment for introductory Biology lab courses.

We also began surveys and interviews of students in General Biology I and General Chemistry I and II. Students were asked to explain what an enzyme is and knowledge about structure and function. We analyzed these surveys and interviews by comparing answers to the content of their lectures to determine what information was learned and retained. Through analysis of the data collected from the undergraduate students, it became clear that most students understood the basic function of enzymes, such as acting as catalysts by lowering the activation energy. However, most students had difficulty explaining the concept of protein-substrate interactions. Undergraduate and graduate student feedback will allow us to make changes before presenting the RINRUS assignment to introductory Biology students, which we anticipate will enhance student understanding of enzymes.

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Exposure to a Pandemic: Effects of Telehealth Acceptance

Global Health - Time: Tue 3:30pm-4:30pm - Session Number: 5092

Morgan Gullett, Ji Wan Son, and Dr. Cheryl Bowers Ph.D., Department of Psychology, University of Memphis - Lambuth, 705 Lambuth Blvd, Jackson, TN 38301.

Morgan Gullett

Field (1996) found the use of information and telecommunication technologies to provide and support healthcare, when distance separates the participants, has been receiving increasing attention for a while now. According to a J.D. Power study on Telehealth Satisfaction, before the recent outbreak of COVID-19, only about 10% of healthcare consumers were using Telehealth services (Effler, 2019). While there are several studies that test how effective Telehealth is, there have been few studies to see how a pandemic will affect the acceptance of this technology. The current study sought to fill this gap, hypothesizing that exposure to a pandemic, COVID-19, will increase acceptance of Telehealth. 127 participants completed the Telehealth Study survey at pre-test, while only 50 returned to complete it again in the post test period. Of those, 25 participants fully completed both assessments and were used in our analysis. At both pretest and posttest, participants completed assessments to measure acceptance of Telehealth, knowledge of technology, and involvement with COVID-19 knowledge and precaution. The interaction between Telehealth acceptance and pretest COVID-19 involvement was significant. The interaction between Telehealth acceptance and posttest COVID-19 involvement was also significant. The data shows that while Telehealth acceptance did not significantly increase from pre to post test, the level of COVID-19 involvement of each participant has an effect on their acceptance of Telehealth.

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The Effects of Musical Nuances on Cognition

Psychology - Time: Wed 1:30pm-2:30pm - Session Number: 6586

Wesley Roberts and Dr. Gina Caucci, Department of Psychology, University of Memphis, 3720 Alumni Ave, Memphis TN 38111

Wesley Roberts

Previous research has found contradictory evidence regarding the effects of music on spatial ability, while largely ignoring important contributing factors of musical complexity and musical training. The purpose of this study is to establish conclusive evidence of the effects of music on spatial ability. Furthermore, this study aims to properly operationalize musical complexity while also furthering the evidence that musical complexity and musical training significantly increase an individual's spatial ability. Participants will consist of university students that differ on their amount of musical training. Participants will listen to musical pieces of varying complexities defined by the musical difficulty grading scale utilized by various states and composers. Participants will then complete several trials of a virtual mental rotation task to measure the concept of spatial ability. It is hypothesized that participants will exhibit improved spatial ability after listening to high musical complexity music and that participants with musical training will exhibit greater spatial ability over participants with no musical training. The potential implications for this research include defining musical complexity, providing support for the hypothesis that music enhances spatial ability, and furthering the research that musicians have greater spatial ability compared to people with no musical training. With the expected outcomes, we could provide supporting evidence that both musical complexity and musical training have positive influences on cognitive processes.

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Visual Imagery: Comparing Object & Spatial Working Memory

Psychology - Time: Wed 1:30pm-2:30pm - Session Number: 6615

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The condition of aphantasia is the absence of visual imagery. Individuals who have aphantasia may have

difficulty voluntarily generating visual images. Researchers found that individuals with aphantasia reported significant reduction in sensory stimulation across a range of mental processes (Dawes et al., 2020). Individuals with aphantasia have consistently reported below average visual OWM (object working memory) scores (Bainbridge et al., 2019; Jacobs, Shawarzkopf, & Silvanto, 2018; Keogh & Pearson, 2018). However, those same researchers have found differing results on spatial working memory suggesting the need for future research. We hypothesize that college students with weaker visual imagery vividness will perform better on a SPW task than on an OWM task. 47 college students completed three online assessments. The Mental Rotation Assessment is a 10-item multiple choice assessment that measures ability to mentally rotate representations of three-dimensional in OWM. The OWM assessment measures short-term memory using object recognition, where participants are shown 15 simple line drawings of objects and then identify those 15 of 30 objects. The Vividness of Visual Imagery Questionnaire consists of 15 questions that explore how vividly a person can see mental images. Paired t tests found no significant differences between mental rotation scores and OWM scores for either the low visual imagery group ($t(11) = .62, p = .55$) or the high visual imagery group ($t(29) = -.57, p = .57$). A one-way MANOVA found no significant differences between the low and high groups on either test. However, there was a bigger discrepancy between mental rotation scores and OWM scores for those in the low visual imagery group than those in the high group. While there was no significant difference, the low group performed much more poorly on the OWM test than the mental rotation test, which is in the direction we predicted.

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