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HyperLynx

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Abstract:
Hyperlynx is a multidisciplinary project which includes students from both the University of Colorado Denver and Metropolitan State University. The ultimate goal of the project is to build a high-speed, vacuum-compatible electric vehicle and take part in the 2019 SpaceX Hyperloop Pod Competition. Over 200 teams from around the world submitted an intent to compete. In February 2019, Hyperlynx was selected by SpaceX as one of 21 finalists worldwide.

The 2019 pod design followed the philosophy of "Steamline and Execute". To be selected, teams need to prove that their design was not only innovative, but also achievable. By streamlining the 2019 design and focusing on execution during manufacturing, the team has put together what will hopefully be the fastest American vehicle. The pod uses a 100kW (135hp), 240N-m (177ft-lb) electric motor to propel itself to 396 ft/s (270mph). The competition happens in a 4150ft (1.25km) tube which is capable of evacuating atmosphere to 1/100th 'normal' atmospheric pressure. This near-vacuum condition requires the pod to be autonomous. Autonomy is achieved via a State Determination Algorithm (SDA) fed by a network of sensors and crew inputs. In order to reach top speed and stop safely within the allotted distance, the braking system will create a 7g deceleration with twelve spring-actuated, pneumatically-retracted, custom machined brake cylinders. Finally, the 269lb pod is designed to carry a 270lb payload,

proving that the system can scale to achieve the ultimate goal of the Hyperloop; high-speed, long distance transportation for the future.

Can overwintering insects actively limit the energetic costs of warming climates during dormancy?

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Abstract:
Winters are generally becoming shorter and warmer as our climate warms. This poses a risk to organisms that go dormant (e.g., hibernate) during winter, because warmer temperatures generally lead to higher metabolic rate (especially in ectotherms), which in turn depletes energy reserves. We used temperature-controlled laboratory experiments to ask two questions about regulation of metabolic rate in Rhagoletis basiola, a fruit fly native to Colorado that overwinters in diapause (dormancy in insects) and whose metabolism is highly temperature-sensitive: 1) does long-term exposure to warm temperatures lead to active suppression of metabolic rate, 2) do populations at low and high altitudes that experience different temperature conditions exhibit differences in the capacity to suppress metabolic rate?

Suppression of metabolism is a common strategy for energy conservation during diapause, but it is unclear whether and how it might be buffered against temperature changes. Respirometry is a way to measure carbon dioxide production in individual pupae and is a reliable way of estimating metabolic rate. By measuring metabolic rates via respirometry during short- and long-term exposures to warm temperatures, we assessed different strategies that the pupae utilize to mediate diapause metabolic rates. Populations at higher altitudes spend most of the winter under an insulating layer of snow, while those at lower elevations experience greater temperature fluctuations. Therefore, we also tested whether populations sampled from high and low elevations use different modes of metabolic regulation to deal with these different environments.

Proton Transport in E. coli CLC Transport Protein by Adaptive QM/MM Dynamics Simulations

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Chemistry

Faculty Mentor(s):
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Chemistry

Abstract:
The CLC transmembrane proteins are Cl− channels and Cl−/H+ antiporters. Highly conserved in all domains of life, CLCs serve a variety of functions, including high-acid response, controls of cell volume and neural resting potential, and lysosome acidification. It has been established that a prototypical E. coli CLC (EcCLC) transports Cl− and H+ stoichiometrically 2.2:1, but many details are not completely clear for the actual H+ translocation process. Here we apply multiscale combined quantum-mechanical/molecular-mechanical (QM/MM) simulations to study H+ migration via the Grotthuss mechanism through the transmembrane domain of EcCLC. In particular, we employ the novel adaptive QM/MM algorithm, which reclassifies atoms as QM or MM on-the-fly in a continuous and smooth manner during molecular dynamics simulations. This is the first time that adaptive QM/MM is applied to model H+ translocation through a biological channel. Our data suggest that the H+ relay dynamic described by adaptive QM/MM is essentially the same as that revealed by conventional QM/MM, but with potentially much reduced computational costs.

Role of the dorsal striatum in fear extinction and relapse

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Abstract:
The poor long-term success of fear extinction-based exposure therapy is often caused by the relapse of previously extinguished fear. We have established that when activated during fear extinction, the nigrostriatal dopamine (DA) pathway enhances extinction memory and reduces renewal. Although the specific neural circuits attributed to this effect are unknown, their identification could pave way for the development of innovative methods to reduce fear relapse in clinical settings. A target of nigrostriatal DA is the dorsal striatum, which consists of two regions: The dorsomedial striatum (DMS), responsible for goal directed learning, and the dorsolateral striatum (DLS), concerning more inflexible, habitual behaviors. Using a GABAA/GABAB agonist cocktail, we temporarily inactivated the DMS or DLS in adult, male Long-Evans rats during fear extinction to investigate the roles of these regions in extinction

learning and memory. Inactivation of the DLS enhanced fear extinction memory, while inactivation of the DMS reduced renewal. To investigate the involvement of DA, D1 receptor signaling was blocked in either the DMS or DLS during fear extinction. D1 blockade in the DMS impaired extinction retrieval in the extinction context, but the extinction memory remained susceptible to renewal. D1 blockade in the DLS had no effect on extinction memory or renewal. This suggests that the DMS supports context-specific fear extinction through a mechanism involving D1 receptor signaling, whereas fear extinction supported by the DLS is resistant to contextual modulation and fear renewal, but D1 receptor signaling does not contribute to extinction learning in the DLS.

The Piece Between Us; A Video Series on the Israeli-Palestinian Conflict

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History

Abstract:
The purpose of this project is to create a platform where Israeli and Palestinian youth can come together to talk about their differences and find common ground. Through a series of questions, open discussions and personal narratives this video series touches on themes of identity, culture and belonging while simultaneously tackling the issues that have caused great conflict between Israelis and Palestinians for almost a century: Palestinian Refugees and the Right of Return, Israeli settlements in Palestinian territory, the Status of Jerusalem, Terrorism and Violence, and Water Distribution.

This video series was created for anyone struggling to understand their place in the Israeli-Palestinian conflict and anyone who simply wants to educate themselves on the issue. This video series is meant to serve as a symbol of coexistence and aims to break negative social stigmas and stereotypes regarding Israeli and Palestinian collaboration. Ultimately, this project is intended to advocate for a future-focused, inclusive Israeli and Palestinian community.

Quantitative Assessment of Equilibration in Molecular Dynamics Simulations

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Biology

Faculty Mentor(s):
Hai Lin, Professor
Department of Chemistry

Abstract:
Molecular modeling and simulations play an important role in modern chemical research by providing detailed atomic-level descriptions and understanding of the mechanisms and dynamics for chemical processes. Many simulations require the model system to be in equilibrium (a stable state) before the thermodynamic properties (e.g. energy) can be accurately calculated. However, it is not trivial to determine if a system has been properly equilibrated, and many studies only carry out simple qualitative assessments such as visual inspections of the simulated trajectories and/or the plotted time series of thermodynamic variables such as energy and temperature (Grossfield and Zuckerman, 2009). Algorithms for quantitative assessments have been published (Schiferl and Wallace, 1985), but their application has been hindered by the lack of user-friendly computer programs that are freely available. To address this issue, we have developed a program called EquCheck to determine equilibration based on statistical analyses of time series of thermodynamic variables, and we will make it freely available to the scientific research community. Four test-statistics are implemented: the Mann-Kendall test for trend (Bradley, 1968), Shape test for normality (Snedecor and Cochran, 1967), Shapiro-Wilk test for normality (Shapiro and Wilk, 1965), and Von Neumann test for correlation (Hald, 1952). Our code is supplemented by 6 test runs and one user's manual.

The Man Upstairs - Personal and Shared Perspectives, through the eyes of one man

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Film and Television Production

Faculty Mentor(s):
Jessica McGaugh, Professor
Film and Television Production

Abstract:
The Man Upstairs is a short documentary that is meant to raise questions about how we perceive reality. The film follows a man, Roger G. Scott, a quirky landlord who has been employed by a yoga organization for the last 40 years. We follow him and his unconventional life; from his unorthodox living conditions, his daily habits, the contact he has with his family, and his view on the world. Although not successful by common definitions of success that involve material wealth or spiritual development, Roger's view of the world challenges how we view others and how we view success, and as viewers, we are encouraged to think about our own commonly held definitions of the world around them, the effect that a subjective perspective has on them, and the way we think about how reality is perceived and interpreted by shared perception.

Discovering Circular RNAs in Mouse Embryonic Stem Cells via Nanopore Sequencing

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Biology

Faculty Mentor(s):
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Abstract:
While circular RNAs (circRNAs) are a diverse group of non-coding RNAs, there is limited research on their features and functions. The primary objective of this project was to isolate circRNAs from wild-type (WT) and Glycogen Synthase Kinase-3α-/-; β-/- double knock-out (DKO) mouse embryonic stem cells (ESCs). This was innovative research as it was the first time circRNAs in mouse ESCs were studied using Nanopore sequencing technology. Quantitative analysis of data obtained from these experiments showed that 3.0% of total RNA species in WT ESCs were circular, while the amount of circRNAs in DKO ESCs was approximately 1.3% of total RNAs.

Later, isolated circRNAs were sequenced and aligned against the mouse reference genome. Through these processes, numerous genes in the mouse genome were found to form circular RNAs. According to this data, some of the histone genes in mouse ESCs form circular RNAs. Several of these aligned genes have been reported previously to generate circular RNAs, which validated our experimental approach. One of these genes is RPPH1, which has been suggested as a prognostic biomarker for the diagnosis of gastric cancer. In order to confirm the results obtained from Nanopore sequencing, we designed PCR primers for thirteen genes that are predicted to form circRNAs; the primers were designed as to only detect circRNAs. To definitively identify the regions of these genes that form circRNAs, we cloned and sequenced 6 circRNA PCR products. Analysis of the DNA sequencing revealed the nature of these circRNAs genes. In summary, this research concludes that circular RNAs represent a diverse, stable and abundant group of RNA in mouse ESCs.

Equity in the Pre-health Application Cycle: An Analysis of Two Financial Assistance Programs

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Health Professions Program

Abstract:
Two programs offset the costs of applying to medical and dental schools: Fee Assistance Programs (FAPs) provide funds towards entrance exam and application fees for low-income pre-medical/pre-dental applicants; the Bardwell Donachy Family Opportunity Fund (B-D Fund), a CU Denver program, provides funds for interview expenses to committed, diverse and low-income pre-medical/pre-dental/pre-physician assistant (PA) applicants invited to interview. We conducted a mixed-methodology study consisting of a survey administered to CU Denver pre-medical/pre-dental students (n = 112) and one-on-one semi-structured interviews with CU Denver pre-medical/pre-dental/pre-PA applicants (n = 18) to evaluate the effectiveness of FAP and the B-D Fund based on the number of schools one applied to, number of interviews attended and support of underrepresented students in medicine (UIM) (i.e. racial/ethnic minority, first generation, etc). We found no significant difference in the number of MD/DO/PA schools one applied to between applicants who received FAP and applicants who did not receive FAP. After controlling for overall grade point average, Medical College Admission Test score and the number of schools one applied to, receiving the B-D Fund was associated with attending two more interviews, compared to non-recipients. Themes from the interviews included applicants' lack of knowledge of application costs, financial assistance relieving stress but not sufficient for the application process. Both the FAP and B-D Fund were effective in aiding pre-medical and UIM applicants in the application process, but more data is required to assess the effectiveness of these programs for pre-dental and pre-PA students.

Nogales Border Field Research

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Abstract:
The issue of immigration in our country has continued to be an ongoing discussion, the mass militarization at our U.S-Mexico border and the violation of human rights against communities of color raises the question as to why the negative sentiment against immigration and immigrant communities continues to be pushed in today's modern day political agendas. Our study intends to analyze the conditions in which our current political climate have produced statutes and laws in border communities and the implications thereof that in which they have on their populace. Our project raises ethical questions about the morality of immigration policies and border control. The violations of human rights

were apparent with the death and disappearance at the border, privatization of detention centers, border violence, and we evaluated the organization of the border social movement, as well as the relation of immigrants with the United States. At the end of our field research, we determined that the violation of human rights within the border communities and of immigrants continues to happen. The deaths, disappearances, and overall violence targeted at communities who are predominantly living under the poverty line and come from ethnic backgrounds has led to the overall social movement against the border wall and the current political climate.

Sex differences in voluntary exercise

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Psychology

Abstract:
Allowing access to running wheels increases physical activity status in laboratory rodents. The effects of wheel running in rats resembles many of the health benefits of exercise in humans. Current literature focuses on effects of exercise in male rats, thus wheel running behavior in males is well characterized. The goal of our study was to characterize the pattern of wheel running behavior in female rats. Adult, male and female Long Evans rats (n = 64) ran voluntarily in running wheels for 4 weeks. Males displayed a typical pattern of escalation of nightly running distance followed by a plateau occurring around week 3. In contrast, female nightly running distances exceeded that of males. Females also escalated faster; reaching a plateau after 1 week. Female running distances depended on the phase of estrous cycle. Females in proestrus, when levels of ovarian hormones are highest, began running prior to the start of the active (dark) cycle, whereas males and females in other estrous phases began running at the start of the active cycle. Most interestingly, if females were in the proestrus phase during the start of running (day 1 or 2), these females displayed greater running distances on subsequent days compared to females who started running in other phases of the estrous cycle. These data reveal novel sex differences in voluntary wheel running behavior and suggest that ovarian hormones have a profound influence on voluntary exercise. Future experiments can use this knowledge to further investigate sex differences in the effects of exercise.

Development of multiple-particle tracking capabilities for translational research investigating complex biological fluids

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Abstract:
One consequence of chronic pulmonary diseases, such as asthma, is decreased mucociliary clearance (MCC), a critical defense mechanism for protecting the lungs from the injurious effects of inhaled pollutants, allergens and pathogens. These deficiencies lead to accumulation of mucus in higher than normal concentrations on airway surfaces and result in clinically significant events such as airflow obstruction or chronic infections. Preclinical studies show that reduction of mucus viscosity may increase MCC. However, more research is required to determine how mucus production and secretion are influenced by these new therapeutic options. To enable investigators to answer questions about MCC dysfunction in pulmonary diseases, we performed multiple-particle tracking (MPT) experiments that follow fluorescent bead movements in biological fluids, such as mucus, to evaluate the viscoelastic properties of these materials before and after treatment. First, fluorescent plastic beads were treated with a polymer coating (poly (ethylene glycol) to block nonspecific interactions between the beads and the suspending fluids. Measurements show this coating was successfully applied (7.76 nm difference in radius between uncoated and coated beads). Next, videos of coated fluorescent bead movement were collected using an Olympus BX-63 microscope. Then a custom software program was used to combine data from multiple movies, calculate the mean-squared displacement (MSD) of each particle track averaged over time, convert the MSD to a self-diffusion coefficient and substitute the values into the Stokes-Einstein equation to calculate the viscosity of the suspending fluid. Here we showed that the custom program was functional using water as a standard. An average viscosity of 0.84 mPa/s was obtained which is within 10% of the dynamic viscosity of water (0.89 mPa/s). Collectively, these results show that it is possible to use the software written for this project to obtain the viscosity of suspending biological fluids using MPT. Future work will focus on additional verification using mucus samples obtain from animal models before and after treatment.

Japanese Beetles and Bees: Examining Pesticides Recommended by Garden Centers and Stores

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Faculty Mentor(s):
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Geography

Abstract:
Pollinator populations have been under stress due to loss of habitat, infectious mites, food shortages, and pesticides. The Japanese beetle, an invasive species, has been moving into the Denver metro area, drawn to its irrigated landscapes and abundance of ornamental plants. Pesticides are used by homeowners and landscapers to control populations of Japanese beetles. Since Japanese beetles use the same plants as bees, the pesticides the bees take back to the hive can weaken or kill bee colonies. For this study, ten garden centers and stores were surveyed to see what pesticides were recommended for Japanese beetles. The store recommended pesticides were examined against a pesticide listing provided by the Colorado State University Extension Service that notes the toxicity levels of pesticides to pollinators. From the ten garden centers in the Denver Metro area, nine of them recommended pesticides with highly hazardous active ingredients. The most recommended pesticide was Sevin, containing Carbaryl which remains lethal days after application. Only one garden center recommended the non-hazardous biologic, called Milky Spore, which contains no chemicals because it is a bacterium that damages the beetle's digestive tract. These research results suggest that big-box stores are recommending hazardous chemicals for Japanese beetles even though less toxic options exist. Future research by the CU Denver Urban Bee Project will be examining the pesticides in beehives and bee products to determine if there is any link between pesticides used on beetles and the health of the bees.

Attentional Learning: Investigating the effect of intertrial priming on the P300 in visual search

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Abstract:
Current models of attention often refer to a dichotomy of top-down, goal-oriented search, versus bottom-up, salience-based search. Relating these to everyday search tasks, we may look for a specific characteristic or a stimulus may capture our gaze. Moving beyond this dichotomy, there is an interest in a third category of attentional guidance, known as intertrial priming. Priming occurs when the target has a characteristic that repeats from over trials, which decreases reaction time. As targets of the same kind continue to repeat, presumably an expectation builds up that leads to these benefits. If the target switches colors after a run of repeated colors, performance is often worse. Our investigation focused on the novelty that is experienced when a switch occurs after different levels of expectations have been built up. To better understand these priming expectations, electrical signals can be recorded and measured from the head. Event Related Potentials (ERPs) are patterns of spikes in electrical activity across the scalp that occur at very specific times after the display of a stimulus. A common ERP component used to measure novelty is the P300, which is a positivity at ~300 ms after the onset of a stimulus. This P300 changes in intensity or latency when an expectation is not met. Our experiment has examined the effects of priming on the P300 and how they are related to attention in terms of learning. Preliminary results show a negative correlation between RTs and number of repeats with a spike in RT for switch trials.

The Effect of Tablet Size on Cognitive Performance: A Randomized Control Trial Using Caffeine

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Abstract:
Background: A capsule's physical design (e.g. shape, size, and color) affects individuals' perception of drug efficacy. This study aims to objectively assess the effects tablet size may have on participant's performance on cognitive tests. Method: 120 participants were randomly assigned to one of four groups: 5 mm diameter sucrose pillule with/without caffeine; and 1 mm pillule with/without caffeine. After 30 minutes post-pill consumption, participants completed the Stroop test, Trial Making Tests (TMT) A and B, and Rey's Auditory Verbal Learning Test (RAVLT). Results: The main study design was not supported; pill size, caffeine content, nor an interaction between the two factors were associated with significantly different performances across the cognitive tests($p's>.05$). Post-hoc analyses revealed significant differences among the testing appointment times for the RAVLT ($F(2,117)=3.104$, $p<.05$) and TMT-A tests ($F(2,117)=3.180$, $p<.05$). Females also performed better than non-females on the RAVLT ($F(2,117)=4.630$, $p<.05$). Discussion: Future studies may increase caffeine doses or adjust pill designs to more familiar disc shapes to possibly enhance the main effects. The post-hoc analyses showed that time of day created varying performances; with the RAVLT, the 8:00am group did worse than the 9:30am group, but in TMT-A the 8:00am group did better than the 9:30 and 11:00am groups. Most likely, simple visual processing is less cognitively taxing than verbal memory storage. Since college students often take early classes, these results support further research into how time of day influences academic performance. Females performing better on the RAVLT may be due to body mass differences influencing caffeine metabolism.

Understanding IRE1-Dependent Decay in Mammalian Cells

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Faculty Mentor(s):
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Abstract:
The unfolded protein response (UPR) is a highly conserved response to endoplasmic reticulum (ER) stress caused by an accumulation of unfolded or misfolded proteins in the ER. Activation of the UPR resolves to protein homeostasis or apoptosis. Inositol-requiring enzyme 1 (IRE1) is an essential ER transmembrane protein that activates the UPR through its RNase enzymatic activity resulting in its

anomalous splicing of X-box protein 1 (XBP1) mRNA. IRE1 also functions in regulated IRE1 dependent decay (RIDD), where IRE1 cleaves Er-associated mRNAs to maintain cellular homeostasis. RNA fragments produced by IRE1 during the UPR has been suggested to cause misactivation of retinoic acid inducible gene 1 (RIG-I), a pattern recognition receptor (PRR). Misactivation of RIG-I causes an inappropriate interferon response, which activated immune cells like macrophages. We propose to identify RNA fragments produced though RIDD that may misactivate RIG-I by identifying IRE1-downregulated mRNAs in XBP1 null cells. We are generating XBP1 knock-out cells using CRIPSR-Cas9 technology, and have validated a ribonucleoprotein complex in vitro. In order to determine IRE1 specific cleavage of RNAs during RIDD, we are using the pharmacologic inhibitor, 4u8C. 4u8C produces comparable XBP1 splicing to basal, even when IRE1 is activated. Finally, we will use mRNA sequencing to determine which RNAs are specifically downregulated by IRE1 during RIDD. Identifying RNAs produced though RIDD is necessary to determine possible endogenous RIG-I activators. These conclusions will allow for a better understanding of how RNA detection by PRRs can contribute to autoimmune disorders.

The Importance of Children's Picture Book Character Development and the Use of Anthropomorphism

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Illustration

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Abstract:
Well-crafted children's picture book characters leave an imprint on the human heart and mind. Successful children's book illustrators focus on ways to establish a point-of-view through memorable and impactful character creation. A picture book exposes a young mind to its first visual representations of narrative and imagery. Characters are literacy advocates, laying the foundation for successful reading comprehension and opportunity. Successful illustrators craft characters with emotive design principles and a contextual relationship to the written word to express concepts such as empathy, friendship, loneliness, etc. This study focused on methods of successful character creation based on first-hand observational exploration of children's literature archives; research in the history of children's books; and a course in character development. The children's literature archives visited were in the eastern United States and London, England. This study was limited to the process work of two author illustrators, Beatrix Potter and Tomi Ungerer, both recognized, prolific illustrators whose work uses anthropomorphism. Through an analysis of Potter's "The Tale of Peter Rabbit" and Ungerer's "Rufus the Bat Who Loved Colors" it is possible to understand how to effectively create an anthropomorphic character. To test these ideas, further study was gained through a book illustration course at the Chelsea College of Arts in London, England. The course focused on the fundamentals of character design, visual sequencing and professional attributes of the book publishing industry. These experiences led to a discovery of the fundamental elements of character development and an exploration of important cultural implications of anthropomorphism. Successful anthropomorphic character creation involves three primary elements: 1) The essence of the creature/object must be understood before attributing human characteristics; therefore, an in-depth study of form, movement and structure of the

animal/object is necessary for it to be anthropomorphized; 2) Environmental narrative and/or experience for the character to interact and exist is crucial for relatability; 3) Expression of personality with facial and/or body movement, and/or the addition of specific accoutrements as indications of likes/dislikes provides depth of character. The study evolved into the creation of an original children's picture book, "Hound Dog and Frog." The creative process includes a prototype or "dummy book" and several full-page color illustrations and spreads formatted to submit for publication. The original story features an illustration of a hound dog who loves to read and lives in an underground den. One day he hears a sound and is drawn up from underground. The sound turns out to be a frog playing the fiddle who inspires the hound to become a writer. Anthropomorphism structures the visual narrative and triggers empathy in the audience as they find the value of friendship and creative inspiration for children.

"Dirty" Energy: The Investigation of Bacterial Communities in Sediment Microbial Fuel Cells and Optimizing Power Production

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Biology and Psychology

Faculty Mentor(s):
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Integrative Biology

Abstract:
Sediment-based microbial fuels cells (SMFCs) are established on the premise that certain types of bacteria (called electrogens) can metabolize organic substrates and transfer electrons extracellularly onto electrodes. The resulting flow of electrons through a circuit from anode to cathode generates an electrical current. If this technology can be perfected, the use of SMFCs as an innovative sustainable energy supply would be ground-breaking. The objective of this project was to identify the bacterial communities found within different SMFC reactors and discern the communities that led to more productive (>100 millivolts, mV) SMFCs. To do this, using graphite fiber felt pads as electrodes, replicate SMFCs were filled with environmentally-available sediments suspected to harbor electrogens including acidic mine tailings and garden soil. The garden soil reactors were saturated with sterile tap water, while the mine tailings reactors were supplemented with either nutrient broth or tryptic soy broth. The reactor voltages were recorded continuously to monitor their power output and to determine if power was sustained over time. Preliminary results showed that garden soil SMFCs as well as mine tailing reactors supplemented with tryptic soy broth could provide voltages up to 440 mV and sustain peak voltages for an average of 6-8 days. Additionally, DNA sequencing analyses (currently underway) on the bacterial communities from the SMFCs will identify the bacterial diversity and species abundance differences between productive and non-productive reactors and among the different sediment types examined. With this data, this project has identified parameters associated with SMFCs that warrant further investigation for the continued optimization of SMFCs as a sustainable source of electricity.

Clustering Neural Spikes Using FGPA

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Faculty Mentor(s):
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Abstract:
Neural activity can be measured via a metal electrode inserted into the brain. When neurons around the electrode fire, the sensor will detect a voltage spike. The same neuron will generate neural spikes with similar temporal shapes each time it fires, and by classifying similar spikes, we determine which neurons around the electrode are firing and when. This method of investigation gains us a deeper understanding of brain activity, which may lead to treatments for neurological ailments such as Parkinson's disease. Previously, clustering of neural spikes was done in software, which is limited by processor speed and complexity. This research implements the clustering algorithm developed by Dr. Tim Lei and Ms. Zeinab Mohammadi in the fabric of a Field Programmable Gate Array (FPGA). The FPGA realizes the algorithm as custom hardware, allowing us to greatly simplify and parallelize the process so that we can achieve the ultra-low latency clustering needed for real-time analysis of neural activity.

Probing the Dynamics of the Villin Headpiece Protein's Subdomain HP-36

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Faculty Mentor(s):
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Abstract:
The folding of many globular proteins and aggregation of non-globular proteins arises from the dynamics of hydrophobic side chain interactions. A headpiece subdomain on villin, HP36, has a hydrophobic core, which is ideal for studying side chain interactions similar to those found in more complex proteins. It is important to obtain the free-energy profiles for flipping of the hydrophobic core residues in order to comprehensively understand the dynamics of the hydrophobic core. Solid-state NMR measurements of the three phenylalanine residues (F47, F51, and F58) implied that the three residues are flexible and frequently undergo ring flipping1. To compare with experimental results, here we use umbrella sampling, a form of biased molecular sampling, to compute the free-energy profiles of these three phenylalanine residues at various temperatures.

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Probing the lipid dependence of Src membrane binding with fluorescence spectroscopy

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Biochemistry

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Chemistry

Abstract:
Src is a non-receptor protein kinase that belongs to the family of tyrosine kinases, it adds a phosphate group to tyrosines. Src may play a role in cell growth and embryonic development; elevated levels of Src are also associated with cancer progression. Src is involved in various signal transduction pathways. Previous studies from the Stith group have shown that Src plays an important role in the events of fertilization of Xenopus laevis by stimulating phospholipase Cγ which triggers other events that eventually affect the intracellular Ca2+ levels. Src is believed to bind lipid rafts via intermolecular and electrostatic interactions. In this study, we test Src's binding ability to different lipid compositions using Fluorescent Resonance Energy Transfer (FRET) and lipid titration. The SH4, unique lipid binding region (ULBR) and the SH3 domains in the N-terminal end of Src bind to negatively charged lipids due to the presence of several lysines and arginines in the SH4 domain.

Preparation of a Deuterated Phosphoserine Analog to Study Morphology Changes within the Aβ-peptide Leading to Fibril Formation

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Abstract:
Alzheimer's disease is caused by the formation of highly structed fibrils that are toxic to neuron cells. These highly structured fibrils arise from the Aβ-peptide undergoing a morphology change from globular to highly structured beta sheets. The cause of this morphology change is not well understood but is hypothesized that post-translational modifications can play a significant role in controlling aggregation. The phosphorylation of serine located in the disordered N-terminal is one of such modifications that can initiate a morphology change and aggregation. Here we describe a method for preparing peptides containing deuterium exclusively on the alpha and beta positions of phosphoserine. This can be used to study the morphology of the peptide leading to fibril formation. To insert this deuterated phosphoserine into the peptide sequence, serine must first be phosphorylated, and the phosphate group needs to be protected. The hydroxyl group will be phosphorylated using a phosphoramidite containing benzyl groups. These benzyl groups will protect the phosphate group during solid phase peptide synthesis. After this deuterated phosphoserine has been inserted into the peptide sequence morphological changes can be studied using 2H-NMR. Trials for creating a protected analog are currently being carried out on a nondeuterated serine.

The relationship between working memory performance and eye movements during memory maintenance

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Abstract:
Visual working memory (VWM) refers to a component of short-term memory responsible for maintaining visual information for a brief duration when the stimuli are absent. While other research has focused on how instructed eye movements during maintenance influence working memory, our research focuses on naturally-occurring, or non-instructed, eye movements. The aim of this study is to analyze how non-instructed eye movements during a VWM task influence performance. The participants engaged in a VWM task where on each trial two, four, or six squares appeared in different colors and locations on the screen for 200 milliseconds., The squares disappeared and after 1,000 milliseconds, one square reappeared. The participants then had to indicate if the square matched the color of the previously-shown square in the respective location. We calculated the mean number of eye movements occurring during the delay period with respect to accuracy at the end of the trial. Participants showed significantly fewer non-instructed eye movements throughout the delay period for accurately-performed trials compared to inaccurately-performed trials. This data supports previous research that has identified an association between eye movement generation and VWM maintenance. Thus, differences in eye movements may contribute to VWM performance across trials. We will conduct further analyses to investigate how eye movement strategy differences may explain individual differences in overall working memory performance.

The role of mTOR signaling in enhanced fear extinction produced by acute, voluntary exercise

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Abstract:
Exercise has beneficial effects on mental health, such as enhancing the extinction of a traumatic memory. In rats, a single, two-hour bout of voluntary exercise after fear extinction training can enhance extinction memory. Identifying mechanisms by which acute exercise augments fear extinction could reveal novel targets for the treatment of trauma-related disorders, such as Post-Traumatic-Stress Disorder (PTSD). One factor that could contribute to enhanced extinction memory following exercise is the mammalian target of rapamycin (mTOR). mTOR is a translation regulator involved in synaptic plasticity, and is a target of cellular signals sensitive to exercise. mTOR is also increased after chronic exercise in brain regions involved in learning and memory. Therefore, mTOR is a compelling potential facilitator of the memory-enhancing effects of exercise. The goal of this study was to determine if mTOR signaling is critical for the enhancement of fear extinction memory produced by acute, voluntary exercise. Adult, male Long Evans rats exposed to auditory fear conditioning received intracerebral-ventricular (ICV) injections of the mTOR inhibitor rapamycin prior to fear extinction training and acute wheel running. We observed that, like chronic exercise, acute exercise increased mTOR signaling in extinction-related brain areas. Moreover, ICV administration of rapamycin reduced mTOR signaling and eliminated the enhancement of fear extinction memory produced by acute exercise. These results suggest that mTOR signaling contributes to the memory-enhancing effects of exercise. Factors that increase mTOR signaling could be useful targets for the treatment of psychiatric disorders like PTSD.

The perception of correlations in graphical scatterplots

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Faculty Mentor(s):
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Abstract:
Data is often condensed and presented in graphical representations. Viewing is often self-guided and there are many factors that can influence viewer interpretation of the data as presented. In this project participants will be presented with scatterplots designed to influence viewer perception of information. We will examine fixation times and participant responses to better understand the relationship between what viewers are choosing to look at and their interpretation of the data. Very little research has been conducted investigating the cognitive processes of data interpretation despite graphs being a commonly used means of displaying information.

Metabolic analysis of the lipid preference in cancer cells with increased CPT1A expression

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Abstract:
In recent years, the connection between nutrition and cancer has been established but not explored in depth. Different cancer cells are more likely to obtain energy from different nutrients. If the link between prostate cancer and the conditions that prostate cancer cells thrive in were to be analyzed, the results could potentially suggest modifications that should be placed on the diets of cancer patients to help improve their conditions. Recently, there have been societal trends that state what foods/oils are considered “healthy.” Carnitine palmitoyltransferase 1A (CPT1A) is an enzyme abundant in the liver. It aids in fatty acid oxidation, a process that metabolizes fats to convert them into energy for the cell. Previous studies have shown that CPT1A is found in an excessive amount in prostate cancer cells1,2. Using that knowledge, an overexpression of CPT1A can be carried out in a cancer cell line to imitate prostate cancer cells. They can be compared to a control which has a normal amount of CPT1A expression. Using the Seahorse XFe96 Analyzer coupled with clonogenic assays, the fats that the cancer cells preferred to burn were determined.

What Are You Going to Do With 390 Photographs of Discarded Christmas Trees?

Student Author(s):
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Photography and Art History

Faculty Mentor(s):
Carol Golemboski, Professor
Photography

Abstract:
In the Spring of 2018, I applied for and was pleased to receive a UROP Grant through CU Denver which helped to partially fund my BFA Photography thesis, What Are You Going to Do With 390 Photographs of Discarded Christmas Trees? The project, a direct homage to late author Richard Brautigan and Polaroid inventor Edwin Land, was shot entirely on Polaroid Originals film. Over the course of two weeks, I traversed the Denver metro area in search for abandoned Christmas trees appropriating a short story written by Brautigan of roughly the same title. Due to the vulnerable nature of Polaroid's emulsion, each photograph is its own document of what Brautigan called, "the going away from Christmas." The images will be presented in late April-early May at the Red Line Gallery in Denver, alongside the graduating BFA students of this May 2019. For the RaCAS Symposium, I would particularly like to highlight the temperature vulnerability and unique nature of the individual images as I know there will be many scientists in the crowd! During development, Polaroid film requires shielding from the light as well as particular temperatures to create a "normal exposure." Thus, if the emulsion is colder than "recommended" the hue becomes notably blue. If too warm, a pinker/yellow hue appears throughout the image as well as visible variations in the contrast. Individually, they are simply images of trees. Together however, they culminate in the documentation of a two-week performance, which brought to life a short story by one of literature's famed lost authors.

A Comparison of Dual Military, Male Military Only, and Female Military Only Couples

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Psychology

Faculty Mentor(s):
Dr. Elizabeth Allen
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Abstract:
Female service members have higher divorce rates than male service members. The goal of this study was to explore possible sources/markers of stress for couples where at least one partner was a female service member. Using a large (662 couples) survey study of couples where at least one partner was in the U.S. Army, this goal was accomplished in two ways. First, self-reported marital quality, mental health, and Army specific support/stressors were quantitatively compared for both husbands and wives in three types of couples: Dual Military, Male Military Only, and Female Military Only. The purpose of

this set of analyses is to determine if couples with female service members report significant differences that could be related to their higher divorce rates, such as less Army support, or more conflict between the spouses. Second, themes of stressors were evaluated based on open ended question regarding problems related to military service for couples where the wife was a service member. The purpose of this thematic review is to see what the couples themselves identify as stressors particularly salient to couples with a military wife. Results will be discussed in the context of gender roles and family expectations and how these might interact with the demands of Army life.

Inversion Breakpoint Mapping of Rhagoletis pomonella

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McCall Calvert
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Faculty Mentor(s):
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Dept. of Integrative Biology

Abstract:
Do genetic inversions contribute to speciation-with-gene-flow?

The process of species formation has generated the vast network of biodiversity that makes up our biosphere. Yet, we still do not understand exactly how it happens because speciation events occur in an 'eyeblink' in evolutionary time. However, some examples of contemporary speciation can be observed in nature including our study system, a fruit-infesting fly Rhagoletis pomonella, that has recently evolved novel populations that infest apples introduced to North America ~300 years ago. In this species, populations infesting native fruit are segregating into two genetically distinct populations that infest different fruits, despite continued interbreeding, which should genetically homogenize populations (i.e., prevent speciation).

It has been hypothesized that genomic structural variants, such as inversions, could facilitate speciation in the face of interbreeding. Chromosomal inversions occur when a section of chromosome breaks and becomes oriented in the opposite direction. This orientation prevents the random shuffling of genes that ordinarily occurs during meiosis, prior to reproduction, ensuring that the entire sequence is conserved in future offspring. If these inverted regions contain genes contributing to trait divergence, hybrids would be poorly suited to either parental environment, thus encouraging reproductive isolation (limited interbreeding).

Testing this hypothesis has been historically challenging, but this project leverages new long-read, low-cost DNA sequencing technology to determine if genetic breakpoint locations can be accurately mapped in the genome of R. pomonella for the first time. These data are absent from the literature but are critical for determining the role of genetic inversions in speciation.

Characterization of the Effects of Systemically Increasing Dopamine, Serotonin, and Noradrenaline Levels on the Valuation of Reward vs. Avoidance

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Oniza Chaman
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Faculty Mentor(s):
Erik B. Oleson, Professor
Psychology

Abstract:
Optimal behavior and overall survival require obtaining highly-valued outcomes from our environment. These action-outcome situations are often driven by either the pursuit of reward or the avoidance of harm. The three primary monoamine neurotransmitter systems that modulate such motivated behaviors are dopamine (DA), serotonin (5-HT), and noradrenaline (NA). Of these, the mesolimbic DA system is generally considered to be a reward pathway. However, it is becoming increasingly evident that DA release events also process and influence aversively-motivated behavior. Combining operant behavior with a behavioral economic framework to model behavioral changes in response to increasing price (i.e., lever responses/outcome magnitude), we recently demonstrated that DA release events represent avoidance value and modify the price rats will pay to avoid electrical footshock. Using a similar approach, my current project will perform a broader characterization of the primary ascending monoamine systems in the valuation of reward vs. avoidance. We will pharmacologically target these systems using the selective reuptake inhibitors GBR-12909, fluoxetine, and desipramine for DA, 5-HT, and NA respectively. Based on our previous findings and the existing literature, we predict; GBR-12909 will increase reward and avoidance valuation, fluoxetine will increase avoidance value but decrease reward value, and desipramine will decrease avoidance value without affecting reward. Investigating whether these pathways produce distinct effects on reward vs. avoidance valuation will provide novel insight into how the brain controls these fundamental aspects of behavior. The implications of this work may also advance our understanding of major psychiatric conditions such as depression and drug addiction.

Interactions between transition and alkali metals and 8-oxo-7,8-dihydroxyguanosine or guanosine. The case for: Pd(II), Fe(III), Ag(I), Cs (II), Na, K

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Abstract:
8-Oxo-7,8-dihydroxyguanosine (8-Oxo-G) is a derivative of guanosine present in DNA (Deoxyribonucleic acid) and RNA (Ribonucleic acid) and is a result of oxidation at the C8-position, commonly generated upon oxidative stress. Its presence has deleterious effects and has been linked to the progression/development of neurodegenerative and other diseases. Reactivity of certain transition metals and their potential use as therapeutics to detect this lesion has been tested with DNA but not with RNA. 8-Oxo-G was synthesized from guanosine and the ribose hydroxyl groups were protected with hydrophobic groups at the C2', C3' and C5' positions. Alcohols at C2' and C3' were functionalized with an isopropylidene group, while the alcohol at C5'-position was derivatized with a bulky hydrophobic tert-butyldimethylsilyl group. Reactivity of different transition metals was explored with silver tetrafluoroborate (AgBF4), palladium chloride (PdCl2), iron(III) meso tetraphenylporine chloride (Fe(III)-TTPCl), cesium chloride (CsCl2) and cesium carbonate (CsCO3); and Group-I metals that included potassium bromide (KBr), sodium nitrate (NaNO3) and sodium hexaflourosilicate (Na2SiF6). The results from Guanosine and 8-Oxo-G were compared and analyzed via thin layer chromatography (TLC) and nuclear magnetic resonance (NMR). Guanosine formed a gel-like compound in the presence of AgBF4 and formation of purple plate-like crystals was observed upon mixing of 8-Oxo-G with Fe(III)-TTPCl This research hopes to find a transition metal that forms complex with 8-Oxo-G and can be used as a potential tool for the detection of this toxic lesion.

Increasing Eco-Awareness: Public Artworks on the Denver Light Rail

Student Author(s):
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BFA in Painting and Drawing and BA in Art History

Faculty Mentor(s):
Maria Elena Buszek, Associate Professor
Art History

Abstract:
For my Undergraduate Research Opportunity Program project, Increasing Eco-Awareness: Public Artworks on the Denver Light Rail, I researched public artworks and environmental activism to propose a theoretical exhibit on the Denver Light Rail system. Based on Environmental artist Lorna Jordan's concept that public artworks can be ideas, places, and actions that regenerate the environment while triggering viewers' internal emotions and narratives, the exhibit would tap into the imaginations and narratives in our city's Denver Light Rail riders. I created a call for participation, and curated work that emphasized the surrounding landscape that we all live off of and have an investment in, the common ground serving as a source of Denver identity. I proposed integrating this artwork into the trains to replace the usual advertisements, so as to interrupt the daily dose of consumption imagery. By supplanting ads with images of raw materials from the Colorado landscape, environment, and population, a shared sense of place is set to invoke in their imaginations the value of landscape, and promoting more ecological, rather than consumerist, awareness. Many Eco-Art theorists support the notion that the aesthetic experience can educate viewers to an eco-conscious, anti-consumption lifestyle. Because the artwork is not restricted to the museum space, this project is designed to inspire engagement with a larger, more diverse audience into viewing art in their daily ride, as well as begin a dialogue surrounding raw materials from the state's landscape and how it influences the community.

“Soft-no” as a barrier in the transition from palliative care to hospice

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BS Public Health

Faculty Mentor(s):
Dr. Karen Luftey Spencer
Department of Health and Behavioral Sciences

Abstract:
Hospice care services, while covered under Medicare, are underutilized in the United States. Hospice cares for patients who are estimated to have a life-expectancy of under 6 months, either in their homes or at a center. However, entering hospice is contingent on patients ceasing all active, or curative, treatment. 26 patients receiving palliative care (e.g “comfort care”) and 16 caregivers were interviewed to examine their decision- making process around entering hospice. Decisions surrounding medical treatment are often placed in two categories—acceptance or refusal. However, these two categories do not accurately depict the diversity within the decision-making process. The goal of the study conducted was to identify what and how patients are refusing.

The data suggests that there are two main types of hospice refusal—hard no and soft no. Hard refusals individuals were not open to hospice and explicitly refused. While soft refusal individuals did not explicitly refuse hospice, their actions continue to postpone hospice. The interview data was closely analyzed for soft-no individuals and we determined three drivers in the soft-refusal. These include hospice being viewed as unnecessary, undesirable, or not the patient’s decision to make. Our study analyzes these components and how they contribute to a soft-refusal of hospice.

Targeting the MLL2-Chromatin Interaction to Inhibit Leukemogenesis

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Public Health

Faculty Mentor(s):
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Pharmacology, Pediatrics (Hematology, Oncology, BMT)

Abstract:
Mixed Lineage Leukemia (MLL1) is a gene that can drive acute myelogenous leukemia (AML) when rearranged by chromosomal translocation. Through prior research, it has been shown that both the non-translocated (wild-type) MLL1 allele and its close relative MLL2 play a significant role in leukemia. Specifically, our lab has shown that deleting MLL2, a chromatin-binding protein, slows leukemia cell growth in vitro and in animal models. To expand on the potential of this finding, a peptide was created to selectively target MLL2 and interfere with MLL2 and chromatin binding. It was fused to nuclear localization signals, epitope tags, and inserted into an expression plasmid using cloning techniques. The hybrid peptide was characterized through immunofluorescence and Western blotting to establish a

stable, nuclearly-localized product as predicted by design. The peptide was then expressed in leukemia cells, where it was hypothesized to have an anti-leukemia effect. To test the effect of the peptide on MLL2 function, quantitative PCR was performed to analyze levels of endogenous MLL2 target genes. As a positive control, the results were compared to the effect of MLL2 deletion on gene expression to determine the effectiveness of the strategy. This proof-of-principle experiment will establish whether targeting MLL2 with small molecules, such as this peptide, would be effective in inhibiting leukemia growth. This would serve as a basis for a functional screen to identify molecules that could be developed as therapeutics for acute myelogenous leukemia.

Computational modeling of the absorption spectrum of gold nanorods in explicit solvent

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Abstract:
Gold nanoparticles exhibit unique optical properties that make them suitable for a wide variety of biomedical applications such as cancer diagnostics, drug delivery, and tissue imaging. Gold nanorods are good candidates for cancer therapy due to their low biotoxicity and easy tunability of their surface plasmon resonance (SPR), which is the collective oscillation of conduction electrons in the presence of an electromagnetic wave. Few computational studies have examined how explicit solvent interactions affect the plasmonic absorption due to the high computational cost associated with modeling explicit solvent molecules. Thus, the goal of this study is to determine how the presence of explicit water molecules affects the energy and intensity of the plasmonic absorption of gold nanorods. The nanorods were modeled with quantum mechanics (density functional theory) and the water solvent molecules were modeled with the effective fragment potential (EFP) method. Results show that water molecules tend to interact with the gold nanorod via the oxygen atom. In addition, the most energetically favorable water binding site is at the end of the nanorod. Solvent interactions can induce a shift of the absorption peaks to higher energy compared to the gas phase. In addition, splitting of the absorption peaks may occur.

The effects of post-weaning social isolation on social fear conditioning and the mammalian target of rapamycin (mTOR) pathway

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Abstract:
Learned behavior such as social fear can be mediated through stressful events. Heightened and prolonged exposure to fearful events can lead to stress-related disorders such as PTSD. Individual differences such as prior experiences to traumatic social events can underlie the development of these disorders. Post-weaning social isolation (PSI) is a model of early life adversity where rats are housed in isolation during a critical period of adolescence. PSI has been shown to alter social behaviors. A novel conditioned social fear paradigm was developed in our laboratory in which a foot-shock unconditioned stimulus is paired with a social stimulus (a novel same-sex conspecific) as the conditioning stimulus. The social behaviors of the experimental rats were assessed during re-exposure to the social stimulus during a social interaction test. To investigate the neural mechanisms underlying conditioned social fear, the mTOR signaling pathway was assessed in the medial prefrontal cortex (mPFC) and amygdala, which are brain regions involved in fear learning. Behavioral results from the social interaction test show that conditioned social fear (CSF) in isolated male rats have increased escape behaviors compared to group-housed rats. Phosphorylated ribosomal protein S6, a component of the mTOR pathway, was assessed using immunohistochemistry. There was increased pS6 expression in the medial ventral (MeV) amygdala in CSF male rats and social stimulus only rats compared to foot-shock only male rats. The results show that the presence of a social animal during conditioning increased pS6 expression in the MeV amygdala and decreased pS6 expression in the mPFC.

Optogenetic Stimulation of Substantia Nigra Terminals Projecting Into The Dorsal Lateral Striatum During Fear Extinction Prevents Fear Renewal

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Abstract:
Exposure therapy relies on the process of fear extinction, which represents new learning that the previous fear conditioned stimulus no longer predicts danger. One limitation of exposure therapy is that fear tends to return in contexts different from the extinction context, a phenomenon called fear renewal. Identification of novel strategies to prevent fear renewal could improve success of exposure therapy. We observed that activation of substantia nigra (SN) dopamine (DA) neurons during fear extinction enhances fear extinction recall and blocks fear renewal (Bouchet et al., 2018), but the specific targets in which SN DA acts to enhance fear extinction remain unknown. SN DA neurons projecting to the dorsal lateral striatum (DLS) support the formation of habitual behaviors, which can be resistant to contextual modulation. The goal of the current study was to test the hypothesis that optogenetic activation of SN terminals in the DLS during fear extinction learning will reduce fear renewal. Adult, male Long-Evans rats received bilateral intra-SN microinjections of control virus or AAV-Chr2-hSyn-mChery and optic ferrule cannulas in the DLS. SN terminals in the DLS were then optogenetically stimulated during auditory fear extinction learning. Fear extinction memory and relapse were subsequently assessed in the absence of stimulation. Results indicate that optogenetic stimulation of DLS-projecting SN neuron terminals during fear extinction reduces the renewal of fear in a novel context while having no effect on extinction memory or spontaneous renewal. These data suggest that novel therapeutic strategies aimed at the SN-DLS circuit could be effective adjuncts to exposure therapy.

Exam skills and metacognition: piloting a new exam type.

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Abstract:
Absorption of knowledge within the college setting is crucial to academic success. Student's need to effectively grasp a wide array of information in multiple classes and it is the hope of many teachers that this information will be retained. STEM courses tend to be anxiety inducing in many students and often they feel as though they are unable to preform due to the technical nature of these courses. Exams are a standard measure used to quantify the information that students have retained. The ThinkCheck Exam is a hybrid exam combing open note and multiple choice exams styles. This exam gives one page with broadly worded version of the questions within the exam. During the first portion of the exam students are allowed to use resources such as the book, professor powerpoints or personal notes. During the second portion of the exam students then use the one page of notes to complete the multiple choice exam. While it may see as though this type of exam is too easy the open note portion is vague enough as to provide a challenge. This type of exam provides the flexibility of multiple choice exams for professors but allows for different difficulty levels of questions as defined by Bloomburg's Taxonomy. With these exams metacognition is enhanced and students will see an improvement in their core knowledge which is reflected within an improvement in understanding of the material and an increase in exam scores particularly within STEM courses.

Computation of host-guest free binding energies with a QM-MM mining minima algorithm

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Spanish

Faculty Mentor(s):
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Abstract:
Host-guest chemistry is a subfield of supramolecular chemistry, which deals with the interactions between two or more molecules. The applications of host-guest complexes range from the development of drug delivery systems to cancer treatment techniques. Within the realm of drug delivery systems, a host molecule is defined as a vehicle that encapsulates a drug, which acts as a guest molecule. A significant aspect of this subfield is the amount of energy that is required to bind a guest to its affiliated host. Finding the binding energies of different host-drug systems can aid in the development of models for larger host-guest systems, such as enzymes and other proteins. Host-guest systems are ubiquitous; therefore, gaining more information about the processes and mechanisms of how guests bind to host molecules is crucial. One of the challenges that arises in drug design is accurately predicting the binding energies of host-guest systems due to the weakness of the interactions between them. This research project aims to find a specific method that predicts these energies in an accurate and computationally inexpensive way. The binding energies were calculated using a method called VM2, which was developed by the software company VeraChem LLC. This system was used in order to find a method that includes the lowest possible energy calculations that correspond to the host-guest systems that are being tested.