Purdue University Chapter

The Society of Sigma Xi

Stewart Center, Rooms 214 A-D
February 21, 2018

2:30 to 4:30 p.m. – Poster Setup & Viewing
6:00 to 9:00 p.m. – Viewing and Judging

Purdue University Chapter
The Society of Sigma Xi

Poster Competition

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Graduate Student Posters

BEHAVIORAL AND SOCIAL SCIENCES

SBS 1.

A Market in Education: How Central Exams relate to Quality & Equity

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Dr. Nielsen Pereira (Faculty Sponsor)

Many countries have reformed their education system based on the idea that combining school autonomy with school choice and school accountability would have a positive effect on the quality of education. However, research has indicated that this might be negative for equity in education. Using PISA 2015 data we therefore explored the questions is there a trade-off between quality and equity when there is a market in education? More specifically we looked at central exams as form of test-based accountability, school autonomy, and the percentage of private schools as an indication of school choice. A multilevel regression analysis showed that it is reasonable to assume that there is a trade-off between quality and equity in education, in the presence of a market in education and specifically in the presence of central exams.

SBS 2.

Singapore Art Teachers' Perceptions of Gifted Art Students

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Dr Marcia Gentry

Few studies in the field of gifted education examine issues of identifying gifted art students. Whereas most academic areas have well-established standardized tests, there is no such practice for visual arts. Further, art teachers are often the gatekeepers to gifted art programs. Thus, there is a need to understand what art teachers perceived to be attitudes and behaviors that characterize gifted art students. Thirteen Singapore art teachers were participated in the study. Among the characteristics of gifted art students highlighted by the participants, taking ownership of the learning process and willingness to work were mentioned the most. Although the participants did assess the students' drawing and other art making skills as part of the identification process, this did not carry as much as weigh as did the students' attitudes. Participants also acknowledged the limitations of the selection process, especially being unable to account for curiosity and level of commitment.

SBS 3.

Depression Trajectories in Military Couples

Coppola, E. C., Christ, S. L., Cardin, J. F., Bailey, K., Southwell, K., & MacDermid Wadsworth, S.
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Shelley MacDermid Wadsworth

Studying transitions, or family and individual changes triggered by external events, may elucidate causal mechanisms and processes that contribute to adaptation or dysfunction. During the experience of deployment, military service members and their families undergo a sequence of complex transitions that influence their well-being. While service members and their partners may fall below clinical thresholds for depression at the aggregate level, certain subgroups within this sample may exceed clinical thresholds during discrete phases (i.e., before, during, or after) of deployment. Thus, using longitudinal data, this study had the following goals: (1) To identify distinct profiles for service members and their spouses distinguished by varying levels of depression at discrete phases of deployment, (2) to determine how profiles of service members and their spouses are related, and (3) to predict group membership to each distinct profile from social location (e.g., deployment history, household composition, and demographics).

SBS 4.

Young Children and STEM Enrichment: A Parental Perspective

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Faculty Sponsor: Dr. Marcia Gentry

Pre-kindergarten and kindergarten curricula can be challenging and engaging, but few are strongly grounded in STEM education. However, researchers have shown that young children can benefit greatly from early introduction to STEM education. In this study, the authors examined parental perceptions of the influences of a Saturday STEM enrichment program in one University center on pre-kindergarten and kindergarten students and their attitudes towards STEM learning. Using survey data regarding benefits, drawbacks, and memorable moments, the authors sought to answer three questions: How do parents evaluate their children's experiences in STEM enrichment classes? What do they perceive to be influences in learning? What kinds of behaviors are witnessed after the experiences?

SBS – 5

Exploring differences in self-esteem, moral foundations and personality among adults who sext.

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The current study assessed the prevalence of sexting as well as the methods used and image content for sext messages among adults. In addition, the current study explored the relationship between sexting, moral foundations, self-esteem, and individual differences. Participants were solicited through Amazon's Mechanical Turk and completed an anonymous, self-report survey. The final sample included 508 adult participants; 68% of adults reported sexting behaviors, and both mobile applications and traditional text messages were used to send sext messages. In general, individuals who scored higher on extraversion and lower on conscientiousness, agreeableness, harm, and fairness were more likely to engage in sexting behaviors. Consistent with previous research, results indicate self-esteem is not associated with sexting behaviors. Additionally, results suggest significant differences between individuals who send semi-nude versus nude sext messages.

SBS – 6

Buffering role of social support on the association between maltreatment exposure and changes in externalizing problems during adolescence

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Sharon L. Christ

The present study has the following aims: 1) to test the association of multiple maltreatment types on externalizing trajectories, and 2) examine the buffering effect of social support on these associations. The average EP at baseline 1.907 point out of 5 and there was significant variance between adolescents in changes in EP over time, indicating that some adolescents in the sample had increasing EP over the course of the study whereas others had decreasing EP. Social support and maltreatment were directly associated with levels of EP. Social support was also a buffer for the association between multiple maltreatment types and EP at any given time point. In essence, at high levels of social support, adolescents displayed lower EP even in the presence of multiple maltreatment exposures. This study illustrates that social support is protective both EP and therefore can be an important point of intervention for these at risk children.

ENGINEERING SCIENCES

E1.

Microstructural Limits of Porous Electrode Theory

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Newman-type models, are the most widely used implementation of porous electrode theory to simulate Li-Ion batteries by both industry and academia (Newman and Tiedemann 1975). These models show great robustness, fidelity, and for most applications they require to fit ~80 material parameters to match the measured experimental data. While it is always possible to match the experimental results with these models, a methodology to quantify their veracity and identify the regions of validity remains unavailable. In general, it is necessary to identify the conditions under which the micro and macroscopic scales are decoupled, and conditions where the assumptions associated to using average microstructural properties remain enforced. In this paper, the effect of the microstructure in the modeling and validity of Newman-type models is described by extending the upscaling techniques analytical method proposed by Battiato et al. (2015), with the use of microstructurally averaged properties, e.g., García and García (2016).

E2.

In situ measurement of native extracellular matrix strain

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Sarah Calve, Ph.D.

Cells directly interact with the extracellular matrix (ECM) in their microenvironment; however, the mechanics of the ECM networks are not well defined. Our objective is to quantify ECM network strain *in situ* after mechanical loading. Visualization and testing of the ECM in the native 3D organization is facilitated using decellularized murine embryos as the tissue of interest. Samples were imaged, before and after mechanical loading, using confocal microscopy. Digital volume correlation was used to calculate ECM displacement and strain. The amount of strain experienced by different proteins was significantly dependent on whether the sub-region analyzed was in the developing cartilage or the adjacent connective tissue. Quantification of strain *in situ* is the first step towards developing constitutive equations describing the mechanical properties of ECM networks. In the future, this information could improve the fabrication of physiologically relevant scaffolds by establishing mechanical guidelines for microenvironments that support beneficial cell-ECM interactions.

E3.

The Development of a Wearable Biosensor for Outpatient Drug Rehabilitation Care

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Jacqueline Linnes

The recent opioid crisis has brought attention to the need for better treatment strategies for rehabilitative patient care. Recent literature has explored technological advances to improve patient outcomes in rehabilitation programs. Drug use has been shown to cause short-term changes in the cardiopulmonary system. This provides a unique opportunity for us to monitor drug-use and risk for overdose in real-time using wearable biosensors. The present work aims to improve the diagnostic capability of wearable biosensors, which traditionally only measure heart rate, by adding the capability of measuring respiratory rate and blood oxygen as well. To date, we have compared our prototype device to a number of known standards on healthy human subjects with reasonable agreement. We will proceed with testing on drug rehabilitation patients to assess the capability of our device in correlating changes in heart rate, respiratory rate, and blood oxygen to drug use.

E4.

Characterization of covalent crosslinking strategies for synthesizing DNA-based bioconjugates

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Bernard Tao

A novel single stranded DNA (ssDNA) bioconjugate was synthesized to compare the conventional carbodiimide (EDC) reaction with an adapted strategy using EDC and imidazole (EDC/Im). Matrix assisted laser desorption ionization-time of flight (MALDI-TOF) results demonstrated that the phosphoramidated conjugate is stable for several adys, and that phosphoramidation was exclusively at the 5' end of ssDNA. A reversed phase liquid chromatography (RP-HPLC) method with UV detection was developed to determine the yield of conjugates. The methods coefficients of variation (%CV) were less than 6%, and biases ranged from -5.1% - 1.2%. The conjugate yield via the conventional EDC method was 68.3±2.2%, while that of the adapted EDC/Imidazole method was 79.2±2.4% (n=10). This study demonstrates a convenient, one-pot strategy for crosslinking biological molecules which is useful in diagnostics, biosensor development, and constructing self-assembling macromolecules where there is a lack of flexibility in adjusting reaction temperature or pH.

E5.

Adaptive VR-Based Gesture Recognition System for Improved Rehabilitation of Tetraplegics Due to Spinal Cord Injury

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Bradley Duerstock

Patients with Spinal Cord Injury (SCI) have limited time with supervised therapy in rehabilitation hospitals. This makes continual regular therapy at home imperative. However physical therapy can be tedious leading to a lack of motivation. We explore the use of virtual reality exergames using the HTC Vive to track end-effectors to sub-millimeter accuracy in 3D space. The exergame involves individuals using their upper limbs to track and reach for moving visual virtual targets. We measure various metrics such as range of motion, speed of movement and fatigue/stamina. As these metrics improve, the game adapts and scales the difficulty such that the individual is motivated to push further. Heatmaps are generated from the motion allowing therapists to quantify progress achieved over time and be notified of any compensatory movements that might require attention. Through the use of this system individuals stay engaged longer and can continue their prescribed physical therapy regimen.

E6.

Aminolated and Thiolated PEG-Covered Gold Nanoparticles with High Stability and Anti-Aggregation for Lateral Flow Detection of Bisphenol A

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Lia A. Stanciu

The few lateral flow assays (LFAs) established for detecting the endocrine disrupting chemical (EDC) bisphenol A (BPA) have employed citrate-stabilized gold nanoparticles (GNPs), which have inevitable limitations and instability issues. To address these limitations, a more stable and more sensitive biosensor is developed by designing strategies for modifying the surfaces of GNPs with polyethylene glycol and then testing their effectiveness and sensitivity toward BPA in an LFA. Without the application of any enhancement strategy, this modified BPA LFA can achieve a naked-eye limit of detection (LOD) of 0.8 ng/mL, which is 12.5 times better than the LOD of regular BPA LFAs, and a quantitative LOD of 0.472 ng/mL. This modified LFA has the potential to be applied to the detection of various antigens.

LIFE SCIENCES AND AGRICULTURE

LS-AG 1.

Evenly Distributing Daily Protein Intake Does Not Differentially Influence Weight Loss- and Resistance Training-Induced Improvements in Cardiometabolic Health

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Wayne W. Campbell, PhD

In a randomized, parallel design, we assessed the effects of within-day protein distribution on cardiometabolic health indicator changes after 16 wk of weight loss and exercise in 41 adults (mean±SEM; age: 35±2y; BMI: 31.5±0.5kg/m^2). Subjects consumed 90 g protein/d in either a skewed (10g breakfast, 20g lunch, 60g dinner; n=20) or even (30g each at breakfast, lunch, and dinner; n=21) distribution. Within-day protein distribution did not affect any cardiometabolic outcomes. Among all subjects, body mass decreased by ~8% and whole-body strength increased by ~20%. Fasting glucose (-2.9±1.6mg/dL), insulin (-5.5±1.2µIU/mL), total cholesterol (-21±4mg/dL), and triglyceride (-26±7mg/dL) concentrations decreased ($P < 0.05$). 24-h glucose concentration average (-7.6±2.6mg/dL), variability (-2.7±1mg/dL), peak (-14±4mg/dL), fluctuation (peak-minimum; -13±3mg/dL), and time spent above 100 mg/dL (-242±87min/d) decreased ($P < 0.05$). The effectiveness of weight loss and exercise to improve cardiometabolic health indices is not influenced by within-day protein distribution.

LS-AG 2.

Protein Structural Modeling For Low-resolution Electron Microscopy Maps

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Professor Daisuke Kihara

Proteins are essential to all living organisms. They have a wide range of roles and come in different shapes. Protein's structure is critical to its function. Cryo-electron microscopy is an emerging technology for determining the structure of large macromolecular proteins. However, the limitation of this technology is that it provides low-resolution 3D density images of proteins. These density images cannot provide detailed information about proteins. Thus, new tools need to be developed to analyze protein density maps and produce more valuable information. Our study aims to build a computational method that combines protein low-resolution density images with the atomic structures of their subunits. The accuracy of fitting subunits into density maps is measured using a number of scoring functions such as cross-correlation and mutual information.

LS-AG 3

Computational Methods for Predicting Protein-Protein Interactions in Plants

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Dr. Daisuke Kihara

Protein-protein interactions (PPIs) play an essential role in biological processes and functions. Previously, the identification of PPIs was limited to experimental techniques which is time and labor consuming. As a result, current PPIs derived from experiments only covered a small fraction of whole PPI networks. We developed a complementary computational approach to aid this large-scale PPI prediction in Arabidopsis, soybean, and maize. Here, we considered sequence information, co-expression, functional association, and phylogenetic profile to predict PPIs. Based on six-cross validation results on golden standard dataset, our prediction method achieved 85% accuracy using sequence feature by support vector machine, and 85.4% accuracy using other combined features by random forest. We predicted 91,362 PPIs in Arabidopsis, 126,216 PPIs in soybean, and 6,062 PPIs in maize.

LS-AG 4

Carbonic Anhydrase Inhibitors as a Potential Alternative for Decolonization of Vancomycin-Resistant Enterococci

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Mohamed N. Seleem

Vancomycin-resistant enterococci (VRE) are major healthcare-associated pathogens. VRE can colonize the gut of patients receiving broad-spectrum antibiotics. This is usually followed by translocation of VRE across the mucosal barrier resulting in systemic infections. However, no drug is yet approved for the decolonization of enterococci from the gastrointestinal tract. In a high throughput screening, FDA- approved carbonic anhydrase inhibitors (CAIs) were found to possess potent antibacterial activities against VRE through a unique target. No activity was observed against human gut microbiota. Drugs with lower permeability across gut epithelium (Caco-2) were tested in a mouse model of VRE gut decolonization. Five CAIs successfully reduced VRE colonization (up to 99.99% reduction) in contrast to the anti-enterococcal drug linezolid. The potential target protein was identified using a whole genome sequence analysis. En masse, CAIs represent good candidates for further investigation to be used as agents to decolonize VRE from the gastrointestinal tract.

LS-AG 5

Developing genome engineering tools for anaerobic gut fungi

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Dr. Kevin Solomon

Anaerobic gut fungi isolated from ruminants have drawn recent interest for their ability to break down a diverse range of lignocellulosic materials. However, the application of emerging synthetic biology and metabolic engineering techniques to these fungi has been prevented by a lack of suitable methods for making genome modifications. Namely, appropriate selection markers to ensure only cells with modified DNA survive, as well as methods for inserting DNA into the fungal nucleus have not been identified, in part due to the challenges of maintaining anaerobic environments during benchtop handling. Here, we present an electroporation-based method for inserting DNA into the nucleus of anaerobic gut fungi. A layer of mineral oil is used to impede diffusion of oxygen into the media. Further, we show that geneticin resistance is an appropriate selection marker. In developing these tools, we have provided simple, repeatable methods for future genome engineering of anaerobic gut fungi.

LS-AG 6

Anaerobic gut fungi efficiently degrade renewable plant biomass with variable lignin composition

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Kevin Solomon

Lignocellulose is an ubiquitous source of carbon that is difficult to efficiently use for bioenergy due to large differences in plant composition. Thus, there is a critical need to identify robust and inexpensive enzymes that readily degrade diverse untreated plant biomass. Anaerobic gut fungi isolated from the digestive tracts of ruminants and hindgut fermenters (*e.g*. horse, wildebeest, giraffe) express an array of carbohydrate active enzymes that powerfully degrade lignocellulose under mild conditions. Here, we demonstrate fungal growth on a range of untreated agricultural residues and forestry wastes. We further test glucan and xylan consumption on untreated poplar, with conversions as high as 45% and 48% respectively. In addition to this, we show these fungi remodel protein expression suggesting an evolutionarily adaptation to degrading variable plant material. Exploiting anaerobic gut fungi as a platform for diverse plant biomass hydrolysis has the potential to increase the feasibility of renewable energy from lignocellulose.

LS – AG 7

Repurposing Anthelmintic Drug Niclosamide for Intestinal Decolonization of Vancomycin-resistant Enterococci

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Enterococci are commensal microorganisms present in the GIT of humans. Their prolonged carriage; particularly vancomycin resistant Enterococci (VRE), has been associated with high rates of nosocomial infections and mortality. VRE decolonization represents a key strategy to curb infection. However, there is a dearth of clinically effective decolonizing agents against VRE. Here we confirm that niclosamide; an anthelmintic drug, has potent anti-VRE activity (MIC from 1 to 8 µg/mL). Nicolosamide resistant E. faecium mutants could not be isolated even after 10 serial passages. Adding these results to niclosamide's limited permeability across the GIT, niclosamide was evaluated in a VRE colonization-reduction mice model. Niclosamide, outperformed linezolid, an antibiotic used clinically to treat VRE infections. Niclosamide significantly reduced the burden of VRE (>99%) in the fecal, cecal, and ileal contents of infected mice after only eight days of treatment. Linezolid, in contrast, could not decrease VRE burden in the intestinal tract of mice.

LS –AG 8

Protein Secondary Structure Detection in cryo-EM maps using Deep Learning

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Professor Daisuke Kihara

With the advancements of cryo-Electron Microscopy(EM), the significance of which was highlighted through the Nobel Prize (2017) in Chemistry, in the field of structural biology, determination and validation of 3D structures of macro biological molecules such as proteins has improved over the past few years. For EM maps of medium range resolution (6 – 10 Angstroms), extracting structure information from a map and building a structure model is a challenge. In this work, we aim to make use of deep learning to accurately identify protein secondary structures such as alpha helix, beta sheet, coil/turn from maps of medium range resolution. We developed a deep convolutional neural network architecture (called DeepSSPred) which is trained using simulated EM maps. We use this architecture to then identify secondary structures in the experimental EM maps taken from the EMDataBank. The deep learning architecture makes classification predictions, voxel-wise, on those volumetric EM maps.

LS-AG 9

Phenylthiazoles: Systemically Active Antibacterial Agents Effective Against Methicillin-resistant *Staphylococcus aureus* (MRSA)

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The emergence of antibiotic-resistant *Staphylococcus aureus* poses a serious threat to people worldwide. As most of the antibiotics in the clinical pipeline are derivatives of existing ones, they fail to exhibit activity against methicillin-resistant *Staphylococcus aureus* (MRSA) which makes it imperative to synthesize newer compounds. The current study investigated a series of phenylthiazoles that could be utilized for topical and systemic MRSA infections. The most promising compounds inhibited the growth of clinically-relevant isolates of MRSA *in vitro* at concentrations ranging from 0.5 μg/mL-2 μg/mL. Furthermore, the compounds were found to be non-toxic against the human colorectal cell line (Caco-2) up to a concentration of 32 μg/mL. We also identified two phenylthiazoles that successfully eradicated MRSA inside infected macrophages. In mice, compound **9** demonstrated comparable potency to vancomycin, and at a lower dose, in reducing the burden of MRSA in a systemic, deep-tissue infection, using the neutropenic mouse thigh-infection model.

LS-AG 10

Auranofin combines the antibacterial, antitoxin and antiinflammatory activities in the treatment of *Clostridium difficile* infections

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Clostridium difficile is the most common and costly healthcare-associated infection with approximately half a million cases and 29,000 deaths annually in USA. One new antibiotic, fidaxomicin, was approved in the last 50 years for treating C. difficile infection. However, it has high recurrence rates (24%). Thus, there is an unmet need to develop novel anticlostridial drugs. A library, containing 4,000 FDA approved drugs was screened against C. difficile. Eighteen non-antibiotic drugs were active against it. Auranofin (approved anti-rheumatoid arthritis drug) showed bactericidal activity, in an applicable clinical range, against C. difficile clinical isolates. The MIC at which 90% of clinical isolates were inhibited (MIC90) was 2 μg/ml. Auranofin was superior to the drugs of choice (vancomycin and metronidazole) in inhibiting toxin production by toxigenic strains. Furthermore, it suppressed spore formation which can lower the transmission and recurrence of infection. Results indicate that auranofin warrants further investigation as novel anticlostridial drug.

LS-AG 11

Elastic Network Models for Flexible Protein-Protein Docking

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Daisuke Kihara

Protein-protein docking, the computational modeling of the 3D structure of protein complexes, is a staple of protein structural bioinformatics. Many docking methods have been developed which consider or are tolerant of small-scale flexibility, such as flexibility of side chains or small changes to backbone conformation. However, large-scale conformational changes, such as hinge-like motions, are not handled by current methods. Since it has been shown that accurately modeling large changes in backbone conformation is necessary for reliable protein-protein docking, we developed a flexible protein-protein docking method based on normal mode analysis of elastic network models. Here, we present a case study of docking calmodulin, a protein which binds to many other proteins.

LS-AG 12

A bovine adenoviral vector-based H5N1 influenza vaccine produce a complete protection against a heterologous influenza virus challenge

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Dr. Suresh Mittal

Several human and nonhuman adenoviral (AdV) vectors including bovine AdV type 3 (BAdV-3) have been developed as gene delivery vectors to supplement and/or to elude human AdV (HAdV)-specific neutralizing antibodies (vector immunity). Here we evaluated the vaccine immunogenicity and efficacy of BAdV-3 vector (BAd-H5HA) expressing hemagglutinin (HA) from a H5N1 influenza virus in a dose escalation study in mice using the intranasal (i.n.) or the intramuscular (i.m.) route of inoculation in comparison with the HAdV type C5 (HAdV-C5) vector (HAd-H5HA) expressing HA of a H5N1 influenza virus. Dose-related increases in responses were clearly noticeable. A single i.m. or i.n. inoculation with BAd-H5HA resulted in an enhanced humoral and cellular immune response and conferred a complete protection following the challenge with a heterologous H5N1 virus compared to that of HAd-H5HA. The results suggest that at least 100-fold dose-sparing can be achieved with BAd-H5HA vector compared to HAd-H5HA vaccine vector.

LS-AG 13

Development of novel gene-editing tools

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Kevin Solomon

Gene-editing tools have revolutionized the life sciences by enabling precise DNA modification in many species for the first time. Although the popular tool, CRISPR/Cas9, has accelerated genome engineering, it requires a sequence-specific motif that restricts its use to specific DNA regions. Here, we develop an alternative tool without this limitation. Phylogenetic analysis of the candidate protein suggests it belongs to a previously unclassified group of prokaryotic immune systems characterized by a repA domain absent in all studied family members. Heterologous expression of the protein cleaves DNA randomly, but can be programmed with DNA guides in *E.coli* to target specified regions. We demonstrate that one mutant can be targeted with programmable DNA guides to increase genome editing efficiency in *E.coli* by 55±16%. Collectively, our study provides insight into a flexible new tool for precise gene-editing with expanded applications in basic research, biotechnology, and medicine.

LS-AG 14

Targeting Multi-Drug Resistant *Candida auris* by a combination therapy of sulfamethoxazole and triazole antifungal agents.

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Mohamed Seleem

Recently, *C. auris*- an emerging multi drug resistant yeast pathogen- has been implicated in numerus outbreaks all over the globe, causing high mortality rate (~ 60%) and presenting serious medical challenge. Thus, finding co-drugs to overcome resistance to the frontline antifungal drugs especially azoles would be of prime clinical importance. Herein, we evaluated the ability of sulfamethoxazole/ azole combination to inhibit the growth of azole resistant *C. auris.* Utilizing checkerboard and time kill assays, sulfamethoxazole exhibited potent *in vitro* synergistic interaction with azole antifungal drugs and restored their fungistatic activity in 25 % of the clinical isolates. This activity was further confirmed *in vivo* in a *C. elegans* infection model. Sulfamethoxazole/ azole combination sustained the survivability of the infected worms by 70 %. Notably, our data indicates that the efficacy of this novel combination is dependent on the underlying mechanism of azole resistance. Mutant strains which resist azoles by either over production of/ or decreased affinity to the azole target (ERG11p) were highly susceptible to sulfamethoxazole/ azole combination. However, this synergism was totally lost against mutants which demonstrated hyperactivity of efflux pumps. In conclusion, sulfamethoxazole stands as a promising co-drug that can restore the efficacy of azole antifungal drugs in resistant isolates of *Candida auris*.

LS-AG 15

A Robust *in vivo* model of Brain Metastases of Lung Cancer

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LT Lyle

The blood-brain barrier (BBB) results in ineffective treatment of brain metastases. The BBB shifts to the blood-tumor barrier (BTB) in the presence of metastases. To investigate changes in the BTB in non-small cell lung cancer (NSCLC), we developed a robust experimental model using brain-seeking adenocarcinoma NSCLC cells (A549-Br) to evaluate pathology and identify druggable targets. Brain metastases were evaluated over 1-6 weeks; there was a 3-fold increase in brain metastasis between 3 and 6 weeks. At six-weeks, mice developed an average of 10 metastases. Interestingly, spinal cord metastases were present, causing paralysis. A striking variation in histologic features of neoplastic cells was observed within tissues and single metastases. This is the first comprehensive pathologic description of an *in* vivo model of brain metastases of NSCLC, adenocarcinoma subtype. The shift to the BTB will be evaluated in all models, which will assist in developing effective therapies to improve quality of life.

LS-AG 16

Changes in skin lipid composition in a mouse model of dermatitis analyzed by mass spectrometry imaging

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Skin lipids are both structural components and bioactive molecules involved in cell signaling and activation. Altered lipid composition is associated with diseases like atopic dermatitis (AD). SHARPIN-deficient *cpdm* mice develop a chronic dermatitis with similarities to AD. We used two mass-spectrometry approaches, mass-spectrometry imaging (MSI) and an untargeted profiling strategy, to gain knowledge of changes in skin lipids of cpdm mice compared with wild-type that may have clinical utility. MSI was successful at providing spatial location of lipids. Overlay of cholesterol sulfate against ubiquitous phosphatidylinositol (38:4) images, showed that cholesterol sulfate was restricted to the epidermis and reduced in cpdm compared to wild-type mice. Lipid related to cell signaling and inflammation, like linoleic, arachidonic and docosatetraenoic acid, and plasmalogen pPC(34:0), were increased in cpdm compared to wild-type by both mass-spectrometry approaches. The identification and location of these lipid changes may provide the basis for a new molecular-diagnostic strategy of dermatitis.

LS-AG 17

A genetic approach to pinning down the wanderer: Mapping vagal afferent innervation of the mouse small intestinal mucosa

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Vagal afferents supplying the small intestine mucosa play a role in regulating feeding, yet their morphology and distribution remains largely unknown. Selectively labeling a large proportion of vagal afferents independent of other extrinsic and intrinsic innervation has been challenging. We used a transgenic Nav1.8-Cre-Tomato mouse exhibiting fluorescence in 80% nodose and DRG cells. To estimate the vagal contribution to this innervation, features of nerve fibers in villi and crypts were compared in Nav1.8-Cre-Tomato mice with (VAGX) and without (CON) abdominal-vagotomy. CON mice exhibited a proximal to distal decrease in the mean number of fibers entering a villus, of fiber crossings at a villus mid-height line, and of crypts closely apposed to fibers. VAGX mice showed stable numbers in all measures along the entire small intestine length. These findings suggest most labeled afferents in the mucosa of Nav1.8-Cre-Tomato mice are vagal, especially in proximal afferents crucial for regulating food intake.

LS-AG 18

Studying the Influence of Cobalt and Nickel on Tungsten Toxicity in Zebrafish (*Danio rerio*)

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Tungsten is a heat-resistant metal. In the 1990s tungsten replaced lead in military munitions. Unexpectedly following this replacement, tungsten was detected in soil and groundwater near military bases. Tungsten is used in pure and alloy forms with cobalt and nickel. As a result, there are rising research questions on the toxicity of tungsten alone and/or in mixtures similar to the composition of tungsten alloy. To assess tungsten's acute developmental toxicity, zebrafish embryos were exposed to different combinations of tungsten, cobalt, and nickel. Survival rates were measured and behavior assessment using a visual motor-response test was performed. Although no significant difference was observed in the survival rate between different combinations, all solutions of 10 parts per million cobalt resulted in decreased velocity, distance swam, and time spent moving. This indicates that cobalt controls behavioral changes observed at these concentrations and that tungsten alone had no behavioral effect on zebrafish larvae.

LS-AG 19

The Soil Microbiome Is Impacted by the Decomposition of Different Cover Crop Species

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Shalamar Armstrong

Cover crop adoption is a rapidly emerging management practice in corn (*Zea mays*) agroecosystems, and it is currently unknown how cover crops impact the soil microbiome. The objective of this study was to determine how cover crop species and residue management treatments impact soil microbial community structure during winter cover crop decomposition. Cover crop treatments included hairy vetch (*Vicia villosa* Roth), cereal rye (*Secale cereal*), a hairy vetch/cereal rye mixture, and a no cover crop control. Residue management treatments included no-tillage and a 15 cm spring tillage. Soil microbial communities (Bacteria) were characterized using the small subunit (16S) rRNA gene sequences determined using the Illumina MiSeq system. Results revealed that cover crop species, sampling date, and residue management treatment significantly influenced the soil microbiome ($p<0.05$). This study enhances our understanding of bacterial abundance patterns influenced by agriculture management practices and can potentially help optimize management practices to promote beneficial microorganisms.

LS-AG 20

Metabolomic Profiling of Glioblastoma using Multiple Reaction Monitoring (MRM) Mass Spectrometry

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Glioblastoma (GBM) is the most common and aggressive form of primary brain tumor. Due to its extremely malignant and invasive nature, current treatment options fail to improve quality of patients' lives. Studies have shown that altered lipids and metabolites in GBM may play a critical role in chemo-resistance, cancer cell initiation and progression governed by oncogenic signaling pathways. This research utilized multiple reaction monitoring (MRM) profiling mass spectrometry to investigate altered lipid and metabolite expressions in GBM tissues using mouse models. Our findings concluded that phosphotidylcholine (PC) and sphingomyelin (SM) were significantly differentiated between GBM10 brain tumors and control, and GBM brain tumors and flank tumors. In contrary, drug treatment study showed the most significance on the level of acylcarnitine. Understanding of metabolic reprogramming and differences between GBM10 tumors and control, orthotopic and subcutaneous tissues, and drug effect on tumors might provide knowledge on the therapeutic targets for GBM.

LS-AG 21.

Toxicity and neurophysiological impacts of essential oil components on bed bug (*Cimex lectularius* L.)

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Bed bugs (*Cimex lectularius* L.) are economically and medically important global human parasites. Integrative pest management approaches have been proposed for bed bug control. This study aims to define insecticidal activity and neurophysiological impacts of essential oil components from different plant sources. The topical and fumigant toxicity of 15 different compounds was evaluated against adult male bed bugs. Neurological effects of four toxic compounds; carvacrol, thymol, eugenol and citronellic acid were also investigated using electrophysiology technique. In topical application bioassays, carvacrol was most toxic to bed bugs whereas thymol showed highest toxicity in fumigant exposure bioassays. Spontaneous electrical activity recordings of the bed bug nervous system demonstrated neuroinhibitory effects of carvacrol, thymol and eugenol while citronellic acid produced neuroexcitation. These comparative toxicity and neurological activity findings, coupled with future synergism and target site studies will provide a vital platform for formulating effective essential oil-based insecticides for bed bug IPM.

LS-AG 22.

***In vivo* direct reprogramming restores local circuit connectivity after focal stroke**

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Stroke is a leading cause of severe morbidity and mortality. Neuronal loss is accompanied by a proliferation of reactive astrocytes and the formation of a glial scar, which is a major hurdle to re-innervation and functional recovery following stroke. *In vivo* direct reprogramming is a novel technology that transforms reactive astrocytes into mature neurons by overexpressing the gene, NeuroD1.. We used Channelrhodopsin Assisted Circuit Mapping to measure local circuit connectivity in mouse visual cortex after endothelin-1 induced local ischemia. After focal stroke and without reprogramming, the local connectivity of surviving neurons in the visual cortex was minimal. *In vivo* direct reprogramming transformed reactive astrocytes into functional neurons. These astrocyte-derived neurons demonstrated physiological properties of mature cortical neurons, and had increased circuit connectivity compared to neurons in control animals without reprogramming. The level of connectivity in the reprogrammed animals appears at least comparable to that expected in normal healthy visual cortex. Our work demonstrates that *in vivo* direct reprogramming achieved circuit repair following stroke.

LS-AG 23.

Influence of age and length of exposure to low phosphorus diet on phytase efficacy during the starter phase of broiler chickens

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This study evaluates the impact of age and length of dietary exposure on the efficacy of phytase using growth performance and nutrient utilization as criteria for evaluation. Four dietary treatments were fed at 5 different length of exposure. Diets consisted of two non-phytate phosphorus concentrations and two phytase concentrations. Exposure effect was observed by comparing responses of birds at 14 d and birds at 22 d. Gain to feed ratio improved ($P < 0.01$) in birds supplemented with phytase irrespective of age or exposure length but an increase in exposure length improved ($P < 0.01$) gain from 2 d to 5 d. Increased age from 8 d to 14 d improved ($P < 0.01$) apparent phosphorus and calcium digestibility with phytase supplementation but was lowered ($P < 0.01$) as exposure grew longer than 2 d. In conclusion, phytase efficacy declines with older birds and increased exposure length.

LS-AG 24.

Mapping Soil Spatial Variability at the Agronomy Center for Research and Education (ACRE) to Support Field-Based Phenotyping

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Soil variability is an important factor in field-based plant phenotyping research because a given genotype is likely to express a slightly different phenotype on different soils in the same field. Climate, organisms, relief (topography), parent material, and time are the soil-forming factors that cause soil variation across soil landscapes. Within individual farm fields, however, most of these factors are constant and relief is usually the major factor determining soil variability. Topographic differences influence plant growth and yield through water, nutrient, and sediment movement from higher spots to lower spots in the field. Additional variability is introduced by tile drainage, and by ice-wedge polygons. We are using aerial photography and computer modeling to capture soil variability and develop high-resolution soil maps for ACRE. Aerial photography taken at different times capture soil variability due to plant growth in the original pre-settlement vegetation, tile lines, and ice-wedge polygons.

PHYSICAL SCIENCES

P1.

Efficient Reduction of Disulfide Bonds via Radical Reactions for Facile Peptide and Protein Analysis by MS/MS

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The presence of disulfide linkage in peptides/proteins tends to inhibit the formation of structurally informative fragment ions under conventional collision-induced dissociation. Herein, we report a novel method based on the coupling of a photochemical reduction of disulfide bond and tandem mass spectrometry for facile sequence coverage. The reaction was initiated by photolysis of acetone (photoinitiator) after 254nm light irradiation, which undergoes Norrish type I cleavage to produce acetyl ($\bullet COCH_3$) and methyl ($\bullet CH_3$) radicals. This is followed by hydrogen abstraction from alkyl alcohols (co-solvent) to give hydroxyalkyl radicals. These radicals react with disulfide-linked peptides/proteins (R-S-S-R), reducing disulfides to give free thiols (R-SH) at the cleavage site. Subsequent MS^2 CID of the reduced product gave abundant fragment ions for improved sequence coverage. This radical-induced disulfide cleavage is fast (<5 sec) and selective to disulfides (>95% yield). Furthermore, this method can also be tuned for partial reduction approach for disulfide-linkage assignment.

Post Doctoral Fellow Posters

LIFE, PHYSICAL AND ENGINEERING SCIENCES

PD-LPE 1.

Pathologic Patterns of the Blood-Tumor Barrier in Brain Metastasis of Lung Cancer

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Lung cancer is the leading cause of mortality among all human cancers. In brain metastases, the blood-brain barrier (BBB), which is the tightest and most effective barrier in the body, shifts to the blood-tumor barrier (BTB). Chemotherapy is an ineffective treatment due to the lack of successful delivery across the BTB. Herein, we characterized the molecular differences between the BBB and BTB in brain metastasis of the non-small cell lung cancer (NSCLC). Brain-seeking NSCLC cells were injected into NSG mice via ultrasound guided intracardiac injection to form brain metastasis. Using immunofluorescence staining, we analyzed the components of the BBB and BTB. Our preliminary findings demonstrated that capillaries in BTB are diluted and tortuous. There is a loss of basement membrane, tight junctions and pericytes. These findings will allow us to develop testable hypotheses to manipulate BTB permeability and facilitate effective delivery of chemotherapeutics to treat metastases and improve patient survival.

PD-LPE 2

3D thermo-mechanical modeling of the shock compression of polymer-bonded explosives

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Polymer-bonded explosives are widely used for military applications because of their safety and reliability. However, the strong thermo-mechanical coupling of these materials can lead to a temperature increase in localized regions, called hot-spots, that can cause ignition during handling and manufacturing. At the micrometer length scale, hot-spots can be caused by several mechanisms: crack surface friction, void collapse, plastic dissipation and shear banding. The temperature increase takes place on the microsecond timescale; therefore, the dynamic evolution of the hot-spot is not easily accessible using experiments. We investigate the relative importance of the mechanisms, depending on the load condition, by using dynamic finite element simulations. The crack surface friction turns out to be sufficient to cause ignition for impact velocities around 400 m/s, while plasticity can reduce the temperature increase by relaxing the stress in the material. The developed model is compared to impact experiments carried out at Purdue University.

PD-LPE 3

Tree-fungal interactions help explain plant invasions in temperate forests

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Plant-fungal interactions play an important role in forest community structure and functions; however, the dominant tree-fungal interactions that affect species invasions in forests remain largely unexplored. Using nation-wide forest inventory data, we examined how belowground tree-fungal interactions affect forest soil, and in turn, how the altered forest structure and soil affect understory plant invasions in temperate forests. We found that understory invaders were more abundant in arbuscular mycorrhizal (AM) dominant forests than ectomycorrhizal (ECM) dominant forests, whereas native species had no strong associations with AM tree dominance. Among the soil attributes that were significantly influenced by AM tree dominance, forest litter thickness and soil carbon:nitrogen ratio were significantly associated with understory invasions. Our results suggest that forest structure and dominant mycorrhizal type are closely linked with understory plant invasions. The increased invader abundance in AM dominant forests can further facilitate nutrient cycling, altering ecosystem structure and functions in forest ecosystems.

PD-LPE 4

Phase Separation in Pharmaceutical Formulations – Origin, Characterization, and Implications

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The use of amorphous solid dispersions (ASDs) has become increasingly prevalent for poorly-soluble drugs due to the large solubility enhancement window and permeability advantage. However, ASD performance can be compromised by subtle changes in microstructure, which might be analytically challenging to characterize. Therefore, understanding the phase behavior of drug-polymer blends and its implications on ASD performance are critical to design an optimally performing formulation. In this study, comprehensive investigations on the origin, characterization, and impact on the dissolution performance of different ASDs prepared using solvent evaporation process were carried out. Water was found to induce phase separation even at a trace amount. Advanced high-resolution imaging techniques coupled with orthogonal characterization enabled characterization of ASD microstructure to the nanoscale. The formation of such microstructure was found to improve the dissolution performance of certain ASDs. This study highlights the complexity and importance of formulation microstructure.

PD – LPE 5

PL-PatchSurfer2: a virtual screening method tolerant to receptor structure variation using surface-patch matching

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Computer-aided drug discovery has been an emerging technique to reduce human efforts to find a new ligand. With understanding of protein-ligand interactions, receptor-based virtual screening (RBVS) predicts putative binders of a target protein from a compound library. One of the weak points of RBVS method is that they cannot treat a receptor conformational change properly. Recently, we have proposed a novel RBVS program called PL-PatchSurfer2. The unique feature of this program is surface-patch description instead of all-atom representation in traditional RBVS methods. The chemical characteristics are used to describe surface patch: shape, electrostatic potential, hydrophobicity, hydrogen bonding ability. A complementarity between a receptor pocket and a ligand is obtained by comparing and matching surface patches. Our virtual screening benchmark result showed a better performance with faster speed than DOCK6 and AutoDock Vina, widely-used RBVS methods, especially on holo and modelled structures.

PD LPE – 6

Discovery of a Novel Dibromoquinoline Compound with Potent Antifungal and Antivirulence Activity that Targets Metal ion Homeostasis

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Every minute, three human lives are lost globally due to a fungal infection. Of the most serious threats, species of *Candida* (chiefly *C. albicans*) are problematic given they are a leading source of invasive fungal infections with limited treatment options available clinically. This underscores the need to develop novel antifungal agents with unexploited mechanisms to combat this public health challenge. The present study identified a novel dibromoquinoline antifungal compound (**4b**) that inhibited growth of *C. albicans* at a concentration of 0.5 μg/mL, was non-toxic to mammalian cells at concentrations up to 128 μg/mL, and prolonged survival of *Caenhorhabditis elegans* infected with *C. albicans* compared to the antifungal drug fluconazole. Interestingly, **4b** also demonstrated the ability to interfere with expression of key virulence factors utilized by *C. albicans* to cause infection. Chemogenomic profiling combined with supplementary growth assays revealed **4b** exerts its antifungal and antivirulence effect by targeting metal ion homeostasis.

SOCIAL AND BEHAVIORAL SCIENCES

PD-SBS 1.

To Invest or Not Invest? That is the Advanced Manufacturing Question

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Industry 4.0 describes manufacturing's trend towards automation and data exchange, and includes the Internet of things, cloud computing, predictive analysis, and enhanced auto-response systems. Unfortunately, the seemingly infinite number of high-tech solutions and continuous technology upgrades can leave manufacturing firms overwhelmed, adding to the fact that the ability to accurately estimate return-on-investment is limited. Even more complexity is added to the technology mix when manufacturing firms consider their supply chain partners, as technology and data standards vary across companies. Investing in advanced manufacturing is an important consideration for manufacturing firms who strive to remain competitive in this global economy, but the uncertainty and complexity of where to focus technology investments is a problem facing the majority of manufacturers. The purpose of this poster is to respond to the following question: **What factors influence a manufacturing firm's decision to invest (or not invest) and deploy various Industry 4.0 technologies?**