Purdue University Chapter

The Society of Sigma Xi

Stewart Center, Rooms 214 A-D
February 20, 2019

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 New Way to Interact With Your Gifted Child: Parent-Involvement Enrichment Program

Gray, A., & Lee, H.
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Name of faculty sponsor: Marcia Gentry

The purpose of this study was to explore the characteristics of a university-based enrichment program which was designed as a parent-involvement format. Data from parent surveys ($N = 110$) and teacher interviews ($N=7$) provided insights of what each perceived to be the programs' benefits and shortcomings. Results revealed that parents' satisfaction level with the program had a positive correlation with their motivation level and perceived interaction level with their child. The open-ended part of the parent survey also identified positive responses to the unique program format in which parents were able to observe and interact with their child. Although the in-depth interviews with teachers similarly reported the program benefits of parents interacting with their child in a new learning environment and having quality interactions with their child, they also shared concerns and suggestions related to parenting styles.

SBS 2.

Comparisons with closest and most: Second and fifth graders' conceptions of integer value

Chen Lizhen
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Laura Bofferding

Abstract

Elementary students have difficulty learning integer values as the new knowledge conflicts with their whole number understanding. We administered a pretest and a posttest to 204 second and fifth graders and collected their answers to three types of integer comparison problems: which number is closest to 10, is most positive, and is most negative among three integers. We coded each comparison phrasing for students' integer value mental models and looked at changes in their mental models from the pretest to the posttest. Results showed that second and fifth graders had difficulty determining which of three negative numbers was most positive. They found it relatively easy to determine which of three positive numbers was most positive and which of three negative numbers was most negative. Students had some improvement in their integer value mental models, although their mental model shifts varied by the question phrasing.

SBS 3.

Parents' Perspective of Disproportionate Subject Areas in Enrichment Program: What about Non-STEM Courses?

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Name of faculty sponsor: Marcia Gentry

The purpose of this study was to explore parents' perceptions of enrichment programs to better understand their decision-making and exploring why there is an imbalance in enrichment course offerings in favor of STEM courses. An explanatory mixed methods study, using data from an online survey (N=135) and interviews (N=15), indicated that parents with STEM majors perceive STEM as more important than non-STEM courses, compared to parents with non-STEM majors ($X^2(1) = 4.19$, $p = .041$, $\Phi = .2$). Results showed that parents' enrichment course decisions are influenced by a societal climate that focuses on the importance of STEM, future financial incentives and job opportunities, the rigor of STEM, and a lack of school activities that focus on this. Furthermore, parents take their child's needs and interests into account as the main factors in choosing which courses to sign up for, and they actively involve their child in the decision-making process.

SBS 4.

Assessing Students' Conceptual Understanding of Calculus Using Item Response Theory

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Faculty Sponsor: Chantal Levesque-Bristol

The Calculus Concept Inventory (CCI) is a popular test of conceptual understanding of differential calculus. However, the CCI is lengthy, and studies documented inconsistent findings regarding the reliability and validity of the instrument. Given that item response theory (IRT) has advantages over classical test theory when analyzing concept inventory data, we used IRT to validate a short version of the CCI (S-CCI). We found that the S-CCI is sufficiently capable of assessing students' conceptual understanding of calculus, especially for students with high-level abilities. Next, we compared the effectiveness of using IRT-estimated abilities and normalized gain as measures of learning gains. Our findings showed that the IRT-estimated gain is a stronger predictor of academic outcomes than the normalized gain. Then, we compared the IRT-estimated gains between interactively-engaged approach and lecture-based approach. The result indicated that students in the interactively-engaged sections achieved greater gains than the students in the lecture-based sections.

SBS 5.

Following the Fabric: Vlisco's West & Central African Print & The Other Face of Africa

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This project, *"Following the Fabric: Vlisco's West & Central African Print & The Other Face of Africa"* uses Vlisco, a historical Dutch textile manufacture turned contemporary fashion label, as a site to understand the transnational identity of African print fashion fabric and the constructions of identity that are established through Vlisco's advertising campaigns. By following the fabric, this project intends to grapple with questions of race, authenticity, tradition, modernity, and appropriation. Equally important, by interrogating Vlisco's "Other Face of Africa" campaign, this project seeks to pull out the various gendered and racial work that is being done to promote notions of whiteness as sophisticated and modern against the historical backdrop of African backwardness. More broadly this project wants to address questions of neo- and post- colonial discourses in the 21st century in regards to Africa and Europe.

SBS 6.

Neurotrophin-4 is essential for survival of a large proportion of vagal afferents that innervate the small intestinal mucosa

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Dr. Ed Fox

Vagal afferents supplying the small intestine play a key role in regulating satiation and gastrointestinal function. Neurotrophin-4 (NT-4) is essential for survival of vagal mechanoreceptors innervating intestinal, but not stomach myenteric ganglia. We used Nav1.8Cre-tdTomato (Nav-Tom) transgenic mice to label vagal afferents and bred them to NT-4 KO (-/-) mice to investigate the effects of NT-4 loss on vagal mucosal afferents. Immunohistochemical staining was used to label axons and terminals in villi in the small intestine. NT-4-/- mice had a 60% loss of axons entering a villus and 40% loss of terminal branches at villus mid-height compared to NT-4+/- and Nav-Tom mice.There was no difference between NT-4+/- and Nav-Tom. These results suggest a large proportion of vagal intestinal mucosal afferents depend on NT-4 for survival. Loss of vagal afferents to small intestine muscle and mucosa supports an organ-specific model to study the effects on GI physiology and feeding behavior.

SBS-7.

Study on the imposition of China's tariffs on Indiana hardwoods export

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Name of faculty sponsors: Drs. Mo Zhou and Eva Haviarova

Since 2010, Indiana's hardwood industry has ranked the sixth in the state's manufacturing sector, with exports of hardwoods playing a major role in the overall sales. Specifically, China has been Indiana's largest logs and lumber importer and the third importer of veneer in 2017. In this study, the impact on Indiana's hardwoods industry will be evaluated after China's tariffs employed. The two-stage partial equilibrium displacement model is adopted to measure the vertical linkage between the log and lumber. The results show that the profits for producers of Indiana's hardwoods are devastated by China's import tariffs. However, native customers are the most beneficial part. Besides, China lost most welfare as producer and customer surplus are negative. As joint products in hardwood industry, lumber and veneer show the substitute characteristic. Additionally, the trade diversion effect exists since there exists positive welfare changes for the rest of the world in this trade intervention.

SBS-8.

Automatic Content analysis of Dream Reports: Test of Continuity Hypothesis and detection of gender and blindness

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Richard Schweickert

The statement that dreams reflect the dreamer's waking life, known as the continuity hypothesis of dreaming, is largely supported by dream research. Linguistic Inquiry and Word Count (LIWC), as a well-validated tool for measuring psychological features in language usage, has not gained enough attention from dream researchers. Study 1 tested the consistencies between waking life and dream in terms of gender differences and whether a dreamer was blind or not by word frequency analysis using LIWC. Based on results of Study 1, we built machine learning models to predict the gender and sightedness of dreamers using dream reports. Our study uses a stringent methodology to find evidence for regularity and order in dreams.

SBS – 9.

Exploring First-Year Engineering Students' Reflection Behaviors, Academic Performance, and Their Relationship to Self-Efficacy

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Muhsin Menekse

The purpose of this study is to investigate first-year engineering students' reflection, academic performance and their relationship to their self-efficacy. Students' reflection data were collected via an educational mobile application called CourseMIRROR. Students' reflection data was coded based on reflection rating and reflection elaboration. Reflection rating indicates the level of difficulty that individual student felt. Reflection elaboration indicates how much elaborated that each reflection was. The results indicated that the students' self-efficacy decreased significantly at the end of the semester. In addition, exam 1 and exam 2 scores were positively correlated to the post self-efficacy survey score with the moderate level. Reflection rating at time point 1 was negatively correlated to post self-efficacy survey score with moderate level as well. Reflection elaboration at time point 2 and 3 were positively correlated to post self-efficacy survey with moderate to high level.

SBS-10.

Efficacy of Service Dogs for Reducing Symptom-Severity in Veterans and Military Members with Posttraumatic Stress Disorder

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Dr. Maggie O'Haire

Emerging research has indicated that service dogs trained for veterans and military members with posttraumatic stress disorder (PTSD) may be an effective complementary treatment for reducing PTSD symptom-severity. However, skepticism remains high in facets of society including policy makers, medical providers, and the public, due to the limited number of empirical studies. The present study uses a cross-sectional design to compare symptoms measured by the PTSD Check List (PCL-V). Participants included 186 post-9/11 veterans and military members; 112 receiving usual care in addition to having a service dog and 74 receiving usual care alone while on waitlist for a service dog. Controlling for age, gender, relationship status, children, and pet dog-ownership, analysis identified that participants with a service dog experienced significantly lower symptom-severity than those without a service dog ($p<.001$). Therefore, this study provides reinforcing evidence that service dogs may effectively reduce symptom-severity for veterans and military members with PTSD.

ENGINEERING SCIENCES

E1.

FLUID-STRUCTURE INTERACTIONS AT DROP-DROP INTERFACE DURING DROP-ON-DEMAND PRINTING OF HYDROGEL-BASED SOFT MATERIALS

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Bumsoo Han

Hydrogel-based materials are widely used to be integrated into 3D configurations with varying functional properties. Among various 3D printing techniques, drop-on-demand (DOD) printing enables advanced additive manufacturing of functional soft materials by depositing hydrogel droplets with desired functional properties at desired positions with appropriate timing between adjacent droplets. However, there is limited mechanistic understanding of the droplets' behaviors. In this study, based on a hypothesis that a complex interaction between polymer matrix and interstitial water occurs during this dropwise gelation-dehydration, we characterized the gelation of printed droplets and their subsequent dehydration phenomena experimentally and computationally to establish a mechanistic understanding of water-polymer matrix interactions. The present computational model can provide a mechanistic explanation of the drop-drop interaction, and enable the prediction of spatiotemporal porosity, ultimately functional properties, of printed hydrogels.

E2.

Derivation of Upper Limb Joint Reaction Forces Using Commercial Virtual Reality System

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Bradley Duerstock

Patients with Spinal Cord Injury (SCI) have limited time with supervised therapy in rehabilitation hospitals making regular therapy at home imperative. However, therapy at home tends to be repetitive, and conventional clinical measures of performance cannot be completed. We present the use of a commercially available virtual reality (VR) gaming system with customised hardware to assist in rehabilitation of individuals with SCI. Data collected by playing a customized game on an HTC Vive provides kinematic data from the shoulder and arm. Inverse dynamics calculations allow determination of joint reaction forces. These forces provide information about muscular effort which is relevant to therapy. Clinicians can use this data to determine the improvement in an individual's exertion levels and effort put into rehabilitation.

E3.

Enhancement of intracellular compound from tomato by Pulsed Electric Field

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Raji Sundararajan

Pulsed Electric Field (PEF) is a novel and emerging technology to achieve better cellular disintegration. Exposure of cells to PEF creates temporary pores on the cell membrane which facilitates the mass transfer of intracellular compounds to the surrounding media through the temporarily created pores. Our work deals with the enhancement of intracellular compounds, such as lycopene, polyphenol, and antioxidants in the tomato. PEF with field strength of 1250-5000 V/cm, pulse duration of 100 μs, pulse interval of 100 ms, and 50 pulses was applied to the tomato juice using BTX ECM 830 electroporator. Our results indicate that applying 50 pulses of 5000 V/cm electric field intensity with the pulse duration of 100 μs to tomato enhances the amount of lycopene by 93.75%, polyphenol by 51.08%, and antioxidant activity by 34.30%. Our results indicate that PEF is a promising technique to improve the lycopene extraction and to reduce the extraction time.

E4.

MAGIC: A Fundamental Framework for Gesture Representation, Comparison and Assessment

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Dr. Juan Wachs

Gestures play a fundamental role in instructional processes between agents. However, effectively transferring non-verbal information becomes complex when agents are not co-located. Recently, remote collaboration systems that transfer gestural information have been developed. Nonetheless, these systems relegate gestures to an illustrative role, only transmitting a representation of the gesture. We argue that gestures can provide information of how well the tasks are being understood and performed. While gesture comparison frameworks exist, they rely on gesture's appearance, leaving semantics and pragmatics aside. This work introduces the Multi-Agent Gestural Instructions Comparer (MAGIC), an architecture that represents and compares gestures at the morphological, semantical and pragmatical levels. MAGIC abstracts gestures via a three-stage pipeline based on a taxonomy classification, a dynamic semantics framework and a constituency parsing. This work shows the feasibility of the framework by assessing MAGIC's gesture matching accuracy against other gesture comparison frameworks during mentor-mentee remote collaborative physical task scenarios.

E5.

Accuracy Assessment of Aircraft Transponder-Based Technology for Measuring Operations at Non-Towered Airports

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John H. Mott, PhD

Accurate airport operations counts are important for determining appropriate funding allocations for airport development and improvement. Fewer than 270 of 2,950 non-primary airports in the United States have air traffic control personnel who are available to count airport operations. This project validates a cost-effective counting technology based on a technique that uses signal strength obtained from aircraft transponders to register the occurrence of aircraft operations at non-towered airports. Over 50 million transponder records were collected from two different versions of system, which were installed at three airports in Indiana. The error rates of estimated operations counts based on transponder signals from Version I and II system are ranging from -10.2% to +7.6% and -4.9% to -1.4% respectively when compared with those obtained from the FAA's Air Traffic Data System (ATADS). The test results suggest that this implementation of the technology is an accurate and cost-effective way to count aircraft operations.

E6.

Harnessing Unipolar Threshold Switches for Enhanced Rectification

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Name of faculty sponsor: Dr. Sumeet Gupta

Threshold switches (TS) represent a class of material that exhibit abrupt, electrically triggered insulator ↔ metal and metal ↔ insulator phase transitions. Ag/HfO_2/Pt is a unipolar TS which exhibits such transitions only with positive voltage polarity. The electrical behavior of this material system is quite like a diode. However, the Ag/HfO_2/Pt exhibits hysteresis in its characteristics which can be utilized for interesting applications. We demonstrate the utility of such unique properties of this material in a diode-based circuit called *Cockcroft-Walton* multiplier. We show that, utilizing an ingenious approach involving the hysteresis, we can create 50% larger DC output from this circuit using Ag/HfO_2/Pt based rectifier, compared to a diode-based implementation. We also show that, the benefits become even more pronounced for higher frequency and for larger number of stages in the circuit. This unique rectifier has immense potential to enable efficient rectification in low voltage analog circuit design.

E7.

Stochastic Modeling of Transforming Growth Factor Receptor Formation

Ingle, Michelle[1,*], Madamanchi, Asakiran[1], Thompson, Matthew[1], Wang, Xu[1], Li, Linlin[1], Wu, Tzu-Ching[1], Hinck, Andrew[2], Umulis, David[1]
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David Umulis

TGF-β2 is a small secreted signaling protein vital to cell growth and development in the animal kingdom. Its full signaling capability is through a tetrameric complex made up of two TGF-β type I and two type II receptors. The TGF-β2 pathway relies on a nonsignaling coreceptor betaglycan in order to facilitate receptor interaction. While essential, Betaglycan's mechanism of action is not yet understood. We developed deterministic and stochastic models of betaglycan and TGF-β2 signaling. Through computational screens we are testing alternative hypotheses for betaglycans role in the pathway. Early results suggest that betaglycan functions to alter reaction kinetics to confer the measured boost in complex formation and it cannot function as stronger source of available ligand to receptors. This model will provide researchers with more knowledge on how to exploit the differences in the interaction between receptor species to develop TGF-beta inhibitors for treatment of cancer or fibrosis.

E8.

A numerical method to simulate boiling in two-phase flows.

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Advisor: Sadegh Dabiri

Two-phase flow and heat transfer has a wide variety of applications ranging from nuclear reactors, to computer chip cooling, and the efficient design of these systems requires a clear understanding of the mechanisms by which two-phase flows enhance heat transfer. With the rapid growth in computing power, CFD is becoming an increasingly reliable predictive tool to understand the physics underlying two-phase flow and heat transfer. We identify the two chief phenomena affecting heat transfer in two-phase flows as being the enhanced convection in bubbly flows, and phase change respectively.
The present work is focused on building a numerical model based in the front-tracking framework to simulate boiling/condensation in two-phase flows. We validate the proposed model by comparison with two benchmark cases and two experimental studies. Further, we build a simple physics based model for the initial micro-layer thickness in nucleate boiling and present validations based on two experimental cases.

E9.

On the Economics of Offline Password Cracking

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Jeremiah Blocki

We develop an economic model of an offline password cracker which allows us to make quantitative predictions about the fraction of accounts that a rational password attacker would crack in the event of an authentication server breach. We apply our economic model to analyze recent massive password breaches at Yahoo!, Dropbox, LastPass and AshleyMadison. All four organizations were using key-stretching to protect user passwords. In fact, LastPass' use of PBKDF2-SHA256 with 10^5 hash iterations exceeds 2017 NIST minimum recommendation by an order of magnitude. Our analysis paints a bleak picture: the adopted key-stretching levels provide insufficient protection for user passwords. On a positive note our analysis demonstrates that memory hard functions (MHFs) such as SCRYPT or Argon2i can significantly reduce the damage of an offline attack. Based on our analysis we advocate that password hashing standards should be updated to require the use of memory hard functions for password hashing.

E10.

In situ Observation of Adiabatic Shear Band Formation in Aluminum Alloys

Nie, Y.[1], Claus, B.[1], Gao, J.[1], Zhai, X.[1], Kedir N.[2], Chu, J.[1],
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Prof. Weinong W. Chen

Shear banding can be observed in various materials during impact loading, which plays an important role in material behaviors. In this work, we used high-speed X-ray phase contrast imaging and infrared thermal imaging techniques to experimentally study the formation processes of adiabatic shear bands in aluminum 7075-T6 and 6061-T6 alloys. A modified compression Kolsky bar setup was used to apply the dynamic loading. A flat hat-shaped specimen design was adopted for generating the shear bands at the designated locations. Experimental results show that the 7075-T6 exhibits less ductility and a narrower shear band than 6061-T6. The maximum temperature generated in the shear band was determined at 720 K for 7075-T6 and 770 K for 6061-T6. This local high temperature zone and the resulting thermal instability were found closely related to the shear band formation in these aluminum alloys.

E11.

Fluid-Structure Interactions At Drop-Drop Interface During Drop-On-Demand Printing Of Hydrogel-Based Soft Materials

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Bumsoo Han

Hydrogel-based materials are widely used to be integrated into 3D configurations with varying functional properties. Among various 3D printing techniques, drop-on-demand (DOD) printing enables advanced additive manufacturing of functional soft materials by depositing hydrogel droplets with desired functional properties at desired positions with appropriate timing between adjacent droplets. However, there is limited mechanistic understanding of the droplets' behaviors. In this study, based on a hypothesis that a complex interaction between polymer matrix and interstitial water occurs during this dropwise gelation-dehydration, we characterized the gelation of printed droplets and their subsequent dehydration phenomena experimentally and computationally to establish a mechanistic understanding of water-polymer matrix interactions. The present computational model can provide a mechanistic explanation of the drop-drop interaction, and enable the prediction of spatiotemporal porosity, ultimately functional properties, of printed hydrogels.

E12.

Recognition of Blind Users' Image Exploratory Behaviors Using Spike-timing Neural Networks

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Bradley S. Duerstock and Juan P. Wachs

Individuals who are blind adopt multiple procedures when they are tactually exploring images. Automatically recognizing these procedures is the first step towards the development of intelligent systems that assist users exploring and understanding images more efficiently. For this purpose, we developed a computational framework that classifies these procedures. Translation-, rotation- and scale-invariant features were firstly extracted from the trajectories of users' movements. These features were then encoded by spike-timing neural networks. The framework employed a distance-based classification scheme with Dempster-Shafter Theory fusion to determine the procedure type. A performance of 94.55% classification accuracy was achieved by experimentation using different spiking neurons dynamics. Experimental results indicated that the framework is effective in classifying spatio-temporal data, as compared to alternative approaches such as Dynamic Time Warping and Hidden Markov Models. The proposed framework serves as the fundamental block to development assistive interfaces for exploring and understanding images for the blind.

LIFE SCIENCES AND AGRICULTURE

LS-AG 1.

Nox2/Cybb Is Required For Proper Axonal Pathfinding In Developing Zebrafish Nervous System

Aslihan Terzi, Cory J. Weaver, Haley Roeder, Theodore Gurol, Qing Deng, Yuk Fai Leung, and Daniel M. Suter
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Daniel M. Suter

In the central nervous system (CNS), ROS have been associated with neuronal progenitor differentiation, cerebellar development, neurite outgrowth, and establishment of neuronal polarity. Here, we provide evidence that an ROS-producing enzyme, NOX is required for proper axonal pathfinding in developing zebrafish nervous system. We found that inhibiting Nox enzymes resulted in the disruption of retinal development and retinotectal pathway defects. *nox2*$^{-/-}$ mutants exhibited increased ganglion cell layer (GCL) thickness in the retina, along with mistargeting of retinal ganglion cell (RGC) axons. In situ hybridization with the well-established CNS markers showed that the *nox2*$^{-/-}$ mutants did not have defects in general CNS development but in the formation of specific neuronal connections. In vitro, cultured RGC neurons derived from *nox2*$^{-/-}$ mutant exhibited different growth response to guidance cues slit-2 and netrin-1, suggesting a cell-autonomous relationship between Nox2 and axonal growth and guidance. We are testing this hypothesis by mutating Nox2 in RGCs.

LS-AG 2.

Role of cell adhesion and spreading phenotypes in Lowe Syndrome pathogenesis.

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Faculty sponsor: Dr. R. Claudio Aguilar

Lowe Syndrome (LS) is an X-linked congenital disorder caused by mutations in the gene *OCRL1* that encodes a lipid phosphatase. Patients are born with bilateral congenital cataracts, renal dysfunction and mental retardation. Unfortunately, LS causes premature death of affected children due to kidney failure and has no cure. We previously determined that Ocrl1 deficiency leads to abnormalities in cell spreading and migration- processes critical for embryogenesis. We have recently obtained strong evidence that suggests patient cells have adhesion as well as signaling defects that may contribute to the spreading and migration abnormalities as well as cell death. We hypothesize that these novel phenotypes in LS patient cells contribute to the multi-organ involvement of LS. Importantly, using a drug- repurposing strategy, we have identified an FDA-approved compound that can suppress these phenotypes. This study expands our understanding the molecular mechanism of LS pathogenesis; providing the basis for development of LS-specific therapeutic.

LS-AG3.

Uncovering the Shared Genetic Basis across childhood-onset neuropsychiatric disorders: ADHD, ASD, OCD and TS

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Dr. Peristera Paschou

Attention Deficit/Hyperactivity Disorder (ADHD), Obsessive Compulsive Disorder (OCD), Autism Spectrum Disorder (ASD) and Tourette Syndrome (TS) are four of the most prevalent childhood-onset neurodevelopmental disorders. High comorbidity rates across these four disorders indicate the possible existence of a common etiological thread connecting all of them. In this work, we evaluated pairwise genetic correlations between each possible combination of two, and further investigated potential common genetic basis shared across them through a series of systematic pairwise and joint genome-wide meta-analyses using summary statistics from genome-wide association study (GWAS) of each individual disorder. We uncovered important clues supporting the overlapping mechanisms underlying on these four childhood- and adolescence-onset disorders on single-nucleotide polymorphism (SNP), gene and pathway levels. By reveling the shared genetic basis of all four disorders, we provided further support for the hypothesis of a common etiological basis for a spectrum of correlated neurodevelopmental phenotypes.

LS-AG4.

Identifying the genetic basis of Myasthenia Gravis through analysis of genomewide data

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Dr. Peristera Paschou

Myasthenia gravis (MG) is an autoimmune disease of the neuromuscular junction. Previous studies have revealed variants associated with the disease, but there is not complete overlap between them, indicating that further elucidation is needed. Here, we are using a Southern-European dataset to explore the common and rare genetic variation of the disease, by performing a GWAS and the first CNV analysis in MG. The GWAS identified 156 SNPs, in 8 loci, reaching the suggestive association level (P-value≤1×10−5). The strongest association was in the THEMIS gene (P-value: 1.40×10-7, OR:1.954). 5 genes remained significant after Bonferroni correction of the gene-based analysis. Our results are supporting the previous studies, as the meta-analysis revealed. The CNV analysis revealed 10 rare duplications significantly associated with MG. Overall, our analysis provides an insight into the genetic architecture of MG, as it reveals some novel associated variants and detects associations in known loci.

LS-AG5.

Molecular determinants of the differential modulation of Cav1.2 and Cav1.3 by nifedipine and FPL 64176

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Gregory H. Hockerman

Nifedipine and FPL 64176 (FPL), which block and potentiate L-type voltage-gated Ca^{2+} channels respectively, more potently modulate $Ca_v1.2$ than $Ca_v1.3$. To identify potential strategies for developing subtype-selective inhibitors, we investigated the role of divergent amino acid residues in transmembrane domains IIIS5 and the extracellular IIIS5-3P loop region in modulation of these channels by nifedipine and FPL. Insertion of the extracellular IIIS5-3P loop from $Ca_v1.2$ into $Ca_v1.3$($Ca_v1.3$+) reduced the IC50 of nifedipine significantly, and substitution of S1100 with an A residue in $Ca_v1.2$, accounted for this difference. Substituting M1030 to V in $Ca_v1.3$+($Ca_v1.3$+V) further reduced the IC_{50} of nifedipine. FPL increased current amplitude in $Ca_v1.3$+V and changed activation/inactivation kinetics. We conclude that the M/V variation in IIIS5 and the S/A variation in the IIIS5-3P loop of $Ca_v1.2$ and $Ca_v1.3$ largely determine the difference in nifedipine potency between these two channels, but the difference in FPL potency is determined solely by divergent amino acids in the IIIS5-3P loop.

LS-AG6.

Turmeric: Add Spice to your life, let *Clostridium difficile* not thrive

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Clostridium difficile infection (CDI) poses a significant threat to the public, with ~500,000 infections, 29,000 deaths annually in the USA. Emergence of new hyper-virulent strains with increased prevalence, and high recurrence and relapse rates has made the issue more worrisome. The current study is aimed at testing the efficacy of derivatives of a natural spice, turmeric, to treat CDI. On evaluation against a broad array of clinical isolates, 3 out of 6 compounds screened were found to have anticlostridial activity with their Minimum Inhibitory Concentrations (MICs) ranging from 8 – 32 µg/ml. In addition, derivatives were able to inhibit toxin production and spore formation. The compounds were not toxic to colorectal mammalian cells and had no activity against gastrointestinal microflora. This study provides evidence that turmeric's derivatives have great potential to be exploited for treatment of CDI, and lay a foundation for further analysis and development

LS-AG7.

Breaking Barriers: Blood-Brain Barrier Alterations in Lung Cancer Brain Metastases

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The incidence of lung cancer brain metastases, particularly non-small cell lung cancer (NSCLC), is increasing. The blood-brain barrier (BBB) at the level of microvasculature results in ineffective delivery of therapeutics to brain metastases. We aim to identify structural alterations of the BBB in NSCLC brain metastases. We hypothesized a distinct difference within the BBB of NSCLC brain metastases will be present compared to the surrounding brain and control brains. To identify these changes, we developed an experimental model using brain-seeking patient derived NSCLC (A549). Functional components were analyzed using immunofluorescence microscopy. Our results demonstrate a loss of tight junction adaptor proteins, diminished basement membranes, and decreased reactive pericytes in NSCLC brain metastases compared to controls. Furthermore, astrocytic endfeet were markedly decreased in NSCLC metastatic lesions compared to controls. Identified alterations, including astrocytic end-feet and pericytes may serve as therapeutic targets for treatment of NSCLC brain metastases and improve patient survival.

LS-AG8.

Repurposing Lopinavir For Targeting Azole-Resistant *Candida* Species

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Abstract:

The limited number of antifungals and the rising incidence of azole-resistant *Candida* infections pose a significant challenge to human medicine. Combinatorial therapy is an appealing approach to augment the activity of current antifungals. We evaluated the azole chemosensitization capability of FDA approved drugs against azole-resistant *Candida albicans*. Our screening uncovered a promising azole chemosensitizing activity of lopinavir, an HIV antiviral agent. Lopinavir displayed a broad-spectrum azole chemosensitization activitiy against a wide range of medically important *Candida* species, including *C. albicans, C. tropicalis,* and the emerging multidrug-resistance *C. auris*. At a clinically applicable concentration (4-8 μg/ml), lopinavir displayed a potent synergistic activity with azole drugs, including fluconazole, itraconazole, and voriconazole. Flow cytometry and Nile Red efflux assays revealed a significant efflux inhibitory activity of lopinavir, underlining its potential mechanism of action. This study reveals lopinavir as a novel, potent and broad-spectrum azole chemosensitizing agent that warrants further investigation against *Candida* infections.

LS-AG9.

Microtubule Assembly and Translocation During Axonal Elongation

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Growth cones are highly motile structures at the distal tips of elongating axons. These sensory vehicles migrate to precise targets in the developing nervous system. Previous studies have shown microtubule assembly and dynein-mediated microtubule translocation are required for axonal elongation. However, the relative contributions of microtubule dynamics and dynein activity have not been fully explored. Here, we investigated how microtubule assembly, microtubule movement, and dynein activity relate to elongation of *Aplysia* neurites using phase contrast and fluorescent speckle microscopy. Pharmacologically inhibiting either microtubule assembly or dynein activity reduced anterograde velocity of individual and bulk microtubule translocation as well as neurites. Inhibiting both processes simultaneously had a less negative effect compared to individual treatments, indicating microtubule translocation and assembly are interdependent. This finding was confirmed by immunolocalization of dynein. Our results strongly suggest microtubule assembly is required for dynein-mediated microtubule translocation and neurite elongation.

LS-AG10.

Repurposing non-antimicrobial drugs and clinical molecules to combat drug resistant Neisseria gonorrhoeae

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Gonorrheal infections, caused by drug resistant *Neisseria gonorrhoeae*, continue to pose a significant risk to global public health, resulting in an estimated 78 million new cases worldwide and 820,000 new cases in USA annually. Furthermore, *N. gonorrhoeae* developed resistance to nearly every antibiotic used to treat it, no vaccine exists, and infection is associated with debilitating, lifelong negative outcomes such as infertility and ectopic pregnancy. There is a pressing need for a simple, safe, and cost-effective solution to this problem. This study is the first to report a wide-scale screening effort to repurpose drugs for treatment of *N. gonorrhoeae*. The NIH Clinical Collections containing 727 FDA approved drugs and small molecules previously used in human clinical trials with known safety profiles were screened against multidrug resistant *N. gonorrhoeae*. Our initial screening identified 87 non-antibiotic drugs and clinical molecules. Remarkably, certain potent inhibitors that were not reported before showed activities. Overall, the current study presents novel inhibitors for *N. gonorrhoeae* with FDA-approved safety that warrant further investigation.

LS-AG11.

A novel strategy to combat methicillin-resistant Staphylococcus aureus infection

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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- 4 μg/mL. Furthermore, the compounds were found to be non-toxic against murine macrophage cell line (J774) up to a concentration of 16 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-AG12.

Drug repurposing approach identified Ebselen as a broad spectrum antifungal compound

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Invasive fungal infections, particularly those caused by Candida, Cryptococcus and Aspergillus have become a serious global public health threat. Moreover, the development of new antifungal agents is currently unable to keep pace with the urgent demand for safe and effective new drugs. One strategy, which warrants more attention for identifying new antifungals, is drug repurposing. In this study, a drug repurposing approach explored the antifungal activity of ~ 2,200 FDA approved drugs. Our screening identified Ebselen an organoselenium clinical molecule considered clinically safe but without proven use, as a potent antifungal activity.
Ebselen showed potent activity against different clinical isolates of Candida, Cryptococcus and Aspergillus with minimum inhibitory concentration range 0.5-8 μg/ml. Moreover, ebselen inhibited the biofilm forming capabilities of the tested fungal isolates by 40-60 %. Using Caenorhabditis elegans as an in vivo infection model, ebselen protected C. albicans infected worms compared to the untreated control. The current study strongly suggest that ebselen is a promising antifungal candidate and that warrants further investigation.

LS-AG13.

Anticlostridial Drug Repurposing

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Clostridium difficile is a notorious healthcare-associated infection. The unsatisfactory cure rate and the high recurrence rate are urging to develop novel antimicrobials with improved efficacy. In the current study, we screened 3,200 FDA-approved dugs, out of which Fifty-one drugs inhibited the growth of *C. difficile*. Auranofin (an antirheumatic gold-containing drug) was selected for further investigation. Auranofin inhibited the growth of 90% of the tested isolates at a concentration of 2 µg/mL. Further, auranofin was superior to the drugs of choice in inhibiting toxin production and spore formation of *C. difficile*. Additionally, auranofin had an anti-inflammatory activity against *C. difficile* toxin-induced inflammation. Interestingly, other gold-containing compound had diverse activities against *C. difficile*. As a result, we came up with a structure-activity relationship model that can be implemented in the development of potent anticlostridial drugs. Overall, we present auranofin as a potent anticlostridial and provide a platform for developing better anticlostridial drugs.

LS-AG14.

Characterization of a FIC Protein from the Respiratory Pathogen, *Bordetella Bronchiseptica*

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Bordetella sp. are respiratory pathogens, the most notorious being *B. pertussis* which causes whooping cough in humans. In contrast to the human-restricted *B. pertussis*, another species - *B. bronchiseptica* - has a broader host range, and causes various respiratory disease including kennel cough in dogs. Interestingly, while *B. bronchiseptica* infection in humans is rare, recent reports indicate an increase in the number of *B. bronchiseptica* infections in immunocompetent humans and suggest involvement of novel virulence factors that may not be under the control of the classical BvgAS two-component signal transduction system. We, therefore, sought to test whether the sole Fic protein in *B. bronchiseptica*, BbFic, could be involved in virulence. Fic proteins are a family of conserved adenylyltransferases that are implicated in several cellular processes including bacterial pathogenesis. Using bacterially expressed and purified WT and catalytically inactive BbFic, we biochemically characterize BbFic and describe the kinetics of its nucleotide usage.

LS-AG15.

Protein intakes greater than versus at the RDA differentially affect lean body mass responses to purposeful stressors: A systematic review and meta-analysis of literature.

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Under stressful conditions such as energy restriction (ER) and resistance training (RT), recommended dietary allowance (RDA) for protein of 0.8 g/kg/d may no longer be appropriate. We aim to assess the effects of protein intake greater than versus at the RDA on changes in whole-body lean mass.

Articles were screened using PubMed, Scopus, CINAHL, and Cochrane databases. Twenty-three comparisons from 19 randomized-controlled, parallel studies were included. Among all comparisons, protein intakes greater than the RDA attenuated lean mass loss after ER [0.41 kg (0.15, 0.67); WMD (95% CI), n=15 comparisons], but not without ER [0.23 kg (-0.44, 0.89), n=8]. Protein intakes greater than the RDA increased lean mass after RT [0.77 kg (0.23, 1.31), n=3], but not without RT [0.29 kg (-0.04, 0.62, n=20].

Protein intakes greater than the RDA positively influence changes in lean mass when adults are purposefully stressed by dietary energy restriction and/or resistance training.

LS-AG 16.

Intradermal Delivery of a Novel Combination Adjuvant Promotes Immunity without Local Adverse Reactions

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The dermal layer of human skin is rich in antigen-presenting cells, making it a promising site for intradermal (ID) vaccination. However, most vaccines are administered intramuscularly (IM). Vaccines often contain adjuvants, which are substances added to vaccines to help promote immunity against infections. However, the FDA approved adjuvants are not applicable for dermal vaccination due to their local reactogenicity. Therefore, there is a need for novel adjuvants to access the likely benefits of ID vaccination. Here, we analyzed the immune response to ovalbumin (OVA) in BALB/c mice after ID vaccination with alpha-D-glucan nanoparticles (Nano-11), and cyclic-di-adenosine monophosphate (cdAMP), both which have adjuvant activities. The Nano-11 and cdAMP combination increased Th1, Th2, and Th17 responses and production of OVA-specific antibodies with no display of reactogenicity. This work suggests that the Nano-11 and cdAMP combination is a potent adjuvant for safe and effective intradermal vaccination.

LS-AG 17.

Identifying critical protein- and microRNA-coding genes that when lost, can potentiate *KRAS*/p53-driven lung tumorigenesis

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Lung cancer is the leading cause of cancer-related deaths. *KRAS* and *TP53* are two of the most commonly mutated genes in lung cancer, and their mutations are well recognized drivers of tumorigenesis. Directly targeting these drivers still remains a challenge for cancer therapeutics. Instead, targeting genes that potentiate *KRAS*/p53-driven tumorigenesis is likely an effective alternative. Therefore, we hypothesize that certain protein- and microRNA-coding genes when lost, can drive cellular transformation of two non-tumorigenic *KRAS*;p53/*Kras*-mutated mammalian lung model systems into cancerous states. To address this, we performed functional CRISPR-mediated gene knockout screen in these two systems using the small guide RNA libraries. We found that genome-wide perturbation induced differential growth rate of the human bronchial epithelial cells that harbored $KRAS^{G12V}$;p53-knockdown (HBEC-KP). Certain knockouts could also support anchorage-independent growth. $Kras^{G12D}$*;Cas9* mouse line was also generated and genome-wide knockouts will be induced directly in murine lungs for evaluating genetic contributions to tumor development.

LS-AG 18.

Determination of the E3 Ligase Interaction Site of Regulator of G-protein Signaling Protein 2

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Regulator of G-protein Signaling Protein 2 (RGS2) is a GTPase-activating protein that primarily targets $G\alpha_q$, reducing duration and amplitude of signaling mediated by $G\alpha_q$-coupled receptors. Deficiencies in RGS2 have been implicated in Alzheimer's Disease, Parkinson's Disease, several cardiac conditions, anxiety, breast cancer, and prostate cancer. As RGS2 is rapidly degraded via the ubiquitin-dependent proteasomal pathway, identifying the binding site between RGS2 and its E3 ligase would open a new avenue for development of therapeutics to treat the aforementioned diseases. The E3 ligase that binds to RGS2 has previously been identified as being composed of Rbx1, Cul4B, DDB1, and F-box Only Protein 44 (FBXO44), with FBXO44 acting as the substrate recognition site. Based on previous research, we hypothesize that the N-terminus of RGS2 binds FBXO44. Our data supports our hypothesis and will assist in the development of a peptide tool compound for future use in high-throughput screening.

LS-AG 19.

The cortical representation of illusory contours requires higher-order input

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Visual systems have evolved to recognize and extract objects from a scene. Contour perception is essential to this process. Contours contain essential information about the shapes of objects in the environment. Correct identification of these objects in the visual scene and segregation of them from the background are necessary for animal survival. Consequently, the visual system has developed a robust ability to recognize shapes even in uncertain environments characterized by a diversity of conditions, including various levels of illumination, colors, texture, and crowding. To determine a neural basis of this brain computation, we used Kanizsa illusory contours which induce contour perception despite having no physical counterpart. Using subjective contours that lack physical basis, in vivo electrophysiology, and optogenetics, we demonstrate that higher order input controls neural correlates of illusory contour perception in mouse primary visual cortex. Our results thus suggest that top-down feedback fills-in the missing information necessary for contour perception in challenging conditions.

LS-AG 20.

Elucidating the Mechanism of Electrochemotherapy with Cisplatin in Triple-negative Breast Cancer Cells: A Quantitative Proteomics Study

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Triple negative breast cancer (TNBC) is refractive to standard chemotherapy due to the lack of the three main receptors. TNBCs depend upon glycolysis, which heightens their growth, proliferation, invasiveness, chemotherapeutic resistance and poor therapeutic response. This calls for alternate and novel therapeutic strategies to target metabolic vulnerabilities present in TNBC. Electroporation-mediated chemotherapy, known as electrochemotherapy (ECT) is gaining momentum as an attractive alternative. However, its molecular mechanisms need better understanding. Towards this, label-free quantitative proteomics is utilized to gain insight into the anticancer mechanisms of ECT using electrical-pulses and Cisplatin on MDA-MB-231, human TNBC cells. Results indicate that ECT with Cisplatin caused a switch in the metabolism with downregulation of 14 key glycolysis proteins with upregulation of 34 oxidative-phosphorylation proteins and 18 tricarboxylic acid cycle proteins compared to Cisplatin. Moreover, ECT induced apoptosis by increasing (1.3×) the reactive oxygen species, demonstrating the potential of ECT with Cisplatin against TNBC cells.

LS-AG 21.

Bone Fracture-Targeted Dasatinib Conjugate Enhances Fracture Repair In Vivo

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Approximately 6.3 million bone fractures occur annually in the USA, resulting in considerable morbidity, deterioration in quality of life, loss of productivity, and sometimes death (e.g. hip fractures). No systemically-administered drug has been developed to accelerate the fracture healing process. To address this need, we have undertaken to target a bone anabolic agent selectively to fracture surfaces to concentrate the drug's healing power directly on the fracture site. We report here that conjugation of dasatinib to a bone fracture-homing oligopeptide via a releasable linker reduces fractured femur healing times in mice by ~60% without causing overt off-target toxicity. Thus, achievement of healthy bone strength is realized after only 3-4 weeks in dasatinib-targeted mice, but requires ~8 weeks in PBS-treated controls. We conclude that targeting of dasatinib to bone fracture surfaces can significantly accelerate the healing process at dasatinib concentrations that are known to be safe.

LS-AG 22.

Drug-repurposing reveals fenamic acids as a novel inhibitors of Neisseria gonorrhoeae

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According to the Center for Disease Control, over 550,000 people in the U.S. suffered from gonococcal infection in 2017. This is partially due to the extraordinary ability of *Neisseria gonorrhoeae* (Ng) at acquiring resistance to various antibiotics. Consequently, we have depleted most antibiotic options available in the last few decades, including our last-resort antibiotics. To find a new treatment option, we utilized drug-repurposing strategy and identified fenamic acids, a class of non-steroidal anti-inflammatory drugs, as potent inhibitors of Ng. Fenamic acids and their analogues showed antibacterial activity against isolates of multidrug-resistant Ng, indicating cross-resistance is unlikely to occur. Interestingly, fenamic acids were relatively ineffective against *Lactobacillus gasseri* and *Lactobacillus crispatus*, two essential members of healthy vaginal microflora. Altogether, our study suggests that fenamic acids are potent and selective inhibitors of Ng that may have potential for further structural modification and ultimate utilization as the next drug against Ng.

LS-AG 23.

Energy value of hydrolyzed feather meal for broiler chickens determined by regression method

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The energy value of hydrolyzed feather meal (HFM) was determined with Cobb-500 broiler chickens. On d 21 post hatching, 192 birds were allotted to 3 dietary treatments comprising 8 replicate cages and 8 birds per cage and fed for 5 days. Diets comprised of a corn-soybean meal-based reference diet (RD) and 2 test diets, which contained HFM added at 50 or 100 g/kg. The ileal digestible energy (IDE), metabolizable energy (ME) and nitrogen-corrected metabolizable energy (MEn) concentrations in HFM was determined by the regression method. There were linear and quadratic decreases ($P < 0.05$) in IDE, ME and MEn as the concentration of HFM increases in the diets. The IDE, ME, and MEn in HFM, determined by the regression method were 3,014, 3,190, and 3,124 kcal/kg DM. The study suggests that HFM provides a considerable amount of energy for use by broiler chickens.

LS-AG 24.

Targeting Neuropeptides to Bone Fractures for Accelerated Healing

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Delayed fracture healing is a major health issue involved with aging, and strategies to improve the rate of repair and prevent non-union will substantially improve patient outcomes and lower healthcare costs. It has been observed that nerves that express substance P, vasoactive intestinal peptide, Amylin, and pituitary adenylate cyclase-activating peptide innervate the bone and respond to trauma. These peptides have been shown to have powerful osteogenic effects in vitro. However, these peptides have not been developed as therapies, because their receptors also play roles in the so many systems throughout the body. We found that these bone-fracture-targeting ligands limited these peptides' localization just to the fracture site, thus minimizing their toxic off-target effects, increasing their efficacy to improve fracture healing and allowing for a noninvasive systemic administration via subcutaneous injection. They all show promise as future therapies, as they all significantly improve the healing rate of bone fracture.

LS-AG 25.

Investigation of the Blood-Brain-Barrier with the Atomic Force Microscope

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The Blood-Brain-Barrier (BBB) is a semi permeable tissue that regulates the exchange of molecules between the blood and the extracellular fluid of the brain and the Central Nervous System. The endothelial cells forming the BBB are closely arranged, resulting in tight junctions at the cell interfaces. The healthy BBB prevents pathogens and toxins from entering the brain but blocks most medication, hampering the treatment of brain diseases. Diseases like Multiple Sclerosis, Parkinson's Disease and Alzheimer's Disease are believed to be related to a damaged BBB.
This BBB investigation was conducted on an in-vitro model consisting of human endothelial brain cells. The cells were fixed at different stages of BBB development and investigated using an Atomic Force Microscope (AFM). The AFM enabled three dimensional characterization of the BBB structure at the micro and nano scale. Future investigations will focus on characterizing the tight junctions at the cell interfaces.

LS-AG 26.

Emap2sec: Protein Secondary Structure Detection in Intermediate Resolution 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 Emap2sec) 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 27.

Accelerating protein function discovery using computation tools

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Discovering the function of genes/proteins is the key to scientific breakthroughs in the field of medicine and biology, impacting billions of lives. However, the current paradigm of discovery relies on experimentations, which increases the time (up to months!) and cost with low scalability option. We are working towards developing computational methods which can predict the function of a protein quickly, economically with possibility of annotating hundreds of proteins per day. To that goal, we developed Phylo-PFP, a phylogenetic based method, which combines statistical tools with biological concepts and leverages the power of big data to predict functional terms for any protein. We showed that our method performance is better than other similar methods which were evaluated on a world-wide protein function competition. We have collaborated with multiple experimental teams that have thousands of new genes/proteins, using our tools to uncover their functions, seeking new and interesting proteins.

LS-AG 28.

Understanding complex single molecule emission patterns with deep learning

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Fang Huang

Analyzing single molecule emission patterns plays a critical role in retrieving the structural and physiological information of their tagged targets and, further, understanding their interactions and cellular context. These emission patterns of tiny light sources (i.e. point spread functions, PSFs) simultaneously encode information such as molecule's location, orientation and environment within the specimen. However, to date, retrieving multiple classes of information beyond 3D position from single molecule data remains challenging, due to the difficulties in perceiving and summarizing a comprehensive yet succinct model. We developed smNet, a deep neural network that can extract multiplexed information near the theoretical limit from both complex and high-dimensional point spread functions. We demonstrated that smNet can be trained to efficiently extract both molecular and specimen information, such as molecule location, dipole orientation and wavefront distortions from complex and subtle features of the PSFs, which otherwise are considered too complex for established algorithms.

LS-AG 29.

Perlecan knockdown significantly alters ECM composition during cartilage development

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Perlecan is an extracellular matrix (ECM) protein. We previously demonstrated with a mouse model, using atomic force microscopy, that perlecan knockdown decreased the stiffness of the ECM and chondrocytes in developing cartilage. However, it is not clear what changes occur in matrix architecture to cause the decrease in stiffness. Therefore, we performed mass spectrometry to test the hypothesis that ECM components that contribute to the structural integrity of cartilage will be in lower abundance in mutants than wildtype littermates.

The relative abundance of multiple proteins was significantly higher in mutant vs. wildtype mice. These results contrasted with our original hypothesis that perlecan knockdown would yield decreased ECM protein incorporation, leading to decreased mechanical stiffness. Future comparative studies will assess fibril maturity and crosslinking within the ECM, resolve ECM ultrastructure, and measure the cartilage secretome to elucidate the mechanism of perlecan-mediated cartilage matrix assembly.

LS-AG 30.

FDA-approved Gold drugs for Combating Multidrug Resistant *Neisseria gonorrhoeae*

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Neisseria gonorrhoeae represents an urgent public health threat as described by the Centers for Disease Control and Prevention (CDC). Due to The growing antibacterial resistance and the dry pipeline of antibiotics drug discovery, it might be only a matter of time that an untreatable 'superbug' *N. gonorrhoeae* becomes the norm. The process of drug repurposing is a novel way to reduce both the time and cost associated with antimicrobial innovation. This study builds upon discoveries of the potent bactericidal activity of the FDA-approved Gold drugs in an applicable clinical range (nanogram concentration), against highly multidrug-resistant *N. gonorrhoeae*. Auranofin and other gold thiol drugs, demonstrated excellent activity against 50 clinical isolates of *N. gonorrhoeae* with minimum inhibitory concentration ranges from (0.03 to 0.125µg/mL). A time kill analysis of the activity of the drugs revealed a bactericidal drug action for auranofin and bacteriostatic activity of other gold thiol drugs. Auranofin in combination with other first line treatment drugs shows no signs of antagonism, which suggests the possibility of using Auranofin in dual therapy. Overall the current study strongly suggest that repurposing gold drugs as an antimicrobial agents to treat *N. gonorrhoeae* infections will leapfrog the drug development process and save years of expensive research

LS-AG 31.

An FDA approved Drug as a Potential Cure for Multidrug Resistant Gonorrhea

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The CDC lists Neisseria gonorrhoeae as one of the three most urgent antibiotic resistance threats in the United States. It has developed resistance to nearly every antibiotic used for its treatment. Importantly, a cluster of cases of super-resistant Neisseria were recently reported worldwide that were resistant to last resort antibiotics, highlighting the critical need for new therapeutics. In this study, we evaluated 3200 approved drugs against multidrug-resistant N. gonorrhoeae. We identified Salicylamide as a potent inhibitor of N. gonorrhoeae. Salicylamide exhibited potent activity against 50 clinical isolates. Additionally, it killed the high bacterial inoculum within 10 hours. Furthermore, salicylamide showed a strong selectivity towards N. gonorrhoeae without affecting any vaginal microflora. The synergistic interaction of salicylamide was further investigated against different clinical isolates of N. gonorrhoeae. Notably, salicylamide displayed a synergistic activity with tetracycline resulting in a 2-fold reduction in tetracycline's MIC values. A more in-depth investigation of the structure-activity-relationship of salicylamide and related analogues identified important chemical scaffolds that are expected to be valuable for medicinal chemists to synthesize more potent drugs against *N. gonorrhoeae*.

LS-AG 32.

A Bayesian Semiparametric Approach for Estimating a Bacterium's Wild-Type Distribution: Accounting for Contamination and Measurement Error (BayesACME)

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Antimicrobial resistance is a major challenge to modern medicine and of grave concern for public health. To monitor resistance, agencies analyze "drug/bug" collections of clinical assay results. It is common to assume the underlying distribution of results is a mixture of two subpopulations: a wild-type distribution on the left, consisting of strains susceptible to the drug, and resistant strains on the right. The goal is to estimate the wild-type distribution and its prevalence.

The dilution assay is commonly used and enforces interval-censored results. Various estimation methods account for this censoring and contamination but do not account for the inherent variability of the assay. This omission can have a profound effect on the estimated distribution. We propose a Bayesian semiparametric method to address this omission as well as to quantify readily the uncertainty in our prevalence and distribution estimates. We demonstrate this approach against others through several simulation studies.

LS-AG 33.

Sub-3 Å Apoferritin Structures Determined With Single Position Of Volta Phase Plate and the Full Range of Phase Shift

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Structure determination of small particles is still a challenging task in the cryo-EM field. Volta phase plate (VPP) has been shown as a valuable tool by presenting several high-resolution structures of various sizes of protein. However, despite the fact that VPP has been garnering attention as a compelling solution to enhance image contrast, it remains a largely artful tool whose performance couldn't be precisely controlled. In this report, we report sub-3Å resolution structures of ferritin reconstructed from datasets collected using only a single position of VPP and datasets with a full range of phase shift demonstrating the potential of turning VPP into a plug-and-play device for cryo-EM.

LS-AG 34.

After decades of a shared life with vancomycin-resistant enterococci, is it time to breakup?

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Vancomycin-resistant enterococci (VRE) is the second-most common cause of nosocomial infections and associated with more than 5% of deaths attributed to antibiotic-resistant infections in USA. VRE acquired resistance to all antibiotics used for treatment. Consequently, novel antimicrobials are urgently needed. Repurposing FDA-approved drugs to find new antimicrobials is a novel way to reduce time and cost associated with antimicrobial innovation. We identified auranofin as a potent antimicrobial agent against VRE. It demonstrated potent bactericidal activity against 30 clinical-drug-resistant VRE isolates with MIC_{90} 1μg/mL. Additionally, no enterococcal resistant mutants could be developed after 14 passages. Moreover, it inhibited highly resistant stationary phase cells, VRE virulence factors and biofilm formation on catheters. Consequently, we evaluated its *in vivo* efficacy against linezolid in lethal VRE septicemia mouse model. Both protected 100% of mice. Remarkably, auranofin was superior in reducing the bacterial load in internal organs (liver, kidney and spleen) where it efficiently cleared VRE after 4 days of treatment. Accordingly, these results indicate that auranofin warrants further investigation as a frontline treatment for lethal VRE infections.

LS-AG 35.

Genome-wide association analysis identifies new loci indicated in cranial cruciate ligament rupture in Labrador Retrievers

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Kari Ekenstedt

Cranial cruciate ligament rupture (CCLR) is one of the leading causes of pelvic limb lameness in canids. The aim of this study was to find candidate genetic regions associated with CCLR in Labrador Retrievers. DNA samples were collected from CCLR affected dogs (n = 190) and unaffected dogs (n = 143). All 333 dogs were genotyped directly on or imputed up to a ~600k SNP array. CCLR is likely a polygenic condition, and unsurprisingly multiple loci were found to be associated with this condition. No loci reached genome wide significance after corrections, however, there were over 30 loci with suggestive significance. Using all individuals, heritability (h^2) of CCLR was 0.600297, and, when calculated with only individuals having a cryptic relatedness value of <0.25 (n=288), h^2=0.44013. More research must be performed to confirm these loci. The heritability value for this disease indicates that steps could be taken to reduce its prevalence.

LS-AG 36.

A grape powder attenuates colonic inflammation, inhibits colitis-associated colorectal cancer development and causes favorable changes of gut microbiota in mice

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Polyphenol components of grape like resveratrol have been shown to have anti-colorectal cancer effects in animal models, but the underlying mechanism is not completely understood. In this study, we examined the chemo-preventive effect of a whole grape powder (GP) on tumorigenesis in a mouse colitis-associated colorectal cancer (CAC) model induced by azoxymethane (AOM) and dextran sodium sulfate (DSS), and evaluated the impact of GP on gut microbiota as a potential anti-CAC mechanism. We used male Balb/c mice and divided them into diseased (AOM/DSS treated) and healthy groups, both of which had calorie, fiber, sugar and organic acid-matched placebo control diets, GP at 3% or 10% diet. Overall, 10% GP diet showed CAC chemo-preventive effects as indicated by decreased rectal bleeding, diarrhea and 29% ($P<0.05$) reduction in tumor multiplicity, modulated gut microbiota under both healthy and diseased conditions, and appeared to prevent CAC-associated gut microbiota changes.

LS-AG 37.

Lipid biomarkers for diagnosis and disease progression of canine atopic dermatitis

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Atopic dermatitis is an allergic inflammatory skin disease that is common in humans and dogs. The diagnosis is based on exclusion of other causes of pruritus which is time consuming and expensive. Since alterations in the lipid composition of the skin plays a key role, we used mass spectrometry-based lipidomics to identify a lipid fingerprint that could be useful for its diagnosis. The skin lipid composition substantially distinguished samples of healthy dogs from atopic dogs. A feature selection strategy found triacylglycerides, long-chain acylcarnitines and sphingolipids as predictive lipids that highly correlated (R2=0.89) with the disease severity of patients. The results showed that changes in the lipid composition of the skin are present in atopic dogs even when the skin appears clinically healthy and, that lipids can predict the progression of the disease. The lipid biomarkers identified here are potentially useful for the diagnosis and monitoring of atopic dermatitis.

LS-AG 38.

Signal-biased drugs: a step towards precision medicine for anxiety disorders

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Various G-protein-coupled receptors (GPCRs) are involved in the complex pathophysiology of anxiety disorders, but the complex symptoms, such as anxiety and fear, do not always respond to current medications. Two β-arrestin isoforms (β-arrestin-1 and -2), downstream of GPCRs, have recently gained attention in drug developments. Therefore, we aim to interrogate the role of β-arrestin in the modulation of anxiety and conditioned fear-related behavior in mice. We utilized a 'biased signaling' approach that can selectively target desired cellular pathways. Using signal-biased drugs for β-arrestin proteins, we measured β-arrestin-mediated molecular, cellular, and behavioral responses in wild type and genetic knockout mice. Our results indicated that β-arrestin-2 modulates anxiety-like behavior and downstream signaling in the dorsal hippocampus and the amygdala, and β-arrestin-1 modulates conditioned fear response and downstream signaling in the dorsal striatum and the nucleus accumbens of mice. Our findings provide novel insights into the development of 'precision medicine' for treating anxiety disorders.

LS-AG 39.

Impaired visually evoked oscillations in the mouse model of Fragile X syndrome

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In this study, we explored how experience dependent changes in neural activity are disrupted at the scale of circuits and neural ensembles in the mouse model of FXS. We used a visual-perceptual learning paradigm in FXS mice that induces low frequency oscillatory activity reflecting familiarity with a visual stimulus. We used this paradigm together with a multifaceted experimental approach; including extracellular recordings across all layers of the primary visual cortex, computational analysis of functional connectivity between these layers, and channelrhodopsin-2 assisted circuit mapping (CRACM) of specific connections between layers. Extracellular recordings revealed shorter durations, lower power, and lower frequencies of visually evoked oscillations in FXS mice. Directed information analysis revealed decreased information flow onto layer-4 fast spiking cells in FXS mice, while CRACM demonstrated decreased synaptic strength onto these layer-4 cells. These results reveal how an experienced sensory stimulus is differentially encoded in autism.

PHYSICAL SCIENCES

P1.

Photoinduced Disulfide-Reduction System Coupled with ET-DDC for Top-Down Characterization of Disulfide-Linked Proteins

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Structural characterization of peptides and proteins using tandem mass spectrometers can be challenging due to the presence of multiple disulfide bonds, which significantly reduces the backbone cleavage efficiency for fragmentation. Recently, we reported an acetone/isopropanol photoinitiating system for a rapid and tunable disulfide bond reduction in peptides/proteins. In this work, we integrate this photoinitiating system with a dipolar DC induced collisional activation of electron transfer products (ET-DDC) of peptides/proteins for a top-down MS approach. The photoinitiating system allows to remove the disulfide constraints; while ET-DDC allows for broadband activation with relatively uniform ion heating across a relatively wide *m/z* range. As a result, this approach allowed to achieve rapid and enhanced structural characterization of disulfide-linked proteins.

P2.

Forging Ru–C(sp^2) bonds in paddlewheel complexes

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Diruthenium compounds have been studied for their applications as molecular wires and in memory devices; these feature Ru_2–alkynyl or Ru_2–C(*sp*) linkages. In this work, we report the first examples of M_2–aryl or M_2–C(sp^2) species (M =Ru) of the type $Ru_2L_4(Ar)$ (L = bridging ligand; Ar = aryl). A series of six electronically distinct compounds have been synthesized and characterized *via* electronic absorption spectroscopy, voltammetry, mass spectrometry, magnetism studies and single crystal X-ray diffraction. Each of the six compounds boasts remarkable stability under ambient conditions and exhibits a rich and robust redox profile with up to four reversible oxidation events and one reversible reduction. These new compounds are thus attractive targets for improved device applications. We have also expanded the scope of this chemistry to other paddlewheel species such as $Ru_2L_4Ar_2$, and mixed aryl/polyynyl complexes such as (R-C≡C-C≡C)$Ru_2L_4(Ar)$, a step toward making polyyndiyl-bridged aryl end-capped paddlewheel complexes.

Post Doctoral Fellow Posters

LIFE, PHYSICAL AND ENGINEERING SCIENCES

PD-LPE 1.

Role of interaction between microenvironmental stress and cell nucleus in breast cancer progression

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Abstract Text: High content of reactive oxygen species in the microenvironment of triple negative breast cancer (TNBC) is conducive to oxidative stress (OS). Chromatin organizer, nuclear mitotic apparatus protein (NuMA) interacts with transcription factor lens epithelium-derived growth factor (LEDGF) and with chromatin protein, remodeling and splicing factor (RSF1) that are both up-regulated upon OS. **Our hypothesis is that OS influences NuMA-LEDGF-RSF1 interaction to promote breast cancer progression.** Using the HMT-3522 TNBC progression series (non-neoplastic S1 cells, preinvasive ductal carcinoma in-situ like S2 cells, invasive ductal carcinoma T4-2 cells) we show that expression of NuMA, LEDGF and RSF1 is significantly decreased in T4-2 cells compared to S1 and S2 cells. However, NuMA-LEDGF interaction under OS is decreased in S2 cells and increased in S1 cells, highlighting a different behavior in response to OS in phenotypically normal and cancerous tissues. These findings call for further investigation of NuMA-LEDGF-RSF1 interaction in controlling cell behavior under OS.

PD-LPE 2.

Long Range Wireless Sensor Network solution for Soil Health monitoring in Arequipa region

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This work presents the development of a sensor network based on LoRa (Long Range) technology to monitor soil health. The main advantage of this technology is that long transmission distances can be achieved with low power. The nodes of this wireless sensor network are called Soil Health Monitoring Units (SHMU) and are installed in every location where soil health needs to be monitored. An SHMU consists of a soil sensor, a processing unit, a GPS module and a LoRa radio. The SHMU processes the sensor data and transmits it to a Gateway at the frequency of 915 MHz. The gateway receives data from several SHMUs and uploads it into a server for storage and analysis. The users can view and analyze the location of the SHMUs, soil temperature, moisture and electrical conductivity by using a graphical user interface.

PD-LPE 3.

III-Nitride Materials for Infrared Devices Based on Intersubband Transitions

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Our work is focused on exploiting unique physical properties of III-Nitride semiconductors to produce novel light sources based on intersubband transitions. These materials have the potential to enable new optoelectronic devices for socially beneficial applications in sensing, imaging, and telecommunication. Much of our experimental effort involves exploring the growth of III-nitride heterostructures by a high-purity growth technique known as plasma-assisted molecular beam epitaxy. The fabrication of heterostructures is coupled with the advanced structural characterization using various experimental techniques. From these experiments, we gain new insights into the fundamentals of growth kinetics, elemental distribution, and structural properties of III-nitride alloys. In collaboration with the Infrared Nanostructured Devices Group, we correlate this structural information with the resulted infrared optical properties. In our work, we want to understand the material growth, establish structure-property relationships, and hence bring III-nitride materials to the next level of maturity necessary for commercial infrared applications.

PD LPE 4.

De novo main-chain modeling for EM maps using MAINMAST

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Processor Daisuke Kihara

An increasing number of protein structures are determined by cryo-electron microscopy (cryo-EM) at near atomic resolution. However, tracing the main-chains and building full-atom models from EM maps of ~4-5 Å is still not trivial and a demanding task. Here, we introduce a novel de novo structure modeling method MAINMAST (MAINchin Model trAcing from Spanning Tree) that builds an entire three-dimensional model of a protein from a near-atomic resolution EM map.

The method has substantial advantages over the existing methods: i) MAINMAST directly constructs protein structure models from an EM density map without requiring reference structures; ii) The procedure is fully automated and no manual setting is required; iii) a pool of models are produced, from which a confidence score is computed that indicates accuracy of structure regions.

MAINMAST performed significantly better than existing software. This work has been published on Nature Communications, 9: 1618 (2018).

PD-LPE 5.

PL-PatchSurfer: a virtual screening program for template based modeled structure using molecular surfaces

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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. Therefore, they are not suitable for template-based modeled structures. Recently, we have proposed a new version of PL-PatchSurfer for TBM models. The unique feature of this program is surface-patch description instead of all-atom representation in traditional RBVS methods. 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.

Data Analytics on the Phase Behavior of Oil/Water/Surfactant Systems

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Sangtae Kim (faculty sponsor)

According to BP Statistical Review of World Energy in 2018, total oil production from the US in 2017 was about 13 million barrels per day (MBPD), which is even greater than that of Saudi Arabia (less than 12 MBPD). Thanks to the booming shale oil production, United States has become the world's top oil exporter. In fact, estimates show that up to two thirds of conventional crude oil in mature fields remains unproduced due to the physics of fluid flow. The techniques of chemical enhanced oil recovery could overcome the physical force holding hydrocarbons, and turn these accumulations into oil reserve, which would enhance the US energy security and maintain economic growth. To enhance the oil recovery in the reservoir, many efforts have been made to apply surfactants into the injected water. For the oil/water/surfactant system, the goal is to form a microemulsion phase achieving the lowest interfacial tension, which increases the capillary number and dramatically recovers the remaining oil fraction within the pore. Therefore, it is critically important to understand the phase behavior for the oil/water/surfactant systems. In collaboration with Pioneer Oil Company, our current effort is to optimize the selection of surfactants and the constituents of the surfactant blend, which turns to be a high dimensional problem. In addition to the conventional analysis, we employ machine learning techniques to solve the system as a multinomial classification problem. With reference to HLD-NAC theory (an effective theory for the surfactant selection), classification approaches such logistic regression and random forests are applied to improve feature selection (best performing surfactants), and thus, optimize the mixing of the oil/water/surfactant system.

PD-LPE 7.

Plasma production of liquid nitrate fertilizer for agriculture: from theory to field tests

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Food security and plant nutrition needs are acute in Sub-Saharan Africa, where corn is such a major part of the human diet but where fertilizer is not applied to about 70% of the corn grown.

We have developed a concept that would be a game-changer in this area. We propose to eliminate the need for massive centralized production of nitrate fertilizers and instead to produce the nitrates "on the spot" using only solar power, air, and water, with no added chemicals. The key technology for this novel concept is based on low-temperature plasma that would make NOx in air with low energy cost, which, mixed with water, would produce the liquid nitrate fertilizer. We report on the development of a laboratory-scale plasma nitrate production system and on the successful field test with corn growth conducted at Purdue in 2018. The test demonstrates the viability of the concept

PD-LPE 8.

Neuropilin 1 is required for fibroblast growth factor receptor-mediated tumor progression

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Background: Human epidermal growth factor receptor 2 (ErbB2)-amplified Breast cancers initially response to treatment with targeted antibodies and kinase inhibitors (collectively called ErbB inhibition or ErbBi) at a high rate, but ultimately these tumors acquire resistance and undergo metastatic recurrence. Thus, there is a critical need to uncover metastatic events that drive the failure of ErbBi therapy. We have recently performed global gene expression analyses on several ErbBi resistant cell lines as compared to their drug sensitive counterparts. These data demonstrate induction of epithelial-mesenchymal transition (EMT) which included enhanced expression of fibroblast growth factor receptor 1 (FGFR1) and the axonal guidance molecules known as neuropilins (NRP). NRP1 is transmembrane receptor protein that functions as a co-receptor for a number of extracellular ligands including some isoforms of VEGF, class 3 semaphorins, HGF, FGF and TGF-β. Several recent studies clearly link FGFR1 and Nrp1 to drug resistance and metastasis. Expression of Nrp1 is elevated in more invasive and advanced stages of cancer and the expression of Nrp1 in human breast cancer tissue negatively correlates with patient survival. We therefore sought to address the hypothesis that EMT-driven tumor metastasis is facilitated by an Nrp1:FGFR1 matrixsensing signaling complex. We also aim to determine if pharmacological disruption of this complex can overcome drug resistance and metastasis.

PD-LPE 9.

Discovery of an aryl isonitrile compound with enhanced drug-like properties that is effective in two mouse models of multidrug-resistant *Staphylococcus aureus* infection

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Mohamed N. Seleem

Methicillin-resistant *Staphylococcus aureus* (MRSA) remains a major global source of antibiotic-resistant bacterial infections that necessitates continuous discovery of new antibacterial agents. This study investigated a synthetic aryl isonitrile compound (**35**) as a novel antibacterial agent against MRSA. Compound **35** inhibited growth of MRSA clinical isolates (from 2 – 4 μM) and was non-toxic to human keratinocytes. Importantly, MRSA was unable to form resistance to compound **35**. In a murine skin wound model, compound **35** significantly reduced the burden of MRSA in infected lesions. Relative to the first-generation lead compound, **35** exhibited a marked improvement both in gastrointestinal permeability and stability to hepatic metabolism (half-life exceeded 11 hours). Thus compound **35** was evaluated in a neutropenic thigh infection mouse model where it successfully reduced the burden of MRSA in immunocompromised mice. In summary, compound **35** was identified as a new lead molecule that warrants further investigation as a novel antibacterial agent.

PD-LPE 10.

True colors: Commercially-acquired morphological genotype data as a valuable resource for revealing allele variation among dog breeds

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Data collected from commercially-available canine genotyping panels provide insight into the current genetic diversity status of trait-causing variants present within purebred dog populations. This study aimed to determine the distribution of common morphologic and pigmentation alleles among and within dog breeds and elucidate their resultant implications on diversity and dissemination of trait-causing variants. Mars WISDOM PANEL™ data from 11,790 canids, representing 212 dog breeds and 4 wild species, was evaluated at genes associated with 7 coat color traits and 5 physical characteristics. Allele frequencies were calculated for each breed and phylogenetic grouping. Analysis of the resultant allele distribution demonstrates that: 1) the occurrence of low frequency alleles within breeds reveals the influence of differing selection practices; 2) the mode by which characteristics have spread across breeds during historical breed formation is traceable; and 3) the necessity of addressing conflicting ideals in breed descriptions relative to genetic potential is crucial

SOCIAL AND BEHAVIORAL SCIENCES

PD-SBS 1.

Characterizing Undergraduate Biology Students' Graphing Practices

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Graphing is one practice used by scientists to explore and analyze quantitative data sets to test hypotheses, make inferences, and communicate findings. Graphing in the context of biology often brings knowledge of statistics and biological inquiry together with knowledge of representations and visual processing to make meaning. We analyzed 26 undergraduate biology students' graphs and the verbal justifications for their graphing decisions from semi-structured interviews. Participants were asked to use a novel program to make a graph testing a prediction in the context of conservation biology. The majority of students' justifications referred to plotting raw data in bar or scatter graph and they typically based their graph type selection on data characteristics and ease of visualization. When analyzing their variable selection, 81% of students plotted variables relevant to the hypothesis. This study contributes to our understanding of undergraduate biology students' graphing practices and provides us with potential instructional targets.