



20th Annual Meeting

LBRN



Louisiana Biomedical Research Network

January 28-29, 2022

Table of Contents

Agenda	1
Keynote and Guest Speaker Abstracts	5
Oral PI and Graduate Abstracts	8
Poster Session Abstracts	17
Index	
Oral Presentation	45
Poster Session	47
Core Structures and Committees	53



20th ANNUAL MEETING OF THE LBRN

January 28-29, 2022

Friday January 28th, 2022

#	Name			Time
<i>Introduction</i>				
1	Konstantin Kousoulas (PI) / Ramesh Subramanian (Program Coordinator)			12:40 - 12:45 PM
	Lakshmi Matukumalli - Program Director - Networks and Development Programs, DRCB, NIGMS			12:45 - 12:55 PM
	Steve Cutler - Interim Provost, University of South Carolina - LBRN EAC Chair			12:55 - 1:05 PM
#	Name	Project Type	Title	Time
2	Nicolas Bazan – Director, Neuroscience Center of Excellence	Keynote	Redundancy and Resiliency Signaling for Neuronal Longevity Counteracts Alzheimer's Onset.	1:10 - 2:00 PM
3	Urska Cvek / J. Steven Alexander	Women's Health	Stability in Inflammatory Bowel Disease	2:05 - 2:30 PM
4	Nektarios Barabutis / Yogesh Saini	INBRE-COBRE	Protective Role of Activating Transcription Factor 6 (ATF6) against endothelial barrier dysfunction	2:35 - 3:00 PM

BREAK

3:00 - 3:10 PM

5	Charles Irvin - Director, Vermont Lung Center	Invited Talk	Scientific Misconduct: Crime & Punishment	3:10 - 4:00 PM
6	Poster Session I			4:00 - 5:00 PM
7	Poster Session II			5:00 - 6:00 PM

Saturday, January 29th, 2022

#	Name	Project Type	Title	Time
1	Oliver Garden - Dean, LSU School of Veterinary Medicine	Dean's Remarks	LSU Vetmed Overview	8:15 - 8:30 AM
2	Matt Lee - Interim Executive Vice President and Provost - LSU	Provost's Remarks	Welcome remarks	8:30 - 8:45 AM
3	Krzysztof Reiss - Program Director Center For Translational Viral Oncology	Keynote	Glioblastoma weak metabolic points as a target for new drugs with high potential for Blood Brain Barrier penetration	8:45 - 9:25 AM
4	Jean Christopher Chamcheu	Full	Development of fisetin as a novel inhibitor co-targeting PI3K/AKT/mTOR/Rac1 and IL-17A for Treating Psoriasis	9:30 - 9:55 AM
5	Georgios Matthaiolampakis	Full	miR-mediated Inhibition of Lung Cancer Progression	10:00 - 10:25 AM

BREAK

10:25 – 10:40 AM



20th ANNUAL MEETING OF THE LBRN

January 28-29, 2022

Saturday, January 29th, 2022 - *Continued*

6	Siva Murru	Full	Development of Pyrazoles and Pyrazolones as Anti-Cancer Agents: Design, Synthesis and Anti-Cancer Activity Studies	10:40 - 11:05 AM
7	Devaiah Kambiranda	Full	Proteasomes/immunoproteasome: Role of lipid rafts in compartmentalization / activation in e-cigarettes vapor exposed lung epithelial cells	11:10 - 11:35 AM
8	Kyle Piller	Full	Life in the fast lane: Testing for congruence among transcriptomic signatures	11:40 - 12:05 PM

LUNCH

12:05 - 1:00 PM

Student Flash Talks – 4 minutes each

10	Rizwana Begum	Summer	HSP70 and proteasomes coalesce in lipid rafts to regulate E-cigarette Vapor condensate induced inflammation	1:00 – 1:30 PM
11	Nandini Bidarimath	Summer	Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells	
12	Eric Clifford	Summer	Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females	
13	Denzel El Hage	Summer	Development of a pH-sensitive liposome formulation for targeted delivery of anticancer pyrazolones in lung cancer cells	
14	Tithi Roy	LBRN	The dietary antioxidant Fisetin suppresses Psoriasis-like characteristics in vitro and in vivo in an imiquimod-induced dermatitis in Balb/c mice: Involvement of the central mTOR signaling pathway	
15	April Wright	Full	Modeling Heterogeneous Data Sources for Time-Scaling Phylogenetic Trees	1:35 - 2:00 PM
16	Srinivas Garlapati	Full	Mechanism of translation initiation in protozoan parasite Giardia lamblia	2:05 - 2:30 PM
17	Vonny Salim	Full	Elucidation of Plant-Derived Drug Biosynthetic Pathways and Molecular Mechanisms as Anticancer Agents	2:35 - 3:00 PM
Awards and closing remarks				3:05 - 3:20 PM
EAC meet with Steering Committee				3:25 - 4:10 PM



20th ANNUAL MEETING OF THE LBRN

January 28-29, 2022

LBRN Annual Meeting Poster Summary

iPosterSession Gallery https://lbrn2022am-lsu.ipostersessions.com/Default.aspx?s=lbrn_2022_gallery

ID#	Sess/Rm	Full Name	Poster Title:	Institution
1	I, Rm 1	Abubakar Abdulkadir	Comparative Bioinformatics and Conventional approach reveal some common signaling mediators in DE-particulate exposed A549 and BEAS-2B cells	SUBR
2	I, Rm 2	Mohammad Shohel Akhter	Growth Hormone Releasing Hormone Antagonists Protect Against LPS-Induced Endothelial Hyperpermeability	ULM
56	II, Rm 1	Duaa Alawad	Accurate identification of ncRNA-protein interactions using ensemble deep learning methods	UNO
4	II, Rm 2	Alexis Bardwell	Identification of Spore-Forming Bacteria in a Louisiana Salt Marsh	LATECH
5	II, Rm 3	David Basnet	N-Boc-hydroxylamine as a Boc-donor Agent for the Catalytic N-tert-Butoxycarbonylation of Pyrazoles and Indazoles	ULM
59	II, Rm 4	Rizwana Begum	HSP70 and proteasomes coalesce in lipid rafts to regulate E-cigarette Vapor condensate induced inflammation	SUBR
54	I, Rm 3	Julianna Berger	Comparing Solubility of the catalytic mutant in the lyase-isomerases MpeQ and MpeZ from Synechococcus sp. A15-62 and RS 9916	UNO
60	I, Rm 24	Nandini Bidarimath	Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells	SUBR
			Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells	SUBR
6	I, Rm 4	Samuel Boateng	Biological evaluation, in silico molecular docking and ADMET screening of a small library of phenolic compounds identified novel anti-skin cancer agents	ULM
57	II, Rm 5	Chelsea Bock	Growth inhibitory and apoptotic effects of Graviola (Annona Muricata) fractions in human melanoma and non-melanoma skin cancer in vitro	ULM
7	I, Rm 5	Mary Caldorera-Moore	Assessment of injectable chitosan-genipin hydrogels biomaterial biocompatibility	LATECH
8	II, Rm 6	Joseph Chaney	Applying the Brakes: Understanding the Role of the Conformational Changes in the Kinesin-5 on Processivity and Inhibition	XULA
58	II, Rm 7	Eric Clifford	Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females	LSUS
9	II, Rm 8	Karli Clifton	Electro-chemical Cyclization of Hydroxychalcones for the Synthesis of Flavonoids	ULM
55	I, Rm 6	Loandi Cruz	Heterogeneous Cu@Hal catalyzed [3+2] cycloaddition reactions for the preparation of 1,2,3-triazoles	UNO
10	II, Rm 9	Urska Cvek	Disparities in Breast Cancer Treatment Outcomes: Improving Access with Health Informatics	LSUS
11	II, Rm 10	Devika Dua	Investigating Key COVID-19 Questions by Using Natural Language Processing on Scientific Publications	CCS (HS)
12	II, Rm 11	Samrat Dutta	Diagnostic Cancer Imaging In the Mid-Infrared Using Novel Contrast Agents	XULA
13	II, Rm 12	PJ Erba	Development of Methodology in Microbial DNA Isolation for Characterization of Soil Microbiome	LSUS
14	I, Rm 7	Anup Ghimire	EEG Based Motor Imagery Task Classification Utilizing Spatiotemporal Deep Learning for BCI Applications	SELU
15	I, Rm 8	Matthew Hayes	Complex Germline Structural Variant Discovery Via Discordant Cluster Normalization	XULA
16	II, Rm 13	Bennett Hibner	Computational Investigations Of Stereospecificity In Concerted Electrocyclic Reactions	SELU
17	II, Rm 14	Hunter Hollie	Design and Development of a Low-Cost High-performance Atomic Force Microscope (AFM)	SELU
18	II, Rm 15	Moses Ihachi	Aryl-fused (Imidazole, Pyrazine and Pyrrole) Boronated Dye Derivatives	SELU
19	I, Rm 9	Chelsey Jordan	Assessment of student appreciation for applied bioinformatics and computational drug discovery methods in a project-based course	LSUS
20	I, Rm 10	Supriya Karki	Developmental Stages of Olfactory Sensory Neurons in Neonatal Life vs. Adulthood	LSUS
21	I, Rm 11	Waheed Khan	Using computational drug repurposing methodology to identify promising bicteggravir-based drug candidates for COVID-19	LSUS
22	II, Rm 16	Phillip Kilgore	Racial Disparities in COVID-19 Symptoms in Northern Louisiana	LSUS
23	II, Rm 17	Vladimir Kolesnichenko	Cancer-Specific Magnetic Imaging Agent	XULA
24	I, Rm 12	Khadeja-Tul Kubra	Activating transcription factor 6 modulates endothelial barrier function.	ULM
25	I, Rm 13	James Lee & Matthew Giblin	Heart rate variability and novel torpor states in tent-making bats	SELU
26	I, Rm 14	Laura Lee	Wastewater Analysis and Genomic Sequencing of SARS-CoV-2 Benefit COVID-19 Surveillance	LATECH
27	I, Rm 15	Chi Jing Leow	Accessing the congruency of DNA repair genes among killifishes with different life histories using QuantSeq	SELU
28	II, Rm 18	Raj Letchuman	Identifying Promising Drug Candidates Against SARS-CoV-2 Using Computational Drug Repurposing Methodology	CPM (HS)
29	I, Rm 16	Elahe Mahdavian	An interdisciplinary course on computer-aided drug discovery to broaden student participation in original research	LSUS
30	I, Rm 17	Ethan Manco	Patterns in Electroencephalograms during Meditation	LSUS
31	I, Rm 18	Pearl Merry	Virus-Induced Gene Silencing: In-Vivo Characterization of Anticancer Alkaloid Biosynthetic Genes in Medicinal Plants	LSUS
32	II, Rm 19	Ryan Miller	Whole Cell Biotransformation for Central Intermediate Formation in Anticancer Monoterpenoid Indole Alkaloid Biosynthetic Pathways	LSUS
33	I, Rm 19	Joseph Mondello	Computing Representative Protein Conformations from Molecular Dynamics Simulations	LSUS
34	I, Rm 20	Savannah Montgomery	Identifying Double Minutes Chromosomes within Hi-C and Deletion-Episomes	XULA
35	II, Rm 20	Derrick Mullins	Simulating Double Minute Chromosome and Phylogenetic Tree Evolution using Java	XULA
36	II, Rm 21	Christopher Murray	Alligators as Models for Human Pathology: Neuroendocrine Effects of Methyltestosterone Exposure	SELU
37	I, Rm 21	Kalani Myles	Computer-aided drug discovery for COVID-19 using virtual screening and molecular docking	LSUS
38	I, Rm 22	Jamie Newman	Canonical and Noncanonical Notch Signaling Regulates Adult Stem Cell State	LATECH
39	I, Rm 23	Keelin North	Metagenomic Profiling of Soil Microbiome from Anticancer Compound-Producing Plants	LSUS
41	II, Rm 22	Uchechi Owunna	Synthesis and Biological Evaluation of 1,3-Diarylpyrazoles: in vitro Cytotoxicity Studies on Human Melanoma and Non-melanoma Cancer Cells	ULM
42	II, Rm 23	Erika Perez	Topiramate treatment precipitates and accentuates physical symptoms of nicotine withdrawal in mice.	XULA
43	I, Rm 25	Stephanie Provenzano	Biochemical Characterization of Anticancer Alkaloid Methyltransferases in Medicinal Plant Camptotheca acuminata	LSUS



20th ANNUAL MEETING OF THE LBRN

January 28-29, 2022

ID#	Sess/Rm	Full Name	Poster Title:	Institution
44	I, Rm 26	Prerana Ramesh	Improving Patient Outcomes for Inflammatory Bowel Disease through Physician Interactions during Infusion Treatment : Symptomatic Review of Biologic Therapy in IBD (STABILITY)	LSUHS
45	II, Rm 24	Silvia Robert	Frequency domain approach for improvement of cochlear implant performance	SELU
46	II, Rm 25	Vonny Salim	Elucidation of Anticancer Alkaloid Biosynthetic Pathways in Medicinal Plants: Improved Solutions for Drug Development	LSUS
47	II, Rm 26	Jeffry Shultz	Identifying Lethal Alleles in Human	LATECH
48	I, Rm 27	Bryan Strong	Translation initiation factors from early-branching eukaryote Giardia lamblia can form multifactor complex in the absence of 40S ribosome in vitro	ULM
49	II, Rm 27	Shilpa Thota	Complex interplay between Hsp90 and Beclin-1 regulates TLR-4 mediated autophagy during Pentachlorophenol exposure-in vitro	SUBR
50	II, Rm 28	Billy Tran	Correlations Among Evaluator's Level of Training, Assigned HEART Scores, and Major Adverse Cardiac Events	LSUS
51	I, Rm 28	Marjan Trutschl	Bioinformatics Analysis of Large-Scale Neuroproteomic Data and Prediction of Neurovascular Change	LSUS
52	I, Rm 29	Yuri Voziyanov	Construction of a model cell line to test DNA replacement catalyzed by tyrosine recombinases	LATECH
53	II, Rm 29	Anna Wilson	Comparative transcriptomic analysis of GABAergic versus dopaminergic neuronal differentiation in mouse ES cells	SUBR

Invited Talk : January 28th, 2022 : 1 – 2 PM



NICOLAS G. BAZAN, M.D., Ph.D.

Boyd Professor Ernest C. and Yvette C. Villere at Louisiana State University

Health New Orleans

Chair for the Study of Retinal Degeneration

Redundancy and Resiliency Signalling for Neuronal Longevity Counteracts Alzheimer's Onset.

The onset of neurodegenerative diseases reflects a failure of neuronal cell survival. It is in a way an inability to successful aging, that is to be able to live over nine decades without neuropathologies. Neurodegeneration activates detrimental events, including inflammation that leads to progressive cognitive decline (e.g., dementia, as in Alzheimer's disease (AD)) and sight failure (blindness, as in age-related macular degeneration (AMD)). We have identified novel mediators, the elovanoids (ELVs), that control the unfolding of neuroinflammation, restore homeostasis and function. ELVs are 32C and 34C,n-3 stereospecific dihydroxylated molecules derived from Very Long Chain Polyunsaturated Fatty Acids,n-3 (VLC-PUFA). I will discuss recent results that demonstrate that the targets of ELVs include senescence gene programming, signalling proteins, microglia, Tau phosphorylation, Tau missorting, Netosis, and telomerase activation.

In both brain and retina interdependent cellular systems, neurons-glia (astrocytes and microglia) and retinal pigment epithelial cells-photoreceptor cells (a differentiated neuron) sustain homeostasis. A proof of principle of the bioactivity of lipid mediators yielded our recent unexpected discovery that intranasally delivered lipid mediators are directly associated with rescuing working memory deficits and other homeostatic changes in a mouse model of AD. We also found that insufficiencies of the biosynthetic ELVs pathway in the hippocampus of a knock-in of amyloid precursor protein (APP) and in the 5XFAD model that the ELV and the neuroprotectin D1 (NPD1) pathway are downregulated, preceding neuronal cell loss. Furthermore, ELVs protect human neurons/astrocytes in cultures from oligomeric A β (OA β) peptide-mediated toxicity and arrest senescence gene programming expression, including SASP secretome. In AMD, OA β sets inflammatory events in motion that contribute to photoreceptors cell death. ELVs prevented OA β -induced changes in the expression of genes engaged in senescence, inflammation, autophagy, extracellular matrix remodeling, and AMD. MALDI molecular imaging of early and advanced AMD human retinas showed decreased PC-VLC-PUFAs in macula cone photoreceptor cells. Overall, we find decreased DHA retention, VLC-PUFA formation and ELVs/NPD1 synthesis in AMD and in AD models. Thus, multiple disrupting mechanisms that lead to the onset and progression of AD and the dry-form AMD are targeted in a redundant fashion by ELVs and related lipid mediators. Thus, they uncover fundamental events in the biology of aging ,represent biomarkers of prodromal disease stages and open avenues of therapeutic exploration.

Invited Talk : January 29th, 2022 : 8:45 – 9:25 AM



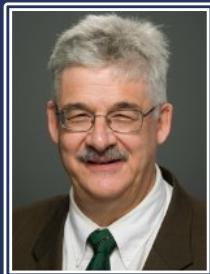
Krzysztof Reiss, Ph.D.

**Professor in the Department Interdisciplinary Oncology
Director of the Neurological Cancer Research Program at the LSUHSC-NO
Cancer Center**

Glioblastoma weak metabolic points as a target for new drugs with high potential for Blood Brain Barrier penetration.

Glioblastomas are the most aggressive and practically incurable brain neoplasms for which treatment options are very limited. The main obstacle preventing development of more effective glioblastoma therapies is the Blood Brain Barrier (BBB), which prevents the majority of anticancer drugs from penetrating intracranial tumor tissue at therapeutically relevant concentrations. Our new anti-glioblastoma therapeutic approach is based on the previously reported anti-glioblastoma activity of a common lipid-lowering drug fenofibrate (FF). FF kills glioblastoma cells by direct interaction of unprocessed form of FF (ester) with mitochondrial membranes. This interaction leads to the severe inhibition of mitochondrial respiration which in consequence triggers depletion of intracellular ATP followed by extensive glioblastoma cell death. However, FF does not cross the BBB and its anti-glioblastoma effects can be attenuated by the elevated glucose content (4.5g/L). Therefore, we have designed and synthesized over 200 new metabolic compounds based on the FF skeletal structure, benzyl-phenoxy-acetamide (BPA). Two of the compounds, three of the compounds, PP1, PP21 and PP23, have physicochemical parameters that indicate high potential for improved BBB penetration. We have also confirmed that the compounds can effectively cross the triple coculture BBB model membranes. Similar to FF, the compounds block mitochondrial respiration, which is followed by an immediate increase of glycolysis. In consequence, glucose is quickly depleted leading to a severe decline of intracellular ATP, activation of AMPK, activation of autophagy, and ultimately, glioblastoma cell death. To improve anti-glioblastoma effects in a high glucose environment, we have tested multiple glycolysis inhibitors, and demonstrated that lonidamine and gnetin H (resveratrol trimer), synergize with PP1- and PP21-induced cytotoxicity in both low and high glucose media. In summary, we have developed a new class of metabolic compounds with improved BBB penetration that can effectively eliminate glioblastoma cells and synergize with the selected glycolysis inhibitors.

Invited Talk : January 28th, 2022 : 3:10 - 4:00 PM



Charles Irvin, Ph.D.
Professor of Medicine, Pulmonary Medicine
Associate Dean for Faculty Affairs
University of Vermont Burlington
Director, Vermont Lung Center

Scientific Misconduct: Crime & Punishment.

Charles G. Irvin, PhD, FERS is a Professor of Medicine, Professor of Physiology and Biophysics, Associate Chairman for Research Department of Medicine and Director of the Vermont Lung Center (VCL) at the University of Vermont. Dr. Irvin's research is focused on understanding the mechanisms of airways dysfunction in patients with asthma. Using a multidisciplinary approach including : cell and molecular biology, animal models and systems, transgenics, physiology, imaging and clinical studies, he and his colleagues seek to understand the pathophysiological basis of asthma in order to both better diagnose and treat patients with chronic airways disease. He has published over 200 peer-reviewed publications and published an additional 125 chapters, reviews and editorials on these topics. Dr. Irvin has been the site PI of the Vermont American Lung Association Airways Clinical Research Center (ACRC) from its inception and is the author or co-author of 37 ACRC publications. Since 2016, Dr. Irvin oversees ethics related issues for the NIGMS IPERT award team at UVM led by Dr. Mercedes Rincon. Dr. Irvin is a pioneer within the IDeA Program. He was one of the first recipients of the COBRE (Center of Biomedical Research Excellence) grant in 2000. One of Dr. Irvin's most significant contributions to the IDeA community has been his efforts to grow the National IDeA Symposium of Biomedical Research – a showcase for the breadth and impact of human biomedical and behavioral research that is done through grants awarded by the IDeA program. In February of 2020, Dr. Irvin received the inaugural W. Fred Taylor PhD Award in recognition of his significant contributions to enhance the impact of the National Institutes of Health (NIH) Institutional Development Award (IDeA) Program.

Project Oral Presentations & Graduate Student Presentations Abstracts

Improving Patient Outcomes for Inflammatory Bowel Disease through Physician Interactions during Infusion Treatment: Symptomatic Review of Biologic Therapy in IBD (STABILITY)

Dr. J. Steven Alexander (Translational Project PI)

Prerana Ramesh, Kelli Morgan, Meher Sindhoora Mavuram, James Morris, Qiang Cai, Phillip Kilgore, Urska Cvek, Marjan Trutschl, J. Steven Alexander

Louisiana State University Health Shreveport LSUHS (Molecular & Cellular Physiology, Gastroenterology and Hepatology), LSUS (Department of Computer Science)

Inflammatory Bowel Disease (IBD) includes Crohn's Disease (CD) and Ulcerative colitis (UC), both of which are characterized by chronic inflammation of the gastrointestinal (GI) tract and extra intestinal manifestations. IBD can be treated by 'biologics' (antibodies) administered via intravenous infusion at infusion clinics with periodic monitoring (colonoscopies and/or abdominal imaging) scheduled during separate clinical visits; based on such screening GI physicians can decide to implement changes in treatment. At LSUHSC-S, IBD patients who received biologic infusions did not routinely meet with a GI physician unless the patient requested this, or upon the infusion nurses' request if the patient was visibly ill. It was observed that many of the IBD patients who did not meet with a GI physician during their infusions would often be absent for their clinical visits. Consequently, these patients' disease progression could not be reliably traced, and alterations that needed to be made in their medication doses, treatment frequency, or therapy plans could go unnoticed. In order to combat this problem, the Department of Gastroenterology implemented patient meetings with GI physicians in the infusion clinics from January 2017 to August 2020 (termed 'STABILITY'). These patients were given anonymous surveys during their infusions to measure their understanding of their disease, how their symptoms had progressed during their treatment, and whether they would want to continue seeing a GI physician during their infusions. Clinical features such as disease severity and colonoscopic evaluations, levels of inflammatory biomarkers (e.g. C-reactive protein, disease activity, rate of hospitalization, etc.) was measured in 110 patients before and after STABILITY. Data analysis revealed significant reductions in disease severity, frequency of hospitalizations, and inflammatory biomarker levels in both CD and UC patients at the end of the treatment period.

Protective role of activating transcription factor 6 against endothelial barrier dysfunction

Dr. Nektarios Barabutis (INBRE COBRE Collaboration / Supplement PI)

University of Louisiana at Monroe

Endothelial barrier dysfunction (EBD) is associated with potentially lethal disorders; including sepsis and acute respiratory distress syndrome. So far approved drugs that specifically target those conditions do not exist, hence the development of novel therapeutics in the corresponding context is of the utmost need. Unfolded protein response (UPR) is a molecular mechanism, composed of three endoplasmic reticulum transmembrane proteins; namely the inositol-requiring enzyme 1 α , pancreatic endoplasmic reticulum kinase, and activating transcription factor 6 (ATF6). Activation of UPR attempts to repair damaged tissues, so to prevent cellular death. In the current study we focus on the role of ATF6 towards endothelial barrier function, to investigate the possibility that activation of this UPR sensor (ATF6) delivers protective effects towards EBD. We reveal that ATF6 inhibition in bovine pulmonary artery endothelial cells (BPAECs) due to ceapin-A7; or siRNA for ATF6; augments the deteriorating effects of cofilin towards actin cytoskeleton integrity. Electric Cell-substrate Impedance Sensing (ECIS) measurements revealed that ceapin-A7 reduced transendothelial resistance; and potentiated lipopolysaccharide (LPS)-induced transendothelial; and paracellular permeability. The latter was measured by Fluorescein Isothiocyanate-Dextran. LPS is the major component of the outer membrane of Gram-negative bacteria. On the other hand, ATF6 inducer AA147 supported the integrity of the BPAEC monolayers by

suppressing the activities of cofilin; and enhancing transendothelial resistance. Moderate concentrations of both ceapin-A7 and AA147 did not affect BPAEC viability. In the following steps of our study we will utilize a murine model of LPS-induced model of acute lung injury, to reveal the effects of ATF6 manipulation in the corresponding pathology. Collectively, we suggest that targeted ATF6 manipulation may deliver a novel therapeutic possibility in EBD-related diseases.

Developing fisetin, a polyphenolic ingredient co-targeting the central mTOR pathway and IL-17A for Treating Psoriasis

Dr. Jean Christopher Chamcheu (Full Project PI)

Tithi Roy¹, Sergette Banang-Mbeumi¹, Samuel Boateng¹, Stephane Esnault², Roxane-Cherille Chamcheu¹, Shile Huang³, Kousoulas Gus Konstantin⁴ and Jean Christopher Chamcheu¹

University of Louisiana at Monroe 1. University of Louisiana at Monroe College of Pharmacy, 2. University of Wisconsin Madison School of Medicine, 3. LSU-HSC-Shreveport School of Medicine, 4. LSU Baton Rouge School of Veterinary Medicine

The PI3K-Akt-mTOR signaling pathway that plays critical roles in cell growth, autophagy, apoptosis, and angiogenesis has emerged as a clinically relevant disease targets in psoriasis, an incurable inflammatory dermatosis afflicting \approx 8 million Americans. This has led to new therapeutic strategies, thus the need for improved understanding of dysregulated pathway in psoriasis. We will affirm the pathways' regulatory role, and develop fisetin (3',4',7-trihydroxyflavonol), as an effective treatment approach for psoriasis. In pursuit of effective psoriasis drugs, we observed that fisetin is endowed with prodifferentiation, antiproliferative and anti-inflammatory properties, and inhibits the activated PI3K/Akt/mTOR components in vitro (Cells. 2019 Sep 15;8(9):1089.), stressing its potential in controlling psoriasis. Here, we assessed the effect of fisetin compared to rapamycin (known mTOR inhibitor) on activated immune- and skin cells, and in imiquimod (IMQ)-induced Balb/c mice psoriasis-like disease. Fisetin and its potent analogs we recently reported (Bioorg Chem. 2021 Feb;107:104595) and bimiralisib, dock and strongly bind to IL-17A, Rac1, and PIK51 α all dysregulated in psoriasis. Fisetin alone or in-combination with immune and skin cells activators eliciting psoriasis-like features, suppressed i) mTOR activity in skin cells (NHEK), and ii) secretion of pro-inflammatory cytokines (IL-17A and IFN- γ) by CD4+T cells primed with IL-1 \square /IL-23, or co-cultured with NHEKs. We have also generated mTOR and Raptor CRISPR/Cas9 knockout NHEKs, and are characterizing these prior to use in testing drugs. We are also analyzing by RNA-Sequencing the effect of treatments to be presented. Furthermore, topical administration of fisetin or rapamycin resulted in marked improvement in IMQ-induced mouse psoriasiform dermatitis, including inhibition of the levels of multiple immune-mediators and activated Akt/mTOR. Overall, our data suggest fisetin could be developed to treat psoriasis.

Micro-RNA therapy against cell cycle progression for Lung Cancer treatment

Dr. George Matthaiolampakis (Full Project PI)

University of Louisiana at Monroe

Lung cancer (LC) is the leading cause of cancer-related deaths in the US, with estimated 131,880 deaths in 2021. Regulation of cell cycle progression is a promising approach for cancer treatment and has translated to patient care. More specifically, three FDA-approved CDK inhibitors are currently used for specific breast cancer subtypes. Interestingly, this methodology has not translated towards LC patient treatment. Recent advances in

molecular therapeutics have brought prominence to nucleic acid-based therapeutics and their potential use in many diseases, including cancer treatment. Among the different types of nucleic acids, micro-RNAs (miRNAs) are natural short nucleic acids capable of regulating gene expression and, thus, pathway activity. We focused on two miRs, miR-143 and miR-506, that regulate CDK1 and CDK4/6, respectively. Gene expression analysis presented that the miRs downregulated these genes and have the capacity to control cell cycle progression in LC cells, in a comparable activity to commercially available CDK inhibitors. This activity was accompanied by an increase of the apoptotic cell population at both 24 and 48 h post-treatment, as detected by an Annexin V/PI analysis. Our future work is to further confirm and decipher the activity of the two miRNAs, creating stable transfection to LC cells. Our work so far strongly supports that the two miRs have the potential for LC treatment and regulating the cell cycle progression. We will expand our analysis with stable transfusions and evaluate the miRs' potential for LC treatment.

Design, Synthesis and Evaluation of Pyrazole Derivatives as Potential Anti-Cancer Agents

Dr. Siva Murru (Full Project PI)

Prof. Seetharama Jois, Dr. JeanChristophe Chamcheu, Dr. Jayalakshmi Sridhar

University of Louisiana at Monroe University of Louisiana Monroe, Xavier University of Louisiana

Cancer is the most difficult ailment and leading causes of death around the world. Anticancer agents that target DNA are some of the most effective agents in clinical use, but they are extremely toxic. Consequently, much effort has been put into finding robust inhibitors that are more selective, less toxic and less susceptible to drug resistance. The general aim of our project is to design, synthesize and evaluate nitrogen heterocyclic compounds and their metal complexes as potential anticancer agents. Nitrogen heterocyclic compounds are an integral part of a huge number of natural and synthetic compounds that play important roles in the biological systems. Among those, pyrazole derivatives can be fine-tuned to achieve desired electronic and steric effects that are essential features required for the desired biological activity. Currently we are working on synthesis and biological evaluation of pyrazole, pyrazolone, and phthalazinone based small molecules as potential anticancer agents. We have recently identified a set of compounds exhibiting anticancer activity particularly towards non-small cell lung cancers (NSCLC). Until now, treatment of NSCLC has had limited success and new therapeutics are desperately needed. We have synthesized several derivatives of lead molecule(s) and tested the in-vitro antiproliferative activity using Cell-titer Glo assay. A few compounds have shown good potency against two lung cancer cell lines i.e. human lung carcinoma (A549) and human adenocarcinoma (NCI H522) while being less toxic to non-cancerous Human Lung Fibroblast cells. We have also tested a set of pyrazole and pyrazolones compounds against cutaneous melanoma (GFP-A375 and SKMEL-28) and non-melanoma (GFP-A431 and SCC-12) cell lines with HaCaT keratinocytes as a control. In addition to that, we performed cell cycle analysis and obtained data from kinase profiling studies. We will present the data and results from our synthetic approaches and biological assays.

Proteasomes/immunoproteasomes: Role of lipid rafts in compartmentalization/ activation in e-cigarettes vapor exposed lung epithelial cells

Dr. Devaiah Kambiranda (Full Project PI)

Rizwana Begum, Shilpa Thota, Lauryn Langley, Sanjay Batra

Southern University and A&M College Southern University Baton Rouge

Cigarettes and other tobacco-based products are addictive. However, due to their projection as less harmful alternatives, e-cigarettes gained popularity in the US markets rapidly. Earlier studies demonstrate that lipid raft proteome contained a marked representation of the ubiquitin-proteasome system in murine macrophages.

Interestingly, lipopolysaccharide exposure selectively activated the proteasome system in membrane rafts in murine macrophages, while its inactivation was observed outside the raft entities. Based on these facts, we hypothesized the important role of lipid rafts in compartmentalization/activation of proteasomes during exposure to e-cigarette vapors. Using human alveolar epithelial cells (A549) exposed to tobacco flavored e-cigs vapor condensate (TF-ECVC) we observed: a) increase in the transcription and translation of lipid raft-associated proteins (caveolin-1, flotillin-1, and flotillin-2) and inducible proteasome subunits (LMP7/PSMB8, LMP2/PSMB9, MECL-1/PSMB10); b) reduced expression of constitutive proteasome subunits (β 1/PSMB6 and β 2/PSMB7); c) increased expression of NF- κ B and MAPK genes; and d) elevated production of pro-inflammatory cytokines/chemokines in A549 cells. In terms of nutrvention, cells pretreated with 5 μ M concentrations of ellagic acid metabolites- Urolithin A (Uro-A) or Uro-C showed significant rescue of TF-ECVC-induced expression of inducible proteasome subunits and lipid raft proteins in our study. Additionally, we observed localization of β 2 and LMP7 subunits in lipid raft fractions of TF-ECVC challenged alveolar epithelial cells. Based on our results, identifying the role of lipid rafts in the activation of proteasome/immunoproteasome and the downstream signaling during TF-ECVC exposure is an interesting and novel objective of the current study. Further studies are in progress to determine the localization of other immuno- and constitutive-proteasome subunits in lipid rafts entities from ECVC challenged cells.

Life in the fastlane: Testing for congruence among transcriptomic signatures in model organisms

Dr. Kyle Piller (Full Project PI)

Southeastern Louisiana University

Traditionally, species are developed as model organisms because they possess interesting life-history features or unique genetic attributes that make them amenable to laboratory studies and testing. The Turquoise Killifish (Nothobranchiidae: Nothobranchius furzeri) is a recently developed model that is being used to investigate the process of aging and age-related diseases. The most intriguing aspect of this species, and the reason that it was developed, is because it is an annual species that can complete its entire lifecycle in between 10 and 31 weeks. However, it is unclear as to whether or not the same expression patterns of this species are unique or whether they are widespread throughout other groups of vertebrates. Annualism is a relatively rare life-history trait among vertebrates, but other species of closely related cyprinodontiform fishes in the families Nothobranchiidae and Rivulidae also contain annual species, as well as non-annual species. Therefore, the overall objective of this study is to assess congruence in the genetic architecture of the Turquoise Killifish to other species in these families with different life-histories traits (annual, facultative annual, and non-annual). Congruence in genetic characteristics of species with similar life-histories would represent strong support for the use of the Turquoise Killifish as an appropriate aging model. This will be accomplished through the generation of RNA-Seq data (Illumina), and validation through the examination of a subset of differentially expressed genes using digital PCR methods. It is well known that replication and congruence are important in the sciences and in the case of potential model organisms, such as the Turquoise Killifish and relatives, congruence among genes, across life-cycle variants, provides stronger evidence for their importance in the aging and age related processes.

HSP70 and proteasomes coalesce in lipid rafts to regulate E-cigarette Vapor condensate induced inflammation

Dr. Rizwana Begum (Graduate Student)

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Electronic cigarettes (e-cigs) and other tobacco-based products are addictive. However, due to their projection as less harmful alternatives, electronic smoking devices or e-cigs gained popularity in the US markets rapidly. Earlier reports suggest that HSP70 interacted with the ubiquitin-proteasome system (UPS) to eliminate the damaged and malfunctioning proteins in the cell. In addition to protecting the cellular proteome, HSP70-the primary stress-inducible heat shock protein has been demonstrated to interact with lipids. In light of these facts, we hypothesized the important role of lipid rafts in-a) compartmentalization of HSP70 and proteasome/immunoproteasomes; and b) regulating inflammatory responses-in e-cig vapor condensate (tobacco flavor; TF-ECVC) challenged human lung epithelial cells (A549). Our experiments revealed TF-ECVC mediated increase in-1) transcription and translation of lipid raft-associated proteins (caveolin-1, flotillin-1, and flotillin-2); 2) inducible proteasome subunits (LMP7/PSMB8, LMP2/PSMB9, MECL-1/PSMB10); c) expression of NF- κ B and MAPK genes; d) transcription and extracellular accumulation of HSP70; and e) production of pro-inflammatory cytokines/chemokines in A549 cells. We also observed a decrease in the expression of constitutive proteasome subunits (β 1/PSMB6, β 2/PSMB7, and β 5/PSMB5). Also, the localization of HSP70, β 2/PSMB7, and LMP7/PSMB8 subunits was observed in lipid raft fractions of TF-ECVC challenged alveolar epithelial cells. Furthermore, using siRNA mediated approach, we observed a decrease in the expression of lipid rafts associated protein flotillin-1 and proteasome subunit β 1/PSMB6 in HSP70 knockdown A549 cells challenged with ECVC. Overall, our findings provide critical information about the role of lipid rafts and HSP70 in ECVC-induced inflammation. Studies are in progress to identify the detailed molecular mechanisms.

Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells

Dr. Nandini Bidarimath (Graduate Student)

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Dr. Sanjay Batra

Pentachlorophenol (PCP), an anthropogenic chlorophenol compound, was primarily used as a wood preservative and in formulations of fungicides, insecticides, and herbicides. Household and occupational exposure to PCP via inhalation and/or ingestion has been associated with immune modulation in humans. However, the genetic and molecular mechanisms regulated during PCP exposure are still not completely understood. To cover the gap in our understanding, we conducted a high-throughput RNA sequencing for determining the potential molecular mechanisms associated with PCP-induced immune regulation. We exposed human lung (A549) and liver (HepG2) epithelial cells to PCP (10 μ M) for determining the effect on transcript abundance and transcriptomic profiles. Two independent RNA-sequencing pipelines were run for identifying differential gene expression (DGE), while Principal component analysis (PCA) was performed independently to understand the variation and pattern in each dataset. This was followed by Gene Set Enrichment analysis (GSEA), Gene ontology (GO) term, KEGG pathway and network/pathway (GAGE-Generally applicable gene set enrichment) analyses to assess the biological implications. The DGE analysis of HepG2 cells revealed 17 significantly upregulated and 49 downregulated genes, while A549 cells revealed 6 upregulated and 16 downregulated genes following PCP-exposure in our preliminary studies. The GSEA and KEGG analysis on HepG2 cells yielded a distinct cluster of significantly expressed genes associated with hepatocellular carcinoma, MAPK signaling, xenobiotic metabolism and steroid hormone biosynthesis-highlighting altered biological mechanisms during PCP-exposure. While A549 cells showed altered VEGF signaling pathway, Hippo signaling pathway, oxidative phosphorylation, neutrophil extracellular trap formation-highlighting altered immune signaling. Further studies are in progress to determine the molecular mechanisms associated with PCP-induced immunotoxicity.

Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females

Mr. Eric Clifford (Graduate Student)

Phillip Kilgore, Urska Cvek, Marjan Trutschl, Nadejda Korneeva, Steven A. Conrad, Thomas Arnold

Louisiana State University Shreveport LSUS (Department of Computer Science and Laboratory for Advanced Biomedical Informatics), **LSUHS** (Department of Emergency Medicine)

Dr. Urska Cvek

LSU Health Sciences Center in Shreveport serves a largely minority-based, urban population. Prior analysis of emergency room urine drug screen results from 1998-2011 found that the African American population tested positive for cannabinoids, opiates, and cocaine at high rates, while the Caucasian population tested positive for cannabinoids, benzodiazepines, and opiates at high rates. The focus of this study was to determine connections between visit reasons and rates of positive drug screens, tracked by race and age, among 18-35 years old females during 2012-2019. Similar to the 1998-2011 general population study, Caucasian and African-American females tested positive mostly for cannabinoids and opiates during 2012-2019. Caucasian females also tested positive for amphetamines and benzodiazepines at higher rates than African American females. African American females tested positive for cannabinoids and cocaine at higher rates than Caucasian females. From 2012-2016, Caucasian females tested positive for opiates at higher rates. Beyond 2016, African American females tested positive for opiates at higher rates. Most visits in both populations were for pain, pregnancy, or psychiatric/neurologic reasons. About 30% of pregnancy and gynecologic visits were associated with cannabinoid use, followed by opiates. Gastroenterology patients tested positive for cannabinoids in over 40% of cases and for opiates in 20%. Psychiatric/neurologic patients tested positive mostly for cannabinoids and amphetamine (36% and 15%, respectively). Sickle Cell patients (all African American) tested positive for opiates at a rate of 72%. GatewayNet analysis indicated that cannabis use likely precedes cocaine, amphetamine, benzodiazepine, and opiate use. This work is supported by the 2021 Summer Research Program of the Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20 GM103424-19.

Development of a pH-sensitive liposome formulation for targeted delivery of anticancer pyrazolones in lung cancer cells

Mr. Denzel El Hage (Graduate Student)

Jafrin Jobayer Sonju, Prof. Seetharama Jois, Dr. Siva Murru

University of Louisiana at Monroe University of Louisiana Monroe

Dr. Siva Murru

Cancer incidence and mortality are rapidly growing worldwide. The World Health Organization and the US National Cancer Statistics reports indicating this multifaceted global health issue as the second most common cause of death in the World. Consequently, much effort has been put into finding robust anti-cancer agents that are more potent, selective and less toxic. Along those lines, we synthesized a library of pyrazolone compounds and screened them against lung and breast cancer cell lines. Based on their antiproliferative activities, we have identified a set of highly potent pyrazolone compounds that are lacking selectivity because they are equally affective against both cancerous as well as non-cancerous cells. To improve their selectivity and anticancer activity, we have been working on developing a pH-sensitive liposomal formulation to cargo the pyrazolone compound and release in the tumor microenvironment which is acidic in general. The pH-sensitive liposome-pyrazolone formulation showed optimum size for accumulation into the tumor microenvironment with homogeneity of particles. Zeta potential also indicates stable dispersion of particles with less undesirable

interaction with other serum proteins. Our preliminary in vitro release study indicated the pH-dependent release of pyrazolone in an acidic environment that can possibly improve the selectivity and reduce the side effects.

The dietary antioxidant Fisetin suppresses Psoriasis-like characteristics in vitro and in vivo in an imiquimod-induced dermatitis in Balb/c mice: Involvement of the central mTOR signaling pathway

Ms. Tithi Roy (Graduate Student)

Tithi Roy¹, Sergette Banang-Mbeumi¹, Samuel Boateng¹, Stephane Esnault, Roxane-Cherille Chamcheu¹, Kousoulas Gus Konstantin and Jean Christopher Chamcheu¹

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The central mTOR-regulated networks have recently emerged as a clinically relevant target in the pathogenesis of psoriasis, a chronic and incurable inflammatory skin disorder. Treatment for psoriasis has remains elusive, thus the need to develop nutraceuticals that can inhibit target activities and improve lesions. We earlier reported that the dietary antioxidant fisetin, is a potent mTOR inhibitor that attenuates keratinocytes-induced responses. Here, we examined the effect of fisetin on activated immune and skin cells, and in an imiquimod (IMQ)-induced BALB/c mice psoriasis-like skin inflammation model. Fisetin alone or in-combination with immune (anti-CD3/CD28) and skin (IL-22/IL-6) cells activators, which elicit psoriasis-like flares in vitro, resulted in the suppression of i) mTOR activity in normal human epidermal keratinocytes (NHEK), and inhibition of the secretion of Th1/Th17 type pro-inflammatory cytokines (IL-17A and IFN- γ) induced by anti-CD3/CD28-activated; ii) peripheral blood mononuclear cells (PBMCs), iii) CD4+T cells that were primed with/without IL-1 \square /IL-23, and iv) CD4+T cells co-cultured with/without NHEKs. Topical application of aldarac cream induced mouse psoriasiform dermatitis associated with activation of Akt/mTOR pathway components. We observed that topically applied fisetin resulted in improvement in IMQ-induced dermatitis including hyperplasia, erythema, ear swelling, scaling, inflammatory mediators and phosphorylated Akt/mTOR versus controls. Fisetin was also found to inhibited the expression levels of multiplexed immune-mediators versus control mice. Generated myeloid-cell specific mTOR-deficient mice are being tested for the role of fisetin as inhibitor for psoriasis control, and this will provide preclinical translational data that could benefit patients with psoriasis and other chronic skin diseases. Overall, our data suggest fisetin as a useful inhibitor of mTOR to be developed for treating psoriasis.

Evaluating model selection frameworks for complex hierarchical models

Dr. April Wright (Full Project PI)

Jeremy Brown

Southeastern Louisiana University LSU

As in many areas of biology, phylogenetics researchers often use complex models. For dates phylogenies, these models may be hierarchical, meaning that different parts of the dataset are described by different models. In some cases, sub component models may even have dependency structures. This has called into question the ability of common model selection paradigms to usefully discriminate between correct and incorrect models. In this talk, I will present current work assessing Bayes factor model selection, posterior predictive simulation, and reversible jump MCMC for model evaluation in phylogenetics. These results, while focusing on phylogeny, will provide insights for any biologist applying complex models to their data.

Mechanism of Translation initiation in the protozoan parasite *Giardia lamblia*

Dr. Srinivas Garlapati (Full Project PI)

Dr. Yong-Hwan Lee

University of Louisiana at Monroe LSU Baton Rouge

Giardia lamblia is a flagellated protozoan parasite that causes gastrointestinal disease giardiasis in humans and is responsible for major waterborne outbreaks of diarrhea in the United States. The protein synthesis machinery of *Giardia lamblia* differs from its mammalian host and hence could serve as a potential drug target. The ribosomes are smaller, and the mRNAs have unusually short 5' untranslated regions (5' UTRs). In addition, it lacks key initiation factors that are required for recruiting ribosome to the 5' end of the mRNA, and once bound, the ribosome selects the start codon without scanning. In eukaryotes, initiation factor eIF4G plays a key role in recruiting the ribosome as a pre-initiation complex to the 5' end of the mRNA. In *Giardia*, homologs for eIF4E (GleIF4E2) and eIF4A (GleIF4A) have been identified but not for eIF4G. To address how PIC is recruited to the 5' end of the mRNA in the absence of eIF4G homolog, we have used yeast two-hybrid assays to identify potential interactions of GleIF4E2 and GleIF4A with the components of the PIC. The results show that GleIF4E2 can interact with the subunit of the initiation factor GleIF2, and GleIF4A can interact with GleIF3i subunit of GleIF3 complex. These interactions were further confirmed by site-directed mutagenesis of ZDOCK predicted residues of GleIF4E2 and GleIF4A and GST-pull down assays. To confirm these interactions in *Giardia* cells, proximity dependent biotin ligation assays were conducted.

Elucidation of Plant-Derived Anticancer Alkaloid Biosynthetic Pathways

Dr. Vonny Salim (Full Project PI)

Ryan Miller, Paul Erba, Stephanie Provenzano, Pearl Merry, Keelin North, Shandrekia Robinson, Christopher Stratton, Elahe Mahdavian, Urska Cvek, Phillip Kilgore, Shile Huang

Louisiana State University Shreveport Louisiana State University Shreveport, Louisiana State University Health Sciences, Shreveport, Louisiana

Medicinal plants produce a wide array of specialized metabolites with anticancer properties that have been used in chemotherapy. *Catharanthus roseus* and *Camptotheca acuminata*, two plant species produce alkaloids that serve as key targets for drug development. Despite their extensive clinical applications, the isolation and purification of these compounds still rely on the plant source with very low yields. Elucidation of biosynthetic pathways of alkaloids from both plants greatly contributes to synthetic biology approaches in microbial systems. Next-generation sequencing of medicinal plants and further bioinformatic analyses have accelerated the process of identification and functional characterization of candidate genes, especially those involved in anticancer alkaloid production. Integration of transcriptomics, genomics, and metabolomics has allowed the improved functional characterization of camptothecin biosynthetic enzymes in *C. acuminata*. The molecular modeling of these biosynthetic enzymes further demonstrated the possibilities of modulating their substrate specificities to diversify the chemical structures of alkaloids with potential new therapeutic applications. In the process of in-vivo characterization of alkaloid biosynthetic pathways in plants, via reverse genetics approach, silencing of biosynthetic genes was shown to alter the alkaloid metabolism and allow additional access to intermediates, possibly critical substrates of biosynthetic enzymes. Furthermore, successful whole cell biotransformation by *Escherichia coli* to produce the central intermediate of alkaloid pathways, strictosidine strengthens our capabilities to develop efficient platforms in large-scale production of plant anticancer metabolites in microbial systems. The modulation of alkaloid production, such as through soil microbiome studies also empower the biosynthetic capabilities and inform our metabolic engineering efforts towards sustainable production of anticancer therapeutics.

Poster Session Abstracts

Poster Session Abstracts

ID 1 Comparative Bioinformatics and Conventional approach reveal some common signaling mediators in DE-particulate exposed A549 and BEAS-2B cells

I, Rm 1 **Mr. Abubakar Abdulkadir, Dr. Sanjay Batra**
Southern University and A&M College, Southern University A and M College

Diesel exhaust particles (DEPs) contribute significantly to the air pollution caused by motor vehicles. Pulmonary exposure to diesel exhaust (DE) has been associated with multiple adverse health effects, including carcinogenicity, hypertension, chronic obstructive pulmonary disorder (COPD), bronchitis, asthma, etc., etc.-with inflammation playing a central role in their manifestation. DE particulates deposited in the lung exert differential bronchial and alveolar epithelium responses. We used human lung alveolar A549 cells with type-II characteristics to study the immune mechanisms regulated by DE particulates and compared our findings with our findings from the bioinformatic study conducted using T-bio server pipelines (Pine Biotech) prepared from the online available data set for BEAS-2B cells transcriptome (GSE155616). Both A549 and BEAS-2B cells have been extensively used for toxicological studies. Although few studies demonstrate the impact of DE particulates in various study models, the comparative analysis of A549 (obtained from carcinomatous tissue) and BEAS-2B cells (obtained from normal bronchial epithelium) will help propose a suitable cell line for future in vitro studies. We hypothesize that DE particulate induces inflammation in both cell lines by engaging similar signaling cascades. We used a hybrid in-silico/in-vitro/bioinformatics approach to determine receptor-mediated signaling events in both cell lines. Using Hex and Autodock vina on the Samson platform, our molecular docking results showed high binding affinities of DE particulates with AHR complex proteins, IL-1R, IL-6R, IL8R, TNFR CBR1/2, TLR4, and AHR. Interestingly, the bioinformatics analysis of the BEAS-2B dataset in T-bio server pipelines and transcriptional expression studies in A549 cells suggest a similar regulation trend for IL1R, IL6R, IL8R, TNFR, and CBR1 in both cell lines after exposure. In contrast, the profiling of TLR4 and AHR was significantly different in the two cell lines.

ID 2 Growth Hormone Releasing Hormone Antagonists Protect Against LPS-Induced Endothelial Hyperpermeability

I, Rm 2 **Mr. Mohammad Shohel Akhter, Antoinette Jaci Leo, Khadeja-Tul Kubra, Nektarios Barabutis**
University of Louisiana at Monroe, University of Louisiana Monroe

Growth Hormone Releasing Hormone (GHRH) is a hypothalamic neuropeptide which regulates the secretion of Growth Hormone from the anterior pituitary gland. Accumulating evidence suggest that GHRH is involved in inflammatory processes and increases the generation of reactive oxygen species (ROS) in human cancers and endothelial cells. GHRH antagonists (GHRHAnt) were developed to suppress cancer growth; and have been associated with anti-inflammatory and anti-oxidative activities in a diverse variety of in vivo and in vitro experimental models. We have recently shown that GHRHAnt support endothelial barrier function and involve unfolded protein response in their actions, so to protect the vasculature against injury. In the current study we utilized bovine pulmonary endothelial cells to reveal that those antagonists oppose Lipopolysaccharides (LPS)-induced activation of cofilin; and the phosphorylation of myosin light chain 2 (MLC2). Cofilin is an essential element of actin cytoskeleton, and MLC2 activation reflects the formation of filamentous actin stress fibers. GHRH triggered the opposite effects, compromising the endothelial barrier function. In a murine model of LPS-induced acute lung injury, GHRHAnt reduced BALF protein concentration of the inflamed lungs; an indicator of edema. Those peptides did not affect cell viability; as measured by the MTT (3-[4,5-dimethylthiazol-2-yl]-2,5 diphenyl tetrazolium bromide) assay. Collectively, we conclude that GHRHAnt may represent a novel therapeutic possibility in illness related to barrier dysfunction. Future investigations will delineate the corresponding molecular events; by employing genetic manipulations and mutant mice.

Poster Session Abstracts

ID 4 Identification of Spore-Forming Bacteria in a Louisiana Salt Marsh
II, Rm 2 **Ms. Alexis Bardwell**, M. Bowles, R. Giorno
Louisiana Tech University, Louisiana Universities Marine Consortium

Spores, highly resistant dormant cells of *Bacillus* and *Clostridium* species, are capable of surviving almost any environmental assault. Spores can be reactivated with nutrients by a process called germination. There is a fundamental gap in our knowledge of spore-forming microorganisms that can persist and possibly thrive in saline and hypersaline environments similar to Mars and other celestial bodies. Additionally, antibiotic resistance is a global health problem, and the environment is an important reservoir for antibiotic resistance genes. Thus, spores associated with saline and hypersaline environments are a concern for contamination of celestial bodies and could add to our understanding of the antibiotic resistance crisis. Our long-term goal is to identify and characterize spore-forming bacteria that can live in extreme environments and add to our knowledge of the environmental resistome. To begin this characterization, we isolated spore-forming bacteria from a Louisiana salt marsh from two different plant stands. The sediment samples, S25 and J25, were treated to enrich for spore formers and then plated onto R2A media and incubated under various combinations of temperature and added NaCl concentrations (25C, 37C, and 50C; 0%, 3%, 5%, and 9%, respectively). Colonies were selected for 16S rRNA sequencing trying to select colonies with novel morphologies. Sequencing results show all colonies selected were from spore-forming genera. The next step in this study is to test for antibiotic resistance in these isolates.

ID 5 N-Boc-hydroxylamine as a Boc-donor Agent for the Catalytic N-tert-Butoxycarbonylation of Pyrazoles and Indazoles
II, Rm 3 **Mr. David Basnet**, Siva Murru
University of Louisiana at Monroe, University of Louisiana at Monroe

The presence of an amino group in various drug molecules and their key intermediates makes protection/deprotection of the amine functionality a necessity during their synthesis. Compared to acylated amines, tert-butoxycarbonylated amines can be deprotected under mild conditions with high purity of products. Moreover, tert-Butyl carbamates are stable in the presence of a wide range of nucleophiles and under alkaline conditions and are very labile under mild acidic conditions to liberate the parent amine. In general, tert-butoxycarbonylation is achieved by treatment of an amine with Boc-anhydride [(Boc)₂O] in the presence of organic/inorganic bases. However, the reported methodologies have various drawbacks such as long reaction times, requirement to prepare the tert-butoxycarbonylation reagents, high toxicity of DMAP and its derivatives. Further, the base catalysed reactions often lead to the formation of isocyanate, urea, and N,N-di- Boc derivatives. With our recent experience in using N-Boc-hydroxylamine (Boc-NHOH) as an aminating agent, we speculated that the above-mentioned disadvantages could be avoided by electrophilic activation of Boc-NHOH in the presence of a Copper-catalyst. We present herein CuCl-pyridine as a highly efficient catalyst for the formation of tert-butyl carbamates from pyrazoles and indazoles at room temperature. We have tested variety of heterocyclic compounds and amines, and performed controlled experiments which will be discussed in the poster. The advantages include (i) the use of a cheap, easy to handle and commercially available catalyst, (ii) room temperature reaction conditions, and (iii) high yields. With the enforcement of tight legislation for environment protection in chemical transformations, the solvent-free reaction conditions employed in the present methodology constitutes a greener protocol for the desired transformation.

ID 6 Biological evaluation, in silico molecular docking and ADMET screening of a small library of phenolic compounds identified novel anti-skin cancer agents
I, Rm 4 **Mr. Samuel Boateng**, T Roy, S Banang-Mbeumi, RN Chamcheu, Mercy E. Agbo, J Fotie,

Poster Session Abstracts

JC Chamcheu

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Skin cancer remains the leading form of cancer in the United State, with about 9,500 newly reported cases daily. The main forms include cutaneous melanoma (CMSC) and non-melanoma skin cancer (NMSC), with CMSC being more fatal, while NMSC is more prevalent. Current pharmacological interventions are limited by their side-effects, drug resistance, low-bioavailability etc. In this project, we seek to address these challenges by identifying new lead compounds against these major skin cancers. Using simplified and improvised methods; C-N/C-C coupling or direct substitution on the aromatic ring and modified Skraup-Doebner-von Miller, about 90 phenolic derivatives were synthesized and screened. Their biological evaluation identified two potent hit compounds APR-5 and CNB-7 showing low micromolar range activities IC₅₀ values; 2.9±0.58 μM (SCC-12), 5.0 ±0.80 μM (A431), 4.9±0.55 μM (SkMel-28), and 6.7±0.47 μM (A375), while having minimal or no effect on control cells (HaCaT). Both compounds were better in activity and selectivity than the positive control drug-Cisplatin. These two also significantly reduced scratch wound healing, colony formation, and activated expression levels of major cancer molecular targets such as RSK/AKT/ERK1/2, S6K1and PIM3 in a dose dependent manner. We observed a significant and dose-dependent induction of apoptosis in SCC-12 and SkMEL-28 cells, evidenced by the downregulation of protein expression levels of Bcl-2 and upregulation of Bax, cleaved caspase-3,-9 and PARP levels. Using Swiss Target Prediction / SwissADME web-based tool, we further identified ROCK 1/2, FYN, MMP9 and LCK dual specificity protein kinase (CLK4) as targets, and identified high GIT absorption, skin permeation (log KP), Log Po/w (below 5), Lipinski rule compliancy and high biodegradable characteristics of the compounds. In surmise, our data highlight promising anticancer potential of these phenolics, to warrant further investigation as potential therapeutics against CMSC and NMSC

ID 7 Assessment of injectable chitosan-genipin hydrogels biomaterial biocompatibility

I, Rm 5 **Dr. Mary Caldorera-Moore**, Claire Colley, Tyler Priddy-Arrington
Louisiana Tech University, Louisiana Tech University

A proactive biomaterials is becoming increasingly necessary to address limitations in current treatments for chronic wounds and tissue regeneration. Previously our group developed chitosan hydrogels crosslinked by genipin at 50°C (termed C-G50 hydrogels). The C-G50 hydrogels were highly absorptive and antibacterial, but they still suffered from the weaknesses of all pre-formed wound treatments in that they can't be injected and don't mold to the wound. Therefore, in this project, we adjusted the hydrogel formula to be able to crosslink at body temperature, instead of 50 °C to enable injection, in situ crosslinking, and cell encapsulation. Herein, to optimize these new C-G37 hydrogels for injection and in situ crosslinking, 5 groups of chitosan-genipin hydrogels were evaluated dependent on time of pre-injection crosslinking (0-hr, 2-hr, or 4-hr) and method of pre-injection crosslinking (loaded or plated). Swelling, absorbance, and gelation studies were performed to characterize and evaluate the 5 groups. The gelation study revealed both 4-hr groups were fully gelled when injected, and they were therefore not further investigated moving forward. Cell biocompatibility was evaluated by exposing plated immortalized human epithelial keratinocyte (HEK) cells to the C-G37 hydrogels over 10 days and performing a live cell count using a CCK-8 assay every 3 days. Cell viability, normalized to the control cells, of all 3 hydrogel groups suffered a small initial decrease. However, at day 4 it then increased and remained above 100% for the remainder of the 10-day study, with a steady increase in cell viability at each time point. The resulting data and subsequent analysis of the studies confirmed that the developed C-G37 hydrogels demonstrate a robust biomaterial that is biocompatible, injectable, and highly absorptive. The ability of the C-G37 hydrogels to be injectable while also providing a viable cell environment presents a viable, minimally invasive wound healing platform.

Poster Session Abstracts

ID 8 Applying the Brakes: Understanding the Role of the Conformational Changes in the Kinesin-5 on Processivity and Inhibition

II, Rm 6 **Dr. Joseph Chaney**, Amaya Sanders (1), Thandiwe Bush (1), Alyria Terry (1), Carolyn Scruggs-Webster (1), Nelson Brown, Kennedy Drake (1), Jada Montley (1), Micquel Downs (2), Edward Wojcik (2), Joseph Chaney (1)

Xavier University of Louisiana, 1. Xavier University of Louisiana, 2. Louisiana State University Health Science Center New Orleans

Human Kinesin-5 (Eg5), an anticancer drug target, is key to the assembly of the bipolar spindle during mitosis. Its promise as a clinical target comes from the fact that they are involved only in metaphase and not interphase like some of the leading clinical drugs. However, the overall mechanism of inhibition in these targets needs further exploration. Inspection of the crystal structures of Kinesin-1 dimers reveals the addition of strands to the central β -sheet is found in one head and absent in the other; this previously unrecognized structural asymmetry between the two heads may suggest a regulatory mechanism involving the N-terminal Neck-Linker (NL) and the C-Terminal Cover-Neck. These structural changes in the neck-linker and cover-neck of Kinesin-5 have not been reported. Thus, the importance of establishing this conformational switch in Kinesin-5 requires additional experiments for understanding and molecular validation. However, we must first understand how changes in the neck-linker modulate kinesin function. We have inserted three residues (+DAL) into various positions of the neck-linker of dimeric Kinesin-5 (1-513) and KHC (1-560). Our results indicate these neck-linker mutants can allosterically regulate kinesin ATPase activity.

ID 9 Electro-chemical Cyclization of Hydroxychalcones for the Synthesis of Flavonoids

II, Rm 8 **Ms. Karli Clifton**, Dr. Siva Murru

University of Louisiana at Monroe, University of Louisiana at Monroe

Flavonoids have a broad distribution in the plant kingdom and they display diverse biological and pharmacological properties. Epidemiological studies suggest that the regular consumption of flavonoids protects humans against diseases associated with oxidative stress such as Alzheimer's disease, arteriosclerosis, cancer, and ageing. Therefore, development of methods for the synthesis of flavonoids has high significance in synthetic organic chemistry. With our on-going interest in flavonoid compounds¹ and electroorganic chemistry, we have developed an electrochemical cyclization approach for the synthesis of flavanones from 2'-hydroxychalcones. Electrochemistry is the study of chemical reactions which take place at the interface of an electrode, usually a solid metal or a semiconductor, and an ionic conductor, the electrolyte. As electron transfer takes place on the surface of the electrodes, the choice of material can have a significant impact on the outcome of a reaction. We have synthesized a set of 2'-hydroxychalcones from the corresponding aldehydes and 2'-hydroxyacetophenones.² We optimized the reaction conditions by screening variety of solvents and electrolytes. Reactions monitored by TLC and products characterized using GC-MS.

ID 10 Disparities in Breast Cancer Treatment Outcomes: Improving Access with Health Informatics

II, Rm 9 **Dr. Urska Cvek**, Urska Cvek, Phillip Kilgore, Eric Clifford, Marjan Trutschl, Tingting Li, Lauren S. Maniscalco, Jane Gulick Sugar, Terry C. Lairmore

Louisiana State University Shreveport, LSUS (Department of Computer Science), LSUHS (Surgery/Oncology and School of Medicine), LTR (Louisiana Tumor Registry)

Breast cancer is the most common cancer diagnosed among US women (excluding skin cancers) and is the second leading cause of cancer death among women, after lung cancer. Breast conservation surgery with radiation therapy was established as the recommended standard of care with equally effective survival rates (NIH, 1990 consensus statement) and thus national mastectomy rates fell steadily through 2006. Cancer outcomes are determined not only by the innate molecular biology of the tumor,

Poster Session Abstracts

but also by potentially modifiable variables including socioeconomic factors, racial differences, and geographical distance from the treatment center. The disparity in cancer treatment and outcomes due to geographic and socioeconomic variables is an increasingly recognized problem. We are interested in identifying these variations and implementing targeted strategies to improve measurable outcome health equity (i.e., incidence, stage at diagnosis, and survival). We used NCI's Surveillance, Epidemiology and End Results (SEER) cancer outcomes database and extracted clinical and demographic data to perform a limited analysis on the national level for over half a million breast cancer patients for the period of 2007-2016. We discovered that mastectomy was the more likely course of intervention for rural breast cancer patients versus the urban patients ($p << 0.001$). We followed our national-level analytics with in-depth analytics and modeling of the effect of distance between the patient's residence and the primary treatment center for more than 42,000 Louisiana breast cancer patients obtained from the Louisiana Tumor Registry database for the period of 2009-2019. In Louisiana, we found that there were significant differences in both the distance to the closest utilized facility and in treatment modality with respect to urban or rural status at the time of encounter.

ID 11 Investigating Key COVID-19 Questions by Using Natural Language Processing on Scientific Publications

II, Rm **Ms. Devika Dua**, Devika Dua, Dr. Norman John Mapes

10

Cedar Creek School, Cedar Creek School, Louisiana Tech University

The title of this study is Investigating Key COVID-19 Questions by Using Natural Language Processing on Scientific Publications. Devika Dua (Cedar Creek School, Ruston, LA) and Mentor John Mapes (Louisiana Tech University, Ruston, LA) are the authors of this study. The COVID-19 pandemic has brought an unprecedented challenge to public health. Numerous scientific publications are published daily on COVID-19 to understand the unexplored facets of the disease. The sheer volume of these publications makes it daunting for researchers to quickly find information and evaluate data related to specific COVID-19 queries. Natural Language Processing (NLP), a form of artificial intelligence, assists in churning these huge piles of data with a sophisticated algorithmic approach. The purpose of this study is to investigate key a COVID-19 question by using NLP on scientific publications. Using the T5 (Text-To-Text Transfer Transformer) model, we analyzed 740,000 journal abstracts for specific answers an important COVID-19 question. We performed qualitative observations, T-Tests (Pvalues and inferences), and accuracy metrics (Precision, Recall, and F1 score) to evaluate the models in this study. As the number of scientific publications increases, our proposed methodology provides an efficient mechanism for performing specific information retrieval for emerging questions, diseases, and related conditions, especially for underrepresented populations.

ID 12 Diagnostic Cancer Imaging In the Mid-Infrared Using Novel Contrast Agents

II, Rm **Dr. Samrat Dutta**, Dr. Thomas Wiese, Mentor

11

Xavier University of Louisiana

The chemical microenvironment of cancer cells is different from healthy cells. An immediate question arises: Is there a way to leverage the unique chemical information from cancer cells to identify them in a straightforward way by infrared microscopy? This is a challenge because the biological infrared image of cells is difficult to interpret due to spectral congestion. Thus, this well-developed technique, which can provide both chemical and morphological data of a sample, is usually ignored by the cancer research community. To address this problem, the PI's team is proposing and implementing research design that exploits the biological transparent zone in the infrared spectrum. In the first phase, the PI's team has shown that the concept can be used to identify bio-organism. Information from the first phase is now translated to identify and distinguish cancer cells. We expect the paradigm shift in our approach to infrared imaging to impact not only cancer research but also bioimaging at large.

Poster Session Abstracts

ID 13 Development of Methodology in Microbial DNA Isolation for Characterization of Soil Microbiome

II, Rm 12
Mr. PJ Erba, Ryan Miller, Stephanie Provenzano, Pearl Merry, and Vonny Salim

Louisiana State University Shreveport

Medicinal plants produce anticancer metabolites that have broad applications in the clinic. Because plants usually manufacture these beneficial compounds in low amounts, understanding the biosynthetic machineries and interactions within their environment are significant. The production of plant specialized metabolites has been known to be largely influenced by the composition of the soil microbiome or rhizosphere. The isolation of soil microbial DNA has been challenging due to humic acid contamination. In this project, we compared various methods to achieve high yield and purity that meet the quality for further 16S rRNA metagenomic analyses. In comparison with the common DNA extraction kits, we demonstrated that the extracted DNA via enzymatic lysis and sonication techniques resulted in significantly greater yield. Further microbial DNA analyses were performed after amplification of 16s rRNA V3 and V4 regions while accurate DNA quantification were done using fluorometric assays. Among the methods that we tested, the most efficient method was the integration of sonication and basic DNA extraction using silica powder with additional advantages of dealing with less harmful materials and generating less chemical waste. The application of this DNA extraction method has been proven to ease the downstream processing of DNA sample preparation for Next Generation Sequencing (NGS) purposes, particularly in microbiome analysis with further implications, such as in identification of pathogenic soil microbes.

ID 14 EEG Based Motor Imagery Task Classification Utilizing Spatiotemporal Deep Learning for BCI Applications

I, Rm 7
Mr. Anup Ghimire, Kazim Sekeroglu, Max Cole
Southeastern Louisiana University, Southeastern Louisiana University

Abstract This study aims to explore the decoding of human brain activities using EEG signals for Brain Computer Interfaces (BCI) by utilizing a multi-view spatiotemporal hierarchical deep learning method. In this project, we explored the transformation of 1D temporal EEG signals into 2D spatiotemporal EEG image sequences as well as we explored the use of 2D spatiotemporal EEG image sequences in the proposed multi-view hierarchical deep learning scheme for recognition. For this work, the publicly available PhysioNet EEG Motor Movement/Imagery Dataset is used. The dataset includes EEG recordings for 109 subjects performing 9 different tasks, including rest. With over 1500 recordings, this is the largest EEG motor movement and imagery dataset. Two different models are proposed. First there is a multi-view 3D Convolutional Model that utilizes Conv3D layers which learn the data from 3 different perspectives. The features learned by these 3D CNN models are then fused together for a final fusion model. Then, a supervised-learning based fusion of hierarchical deep learning models is applied. It utilizes Conv2D layers in a hierarchical structure, where a decision is made at each level individually by using the decisions from the previous level. This method is used to learn the spatiotemporal patterns in the EEG dataset. Both the models perform on par or better than current state of the art EEG Motor Imagery classification models in the binary classification paradigm. For the binary MI left fist versus MI right fist classification, we were able to achieve 86.88% and 82.79% average validation accuracy using different test sets on the 3D CNN and Hierarchical Models respectively. This level of validation accuracy on multiple test dataset proves the robustness of both the model structures. At the same time, the models clearly show an improvement due to the use of the multi-layer and multi-perspective approach.

Poster Session Abstracts

ID 15 Complex Germline Structural Variant Discovery Via Discordant Cluster Normalization

I, Rm 8 **Dr. Matthew Hayes**, Derrick Mullins, Angela Nguyen
Xavier University of Louisiana, Xavier University of Louisiana

Complex genomic structural variants (CGSV) are abnormalities that contain three or more breakpoints, making their discovery a challenge. Many existing algorithms for structural variant detection detect simple variants, but not complex events like deletion-inversions. In this study, we present an algorithm named CleanBreak which employs a maximum clique graph-based strategy to identify collections of simple structural variant (SSV) clusters, and then subsequently identifies overlapping SSV clusters to examine the search space of possible CGSVs, choosing the one that is most concordant with local read depth. We evaluated CleanBreak's performance on simulated and real data, demonstrating it's utility as an effective method to discover CGSVs.

ID 16 Computational Investigations Of Stereospecificity In Concerted Electrocyclic Reactions

II, Rm 13 **Mr. Bennett Hibner**, William A. Parkinson

Southeastern Louisiana University

Successful drug design relies on the synthetic chemist's ability to optimize Structure-Activity Relationships (SARs) of specific functionalizing moieties. Instead of exploring pharmaceutical design via traditional laboratory combinatorial methods, this project proposes to use computational quantum chemical techniques to explore the energetics of reaction pathways of concerted synthetic processes tailored to systems important in drug design. Specific applications include the theoretical investigation of thermodynamic and kinetic control in heterocyclic ring formation intended as drug delivery vehicles. Computational methods will also be used to predict stereospecificity of drug functionalization that results from Diels-Alder and retro-Diels-Alder processes.

ID 17 Design and Development of a Low-Cost High-performance Atomic Force Microscope (AFM)

II, Rm 14 **Mr. Hunter Hollie**, Patrick Moyer (Faculty Advisor)

Southeastern Louisiana University, Southeastern Louisiana University

Optical microscopy and scanning probe microscopy (SPM) are among the most widely utilized techniques in scientific and engineering studies. We are developing our laboratory at Southeastern Louisiana University (SLU), the Southeastern Photon/Probe Microscopy (SPM) lab, to work on leading imaging techniques and image analysis methods with a particular focus on nanoscale size dimensions. The SPM lab will consist of two components: (1) an image acquisition and instrumentation facility comprising laser scanning confocal microscopy and scanning probe microscopy, or atomic force microscope (AFM), and (2) an image analysis component. The imaging instrumentation will be home-built by students and capable of single molecule and single photon fluorescence sensitivity, nanometer localization, and dynamic fluorescence measurements with picosecond temporal resolution. LabView will be the interface for instrument control. This poster is focused on the design, development, and performance of the AFM that has been completed. The key components of this poster are (1) a description of the AFM technique, (2) presentation of the control software, including the PID (Proportional, Integral, Derivative) feedback control, (3) schematic diagram of the instrument, and (4) initial performance data.

Poster Session Abstracts

ID 18 Aryl-fused (Imidazole, Pyrazine and Pyrrole) Boronated Dye Derivatives

II, Rm 15
Dr. Moses Ihachi, Dr. Vicente (Mentor)

Southeastern Louisiana University, LSU

This proposed research is categorized under preventive medicine (new diagnostic tests). The broad purpose of this project is to synthesize boron-based dyes, investigate their photochemical and cellular properties for potential applications in fluorescence labelling and in bioimaging. The new dyes are expected to complement known BODIPYs (boron-dipyrromethenes) fluorophores which have been studied extensively, but absorb only in the visible region of the spectrum. The new proposed dyes are expected to absorb near-IR wavelengths which is an attractive property for deep tissue imaging since light penetration through body tissue is known to increase with increased wavelength. In vivo fluorescence helps the physician to avoid unnecessary cuts during surgery. The proposed aryl fused dimers are expected to display red-shifted absorptions and emissions and enhanced fluorescence compared with BODIPY dyes. Readily available synthetic materials and laser probes will be used in this investigation. To enhance cellular uptake, tumor cell selectivity, and controlled cellular retention, the PI will meticulously choose "R" group substituents to functionalize the proposed dye with water-solubilizing PEG, sugars, sulfonic acid, quaternarium ammonium groups, or amino acids. These would be synthesized in the second phase of the project depending on primary cell studies results using human HEp2 cells. The collaborating investigator is well informed and equipped in this scope of cellular studies. For each compound, the structural features, absorbance spectra, fluorescence quantum yield and triplet state lifetimes will be determined by theoretical calculations. Each dye will also be screened for cytotoxicity, thermal stability and photostability. Later on, these motifs will be cyclized without the boron complex and tested as photosensitizers for Photo Dynamic Therapy application.

ID 19 Assessment of student appreciation for applied bioinformatics and computational drug discovery methods in a project-based course

I, Rm 9
Ms. Chelsey Jordan, Chelsey Jordan, Avery Christensen, Brian A. Salvatore, and Elahe Mahdavian
Louisiana State University Shreveport

Here we report the results of the Assessment of Student Learning Gains Survey (ASLGS) used to evaluate a project-based course on computer-aided drug discovery (CADD). This CADD course, which was launched in 2020 as a summer LBRN program, was offered subsequently in three separate upper-level elective courses at LSUS in 2020-2021. The course centered on computational drug discovery methods for the development of anti-viral agents to treat COVID-19, which allowed students to experience all aspects of the scientific method in a virtual environment. This included devising a hypothesis, proposing experiments to test the hypothesis, collecting, and critically analyzing data, formulating a conclusion, and presenting the project. We implemented an 18-item questionnaire, which was used as both a pre-course and a post-course student self-assessment survey. The pre-course survey was administered at the beginning of the course, and the post-course survey was administered on the last day of class. All data collection procedures were approved by LSUS IRB guidelines. The data from all sessions, comprising responses from all 49 students, were compiled together, and analyzed using Microsoft Excel and Google Spreadsheets. In evaluating the student questionnaires, we defined students who became 'knowledgeable' after taking the course as those who gained both awareness (i.e., that an online database or computational tool exists) and understanding (i.e., of the function of that database or tool). The results of the ASLGS suggest that the CADD course increased student knowledge and enhanced confidence in using applied bioinformatics and computational tools to address the medical challenge of drug discovery for COVID-19.

Poster Session Abstracts

ID 20 Developmental Stages of Olfactory Sensory Neurons in Neonatal Life vs. Adulthood
I, Rm Ms. Supriya Karki, Kathryn Hamilton, Stephanie Villalba
10

Louisiana State University Shreveport, LSUS, LSU Health Shreveport

In mammals, olfactory sensory neurons (OSNs) undergo turnover throughout much of the lifespan. The turnover rate appears to slow significantly with aging, however, and mechanisms regulating the rate remain poorly understood. Here, we have BrdU (Bromodeoxyuridine, a thymidine analog) and immunolabeling to visualize nuclei of proliferating BrdU+/GFP+ cells in young (P7) and mature (P25) GAD65-GFP mice. We also immunolabeled for GFP+/cC-3+ (cleaved caspase-3, neuronal death caspase) to identify dying GFP+ neurons in the same mice. In these mice, the gene promoter for the 65 kDa isoform of glutamic acid decarboxylase (GAD) drives expression of the fluorescent protein, enhanced GFP. In previous studies, we found that the MOE of our mice contained immature GFP+ OSNs, but mature GFP+ OSNs were not found. Nonetheless, the mature MOE was found to express GAD65 mRNA. We hypothesize the GFP+ OSNs stop producing GFP as they approach maturity. Alternatively, they could simply die, leaving GFP levels that are undetectable by immunolabeling but detectable by PCR. Our initial results fail to support the alternative hypothesis. Thus, it seems likely GFP production is switched off in OSNs at or near maturation. In ongoing studies, we will label and quantify BrdU+ and cC-3+ cell numbers in additional young and old mice to determine if the apparent differences reported here are significant. We also plan to label markers for multiple stages of OSN development throughout the lifespan, in order to pinpoint mechanisms regulating OSN turnover. Identifying these mechanisms could further understanding of neuronal plasticity in other neural systems, such as those involved in learning and memory.

ID 21 Using computational drug repurposing methodology to identify promising bictgravir-based drug candidates for COVID-19
I, Rm Mr. Waheed Khan, Elahe Mahdavian
11

Louisiana State University Shreveport, LSUS

Since the deadly outbreak of SARS-CoV-2 in 2020, the global scientific community has focused on research to develop an effective treatment for COVID-19. We used computer-aided drug discovery (CADD) to identify promising drug candidates for COVID-19 based on bictgravir, an existing antiviral drug. Using a virtual screening tool, Swiss Similarity, we identified analogs that share significant structural similarities with bictgravir to build a compound library. We then performed molecular docking using the mCule platform with bictgravir and its structural analogs and a high-resolution structural model of the viral (SARS-CoV2) main protease, Mpro (PDB-ID 6lu7). Compounds that bind tightly to 6lu7 could potentially disrupt interactions with Mpro's natural substrate and thus disrupt the viral life cycle. Compounds with high binding affinity were further profiled for their pharmacokinetic properties using Swiss ADME. We selected two promising compounds with optimal binding affinity and ADME properties for experimental testing.

ID 22 Racial Disparities in COVID-19 Symptoms in Northern Louisiana
II, Rm Mr. Phillip Kilgore, Phillip C.S.R. Kilgore, David Janese, Jenny Jones, Kasi Addison,
16 Raymond Kessler, Rachel Waesche, Mary Ann Edens, Angela Cornelius, Marjan Trutschl,
Urska Cvek
Louisiana State University Shreveport, LSUS (Department of computer Science and
Laboratory for Advanced Biomedical Informatics), **LSUHS** (Department of Emergency
Medicine)

Since the onset of the COVID-19 pandemic, the question of racial differences has been at the forefront of prognostic thought in determination of high-risk groups. We identified a total of 410 unique Medical

Poster Session Abstracts

Record Numbers (MRNs) in a retrospective data collection of patients in the Ochsner LSU Health System (LSUH) in Shreveport and Monroe, Louisiana. Data was collected from a mix of rapid and regular PCR nasal swabs collected at the two locations from 4/1/2020 to 4/30/2020. Data collected included symptoms, race, ethnicity, occupation, gender and age, to determine if there was a statistical difference in presenting symptoms based on race. Black/African American patients were the most represented race (74%) with COVID-19 and most patients were not confirmed Hispanic (70.15%) with a female predominance amongst all races. Gender was evaluated as a covariate, which demonstrated a slight female predominance in symptoms with black females representing 58.73% and black males representing 41.27%. In the uncollapsed data, fever was seen with cough, shortness of breath, headache, arthralgias/myalgias, not Hispanic ethnicity and male sex. In the grouped data, the top 10 rules predicted either shortness of breath or fever with COVID-19 and five of the rules were associated with the black race. White and black patients were noted to have similar rates of anosmia. While evaluating the racial distribution of COVID-19 as it pertained to symptoms, gender, and occupation, black patients were statistically more affected by COVID-19 in Northern Louisiana, which was not observed in Southern Louisiana.

ID 23 Cancer-Specific Magnetic Imaging Agent

II, Rm **Dr. Vladimir Kolesnichenko**, Galina Goloverda, Quincy J. Brown, Thomas Wiese
17

Xavier University of Louisiana, Xavier University, Tulane University

Magnetic nanoparticles with tunable size for solving various biomedical diagnostics tasks are very attractive candidates for research and development, as they can be easily detected by MRI or MPI, and they can be constructed using stable and relatively non-toxic materials, such as iron oxides and/or ferrites. In this project we are developing new imaging agents selectively recognized by cancerous cells. These agents are composed of individual 3-5 nm magnetic iron oxide particles coated with covalently bound organic oligomers, so that overall size of the nanoparticulate adduct will not exceed 15-20 nm. The organic coating for these particles (linker molecules) is composed of coordinating head and amphiphilic spacer consisting of 10-15 ethylene oxide units. These spacers are conjugated at their termini with peptide-vectors responsible for the cell specificity (recognition). The idea is that these small particles will (a) avoid capturing by phagocytes, (b) exhibit fast pharmacokinetics, (c) penetrate through biological boundaries, (d) recognize the receptors at the surface of certain cancer cells, and (e) shorten the proton relaxation rates of the surrounding biological media and thus, act as MRI contrast agents.

ID 24 Activating transcription factor 6 modulates endothelial barrier function.

I, Rm **Mrs. Khadeja-Tul Kubra**, Khadeja-Tul Kubra, Mohammad S. Akhter, Yogesh Saini,
12 Konstantin G. Kousoulas, Nektarios Barabutis
University of Louisiana at Monroe, University of Louisiana Monroe, Louisiana State University

Endothelial hyperpermeability due to inflammatory stimuli contributes to sepsis and acute respiratory distress syndrome (ARDS). Efforts to identify molecular pathways responsible for those pathologies may deliver promising therapeutic targets for diseases related to endothelial barrier dysfunction. The unfolded protein response (UPR) is a highly conserved molecular pathway regulating protein homeostasis, and it is consisted of inositol-requiring enzyme 1 α , pancreatic endoplasmic reticulum kinase, and activating transcription factor 6 (ATF6). In our study, we focus on ATF6, previously shown to be induced by growth hormone-releasing hormone antagonists and heat shock protein 90 inhibitors. We observed that pharmacologic inhibition of ATF6 by ceapin-A7 induces endothelial hyperpermeability since that compound destabilized the actin cytoskeleton of bovine pulmonary artery endothelial cells. Consistent with those findings, suppression of ATF6 by small interfering RNA deactivated the actin-severing activity of cofilin. Moderate concentrations of both compounds did not

Poster Session Abstracts

affect cell viability, as measured by the MTT assay. To further our study, we employed electric cell-substrate impedance sensing (ECIS) to measure transendothelial resistance, and fluorescein isothiocyanate (FITC)-dextran to assess paracellular permeability. Our observations suggest that ATF6 activation enhanced endothelial barrier integrity, while ceapin-A7 potentiated lipopolysaccharides (LPS)-induced endothelial barrier dysfunction. LPS is the major component of the outer membrane of Gram-negative bacteria; inducing hyper-permeability responses. Collectively; our study reveals that ATF6 regulates endothelial barrier function, and activation of that UPR sensor may serve as a strategy to repair the inflamed endothelium. Future studies in mice will further our observations in a model of LPS-induced acute lung injury.

ID 25 Heart rate variability and novel torpor states in tent-making bats

I, Rm Mr. James Lee, Matthew Giblin, Dr. Teague O'Mara
13

Southeastern Louisiana University, Southeastern Louisiana University

Variability in heart rate is a normal and expected occurrence and is a key indicator of cardiovascular health. However, lowering and eliminating variability in heart rate is critical for mammals that use daily torpor. Torpor is a low-reactive state with reduced metabolic rate that lasts for hours (torpor) to days or months (hibernation). The tropical tent-making bat *Uroderma bilobatum* shows multiple short bouts of extreme bradycardia that may also show low variability. These frugivorous bats live at their energetic ceiling, and rely on the energy gained during the night's foraging. We tested the hypothesis that their short bradycardia events are a novel, shortened form of torpor that aids in energy conservation. The number and duration of these events would be predicted by the previous night's energy expenditure. We also test how control is mediated by coordinated branches of the autonomic nervous system and as a cell-mediated directive. The regularity of recurring drops could indicate the normalcy or the abnormality of these drops, and differences between the entrance and exiting heart rate may indicate the tension of nervous control. We used heart rate data collected from free-ranging tent-making bats in Panamá. Each heart rate drop was broken down into entrance, maintenance, and exit to for comparisons among events, days, and individuals. These results show that energy expenditure directly impacts the frequency of bradycardia, and that the changes in heart rate variability across these bouts indicates a true torpor state and highlights the physiological innovation and diversity in tropical bats. Perhaps because of their exposed roosting habitat (under large palm leaves), these bats may not be able to enter long bouts of torpor and instead use many small drops to maintain predator awareness.

ID 26 Wastewater Analysis and Genomic Sequencing of SARS-CoV-2 Benefit COVID-19 Surveillance

I, Rm Ms. Laura Lee, Laura Lee, Michael Foster, Paul Austin, Tom Bishop, Paul Kim, Jamie
14 Newman

Louisiana Tech University, Louisiana Tech University, Grambling State University

Declared a pandemic on March 11, 2020, the COVID-19 pandemic has claimed over 5 million lives worldwide. Quantitative reverse transcriptase PCR (RT-qPCR) and antigen testing have become the predominant surveillance methods for SARS-CoV-2 positivity, the former being more sensitive to viral load and the latter being more efficient. These testing methods are invaluable, but do not provide an accurate assessment of the total caseload in an area. To monitor the on-going pandemic more closely, our lab, like many around the world, is examining local wastewater output to measure presence of SARS-CoV-2 in Ruston and sequencing patient samples to monitor the evolving virus. Wastewater-Based Epidemiology (WBE) allows us to measure genome copy units in wastewater providing a more accurate assessment of virus present in a community as it includes those individuals who do not test or report cases of COVID-19. Genomic surveillance analyzes positive patient tests to identify SARS-CoV-2 variants, allowing public health officials to monitor novel mutations in real-time during emerging and active outbreaks. For SARS-CoV-2, there are numerous mutations of concern and the

Poster Session Abstracts

ability to track their prevalence and correlate with epidemiologic data is invaluable. As sequencing and even WBE has previously only really been available at larger institutions, the ability to run these assessments in rural communities provides a more representative understanding of the virus and pandemic. WBE and genomic surveillance provide novel and predictive insights that can dramatically increase the effectiveness of public health responses to emerging pathogens.

ID 27 Accessing the congruency of DNA repair genes among killifishes with different life histories using QuantSeq

I, Rm 15
Mr. Chi Jing Leow, Chi Jing Leow and Kyle R. Piller

Southeastern Louisiana University, Southeastern Louisiana University

Model organisms are fundamental research components when it comes to the study of ageing. Historically, they were chosen for their repeatability and cost of maintenance. In recent years, new model organisms have been developed based on their unique characteristics. For example, the African Turquoise Killifish (*Nothobranchius furzeri*) is being used in the study of ageing and age-related diseases. This species has an annual life history which is uncommon among vertebrates. The short life cycle (10-31 weeks) is retained in captivity which made them amenable to genetic research. The genome of the Turquoise Killifish has been sequenced and age-related orthologs with humans were identified. However, whether these DNA repair genes are expressed the same way across closely related species remains unknown. The goal of this research is to examine the congruency of these DNA repair genes among killifishes with different life histories including annual, non-annual, and facultative-annual species. This will be achieved by using QuantSeq to produce gene expression data. We hypothesize that annual and non-annual species will possess the same but differently expressed DNA repair genes. Specifically, the non-annual species will have upregulation in genes associated with DNA repair. If the same genes are under positive selection in a set of fishes with different life histories, then it provides evidence that these candidate genes may be worth studying in the human ageing process. Currently, RNA extraction has been done on one annual species and one facultative species in the Nothobranchiidae family. Several more species are being raised to the adult stage in the lab. These RNA samples will soon be sent out for sequencing as more species are acquired in Spring 2022.

ID 28 Identifying Promising Drug Candidates Against SARS-CoV-2 Using Computational Drug Repurposing Methodology

II, Rm 18
Mr. Raj Letchuman, Elahe Mahdavian, Christopher Stratton

Caddo Parish Magnet High School, Louisiana State University of Shreveport (LSUS)

Responsible for over 300 million cases and 5.4 million deaths as of January 2022, the COVID-19 pandemic has disrupted the livelihoods of people across the globe. Research and development have contributed to effective vaccines, widespread safety protocols have aided in mitigating the spread of the virus, and drug discovery has decreased mortality. However, the demand for effective COVID-19 treatments is still significant. In this study to identify promising drug candidates for COVID-19, we focused on inhibition of the viral main protease (nsp5), which is a key enzyme in the viral replication cycle. Using a computer-aided drug discovery approach, we repurposed Beclabuvir, an investigational drug used in the treatment of chronic Hepatitis C. As a seed compound in previous studies, Beclabuvir has been shown to have a high binding affinity with nsp5; however, a large molecular weight paired with low water solubility renders this compound inefficient as a drug. We created a compound library based on structural similarity with Beclabuvir and screened thirty analogs for drug likeness using the Swiss ADME tool. Analogs with promising ADMET properties were then virtually docked with the structural model of the nsp5 (PDB-ID 6lu7) protein to determine binding affinities. The results of this study revealed three analogs of Beclabuvir with comparably high binding affinities with nsp5, thereby providing evidence for three potentially effective drugs against SARS-CoV-2.

Poster Session Abstracts

ID 29 An interdisciplinary course on computer-aided drug discovery to broaden student participation in original research

I, Rm 16
Dr. Elahe Mahdavian,

Louisiana State University Shreveport

This project is focused on the implementation, pedagogical strategies, and evaluation of a new interdisciplinary course on computer-aided drug discovery (CADD). This CADD course was developed in response to a call for alternative programs after the COVID-19 pandemic prompted the cancellation of the face-to-face summer 2020 research internship program sponsored by the Louisiana Biomedical Research Network (LBRN). This course integrates guided research with educational experiences for science students. The primary course objective is to teach students to think like scientists as they navigate through a computational research project in the context of drug discovery for COVID-19. Students learn to use research-based methods and employ active learning with publicly available bioinformatics and computer modeling tools to identify promising anti-viral drugs for use in treatment and prevention of the novel SARS-CoV-2 virus. The inspiration for this course is fourfold: I. The importance of teaching science as science; guided research is merged with course-based instruction to broaden student participation in research; II. The recognition that interdisciplinary research skills in applied bioinformatics and computational modeling are indispensable to a student's scientific education; III. The significant negative impact of the COVID-19 pandemic on public health and hence the urgent unmet need for new antiviral therapeutic agents; IV. Instructional shifts in response to COVID-19 and their impact upon the classroom-based student research experience. The course, which has now been successfully offered four times, combines three modules: lectures including live demos, inquiry-based assignments, and scientific communication.

ID 30 Patterns in Electroencephalograms during Meditation

I, Rm 17
Mr. Ethan Manco, Co-author: Dr. Subhajit Chakrabarty

Louisiana State University Shreveport, LSU Shreveport

Meditation creates a profusion of patterns in electroencephalogram (EEG) recordings. These patterns can be fed into an algorithm in real time to predict whether someone is meditating. There is an abundance of health benefits from meditation, therefore, a tool to help people see when they are successfully meditating could help them in several ways. Previous studies of EEGs have found that brainwaves at certain frequencies will reach values within ranges that indicate meditation. These studies generally reported a large range of higher than normal delta frequencies and slightly higher than normal theta and alpha frequencies. In addition, drowsiness was associated with very high delta frequencies, so there had to be a defined limit on its level. With these indications, an algorithm can separate premeditation, onset of meditation, and post meditation. The Focus Widget included in the OpenBCI GUI was modified to create this algorithm. To do this, Fast Fourier Transform (FFT) bins were added for delta and theta frequencies. These were added so that the algorithm could be modified to determine when these values were within the aforementioned ranges. In addition, two more waveform indicators were added to the graphical interface to show when these frequencies were within the algorithm's range. Playbacks of previous recordings could be processed through this new meditation widget and exported as .csv files. This allows users to see the values of different frequencies before meditation, during meditation, and post meditation. The widget was tested on ten expert subjects from an OpenNeuro EEG meditation study. In pre-meditation, alpha and theta levels were noticeably lower. In post meditation, delta slightly decreased, theta increased, and alpha was relatively unchanged. The algorithm may have over-fit to the testing subjects that were used. An improvement would be to add more participants with different meditation styles, more sessions, and perform better generalization.

Poster Session Abstracts

ID 31 **Virus-Induced Gene Silencing: In-Vivo Characterization of Anticancer Alkaloid Biosynthetic Genes in Medicinal Plants**

I, Rm 18
Ms. Pearl Merry, Paul Erba, Ryan Miller, Stephanie Provenzano, Vonny Salim

Louisiana State University Shreveport, Louisiana State University Shreveport

Medicinal plant *Camptotheca acuminata* produces camptothecin, a monoterpene indole alkaloid that has been extensively used as an effective chemotherapeutic agent. Despite its respected value as a potent antineoplastic agent, to date, the laboratory synthesis of camptothecin has proven exceedingly difficult and time-consuming with high cost. The extraction from medicinal plants remains the primary means of acquisition of camptothecin, while the plants produce such compound in small amounts. To ascertain possible avenues for increasing production and driving down the cost, the identification of biosynthetic genes in the camptothecin pathway is necessary. The incorporation of key biosynthetic pathways into microbial systems provides an exciting theoretical avenue for the mass production of plant specialized metabolites. In this project, we optimized Virus-Induced Gene Silencing methods (VIGS) in order to achieve a timelier efficient reverse genetics approach. We aim to elucidate the complex multilane *C. acuminata* camptothecin biosynthetic pathways by focusing on the in-vivo characterization of biosynthetic enzymes. Furthermore, VIGS will allow access to novel intermediates or substrates that are useful for biochemical characterization of biosynthetic enzymes in camptothecin pathways. The photobleaching phenotypes when the phytoene desaturase (PDS) gene was silenced became the marker to evaluate the effectiveness of VIGS. As candidate genes were silenced, alteration of metabolic profiles and changes of gene expression were observed to better understand the complexities of camptothecin biosynthetic pathways. VIGS will also allow the identification of potential substrates for alkaloid biosynthetic enzymes, as well as purification of novel natural products for future anticancer therapeutic applications.

ID 32 **Whole Cell Biotransformation for Central Intermediate Formation in Anticancer Monoterpene Indole Alkaloid Biosynthetic Pathways**

II, Rm 19
Mr. Ryan Miller, Vonny Salim, Paul Erba, Stephanie Provenzano, Pearl Merry

Louisiana State University Shreveport, Louisiana State University Shreveport

Monoterpene Indole Alkaloids (MIAs) are considered one of the most diverse class of specialized metabolites with ~3000 members produced by medicinal plants, mainly in the Apocynaceae family, such as *Catharanthus roseus* and *Rauvolfia serpentina*. The main central intermediate, strictosidine is the precursor of these MIAs after its glucose moiety is removed followed by carbon-carbon rearrangement. Many of these MIA's, in turn, exhibit an array of useful pharmaceutical effects but are often difficult to synthesize in the laboratory. Currently, the production of several important MIA's is achieved via extraction directly from medicinal plants. This method is inefficient and costly, thus leading us to search for ways to incorporate synthesis of these compounds into microbial systems. Availability of strictosidine is essential for functional characterization of downstream MIA biosynthetic machineries. Yet, strictosidine is, presently, commercially unavailable leading us to search for avenues for large scale production. Strictosidine synthase is an enzyme found in many plant species, particularly in MIA producing species. It is known to catalyze a Pictet-Spengler-like reaction thereby creating strictosidine via condensation of secologanin and tryptamine, its substrates. In this study, we transformed *Escherichia coli* cells to express *Rauvolfia serpentina* strictosidine synthase. Following the culture of bacterial cells expressing strictosidine synthase, the cells were found to take up substrates and secrete the desired product without tedious protein extraction, thus easing the production, isolation, and purification of strictosidine. The effectiveness of biotransformation in the synthesis of strictosidine provides more sustainable ways to produce MIAs and accelerate our metabolic engineering efforts to increase the yield of anticancer MIAs.

Poster Session Abstracts

ID 33 Computing Representative Protein Conformations from Molecular Dynamics Simulations

I, Rm 19 **Mr. Joseph Mondello**, Tauhidul Alam

Louisiana State University Shreveport, Louisiana State University Shreveport

Introduction: There have been significant computational studies in using the SARS-CoV2 main protease (Mpro) protein structure for molecular docking, intending to identifying drug candidates to treat COIVD-19. Ensemble molecular docking utilizes a number of generated conformations from the dynamics of the protein target, known as molecular dynamics (MD), instead of performing docking to a single structure of the target. However, it is computationally inefficient to perform ensemble docking for long MD simulation trajectories. Methods: To address this computation burden, our approach computes a subset of representative protein conformations from MD simulations of the Mpro protein. Employing a dimensionality reduction method, we obtain two-dimensional data from high-dimensional protein conformations of an Mpro simulation trajectory. We then find the optimal number of protein conformations after clustering two-dimensional data. Results: We apply two dimensionality reduction methods, principal component analysis (PCA) and time-lagged independent component analysis (TICA), for reducing protein conformation dimensions to two. The K-means clustering algorithm is implemented to calculate clusters from two-dimensional data and then compute an ensemble of representative protein conformations from all clusters. Finally, we evaluate the performance of our approach by comparing the computed ensemble of Mpro conformations against existing CHARMM and GROMOS ensembles of the same target protein, in terms of Root Mean Square Deviation (RMSD) values for all heavy atoms of the protein structure. Conclusion: Our comparison results show high variations for computed representative protein conformations. These variations validate the distinctive nature of conformations that is necessary for ensemble molecular docking. Acknowledgment: This work is supported by the Louisiana Biomedical Research Network (LBRN) summer research program 2021

ID 34 Identifying Double Minutes Chromosomes within Hi-C and Deletion-Episomes

I, Rm 20 **Ms. Savannah Montgomery**, Angela Nguyen, Dr. Hayes

Xavier University of Louisiana, Xavier University of Louisiana

Double minute chromosomes are extrachromosomal circular fragments of DNA found in some cancer cells. Hi-C data is used to observe the arrangement of chromatin. Hi-C can also be used to infer large mutations known as structural variants. Simple structural variants include deletions, duplications, inversions, and translocations. Knowing where the double minutes are located allows for information such as seeing if the double minute is caused by deletion and amplification of a genomic segment, known as a deletion-episome event. The objective of this research is to use Hi-C sequencing data to determine whether a double minute is formed because of a deletion episome event - when a segment of the DNA has been deleted, circularized, and amplified. This research presents an algorithm that can identify a deletion episome double minute compared to a non-deletion episome double minute. From our research, health care professionals will be able to identify double minutes formed from deletion episomes, which gives information about the formation mechanism of double minutes; this information could better inform anti-cancer therapies in a clinical setting.

ID 35 Simulating Double Minute Chromosome and Phylogenetic Tree Evolution using Java

II, Rm 20 **Mr. Derrick Mullins**, Derrick Mullins, Zoe Mitchell, Matthew Hayes

Xavier University of Louisiana, Xavier University of Louisiana

Double minutes are small extrachromosomal circular fragments of DNA that are acentric and contain

Poster Session Abstracts

oncogenes. Because double minutes have high amplification, they increase the malignancy of cancer present in cells. Double minutes (DM) can be discovered algorithmically, but they are difficult to detect. Thus, it is important that new algorithms for double minute discovery are evaluated on a panel of accurate simulated data. The goal is to simulate double minute evolution to create this evaluation data. The aim is to represent double minute evolution through phylogenetic trees. Because DMs are challenging to detect, we want to simulate them to help create data to evaluate DM discovery algorithms, which can lead to improved cancer treatments in the future. The algorithmic approach to simulating double minutes is to simulate DM evolution via a recursive algorithm. By simulating double minutes using recursion, we create hidden recursive trees like that of a phylogenetic tree. Given a user-input double minute that we consider the ancestor, 2 derivative DMs are produced with each recursive call, each containing different chromosomal locations, start coordinates and end coordinates. The results show an accurate representation of a phylogenetic tree containing double minutes represented in BED format. This helps us gain knowledge on how to identify cancer early, treating cancer before it progresses too far, and benefiting the entire cancer community. Future directions will be creating more methods to simulate and extract double minutes from phylogenetic trees.

ID 36 Alligators as Models for Human Pathology: Neuroendocrine Effects of Methyltestosterone Exposure

II, Rm 21
Dr. Christopher Murray, Tristan Herod, Jorge Lopez-Perez, Karen Maruska

Southeastern Louisiana University, Southeastern Louisiana University, Southeastern Louisiana University, Louisiana State University

The synthetic androgen 17 α -methyltestosterone (MT), used pan-tropically to masculinize tilapia fry for farming and sale, results in the development of intersex crocodilians by masculinizing female crocodiles and is detectable in crocodile egg yolks within natural systems, making MT one of the first environmental androgen endocrine-disrupting contaminants. Biotic and chemical exchange between aquaculture farms and human water sources are often unrestricted, leading to MT being detected in vertebrates throughout the region and pandemic human exposure. The proposed research will result in a behavioral and neuroendocrine understanding of MT as an ecotoxin and its contribution to mechanistic human pathology post exposure. This project aims to determine behavioral effects and brain reception of MT with regard to sexually dimorphic nuclei using alligators as model organisms. This experimental assessment will identify the role of MT as a behavioral androgen, neuroendocrine mechanisms of anthropogenic androgen mimics and how exposure relates to androgen-driven behavioral changes. An understanding of this relationship is key to predicting human symptomology.

ID 37 Computer-aided drug discovery for COVID-19 using virtual screening and molecular docking

I, Rm 21
Ms. Kalani Myles, Elahe Mahdavian

Louisiana State University Shreveport, LSUS, Department of Biological Sciences

Since the onset of SARS-CoV-2 (COVID-19) in December 2019 and its evolution into a worldwide pandemic in March 2020, over 279 million people have been infected worldwide, with over 5 million deaths recorded in at least 188 different countries [<https://coronavirus.jhu.edu/map.html>]. The need for effective treatments to control the severity of the disease and reduce infection rates is urgent. We used a computer-aided drug discovery (CADD) methodology to identify promising drugs for use in treating COVID-19 based on a broad-spectrum antiviral drug, Arbidol. We screened the ChEMBL library on the Swiss Similarity web portal and identified analogs that share >85% structural similarity with Arbidol based on an FP2 metric. We performed molecular docking of Arbidol and these analogs with the structural model of the spike ACE2 (PDB-ID 6M0J) protein using the mCule platform to identify compounds with high binding affinity. Then, using Swiss ADME tools, we screened the

Poster Session Abstracts

pharmacokinetic profiles of the compounds and removed compounds with poor 'drug-like' properties. In this presentation we will discuss the overall CADD methodology and our results in building the Arbidol-based compound library, the mCule docking experiments, and the ADME screens. Future work will include the analysis of binding modes/stability in compound-6M0J complexes and cross-docking experiments (using Autodock vina) to prioritize compounds for in vitro validation experiments. The goal is to select compounds that can serve as inhibitors of the mechanism used for SARS-CoV-2 viral entry and thus viral infectivity.

ID 38 Canonical and Noncanonical Notch Signaling Regulates Adult Stem Cell State
I, Rm **Dr. Jamie Newman**, Taylor Teach
22

Louisiana Tech University, Louisiana Tech University

Notch is a highly conserved, developmental signaling pathway with a complicated and interconnected role in adipogenesis, metabolism, and inflammation. Despite decades of research on Notch signaling, the mechanism through which it controls cell state has only become more uncertain, leaving a critical knowledge gap in the understanding of canonical and noncanonical signaling pathways that control transcription and metabolism during adipogenesis. We use human adipose stem cells to provide an in-depth characterization of the role and mechanism of action that individual Notch receptors have in regulating transcription profiles, self-renewal and differentiation. Here we examine the influence of transcriptional co-activator MED12 in regulating Notch pathway activity, both by looking at Notch receptors and Notch ligands. This work will take a more focused, in-depth approach that not only contributes mechanistic understanding to aid in identifying novel targets for combating the growing problems associated with obesity and metabolic syndrome.

ID 39 Metagenomic Profiling of Soil Microbiome from Anticancer Compound-Producing Plants
I, Rm **Ms. Keelin North**, Ryan Miller, Paul Erba, Stephanie Provenzano, Pearl Merry, Vonny
23 Salim
Louisiana State University Shreveport

Medicinal plants, such as Catharanthus roseus and Camptotheca acuminata produce a class of specialized metabolites, known as monoterpenoid indole alkaloids (MIAs) with wide clinical applications as chemotherapeutic agents. The source of these MIAs is mainly from plants, rather than chemical synthesis that is proven to be time and cost prohibitive. Due to the cytotoxicity of these high-value compounds, plants accumulated them at low levels. The production of plant specialized metabolites was reported to be influenced by the composition of soil microbiome. In this project, we characterized the rhizosphere or soil microbiome composition of MIA-producing plant species, *C. roseus* and *C. acuminata* using Next Generation Sequencing (NGS) of 16S rRNA metagenomics and performed comparative analyses with non-MIA-producing plant. We distinguished specific population of bacteria, such as certain Firmicutes that are accumulated only in *C. acuminata* soil microbiome and unique populations of bacteria in the genus *Bacillus* from *C. roseus* soil microbiome. The microbial populations in the soil may influence the production of MIAs that are highly accumulated in the roots, such as catharanthine of *C. roseus*, an essential moiety of anticancer vinblastine arresting cell division. This study provides additional avenues to increase anticancer metabolites by manipulating the soil microbiome composition and potential applications for metabolic engineering in microbial systems.

Poster Session Abstracts

ID 41 **Synthesis and Biological Evaluation of 1,3-Diarylpyrazoles: in vitro Cytotoxicity Studies on Human Melanoma and Non-melanoma Cancer Cells**

II, Rm
22 **Ms. Uchechi Owunna**, Uchechi Owunna¹, Ramesh Bista¹, Samuel Boateng², Tithi Roy², Jean Christopher Chamcheu², Siva Murru^{1,*}

University of Louisiana at Monroe, School of Sciences, and School of Basic Pharmaceutical Sciences, University of Louisiana at Monroe

The substituted pyrazoles with aromatic and heteroaromatic groups possess numerous biological activities, which makes them particularly interesting. Continuous efforts have been devoted to the development of general and versatile synthetic methodologies to this class of compounds. The existing methods suffered with some drawbacks such as longer reaction times, undesired products formation, and thus difficulty in product isolation and purification. Accordingly, we chose to develop microwave assisted synthetic methods to access these highly useful heterocyclic compounds. We have developed two alternate approaches for 1,3-diaryl pyrazoles i.e. microwave assisted and metal catalyzed approaches. We have initially developed an efficient microwave assisted synthetic approach by optimizing the reaction conditions such as solvent, microwave power and reaction time. A series of pyrazole compounds were prepared using arylhydrazines and dicarbonyl compounds. However, we observed formation of regio-isomeric products in case of unsymmetrical 1,3-dicarbonyl compounds. With the goal of achieving regio-selective synthesis, we have developed a room temperature Co-catalyzed approach which improved the selectivity. All the synthesized compounds were characterized by IR, ¹H NMR, ¹³C NMR, and GC-MS analysis and evaluated for in vitro anticancer activity against melanoma (GFP-A375 and SKMEL-28) and non-melanoma (GFP-A431 and SCC-12) cell lines with HaCaT keratinocytes as a control. Some of the compounds exhibited significant decrease in cell growth/viability compared to positive controls Celecoxib and Cisplatin. The results and data from synthesis and biological characterization will be presented in the poster.

ID 42 **Topiramate treatment precipitates and accentuates physical symptoms of nicotine withdrawal in mice.**

II, Rm
23 **Dr. Erika Perez**

Xavier University of Louisiana

Smoking tobacco is highly prevalent in alcohol dependent individuals. Topiramate is an FDA approved anticonvulsant medication that has been used off-label for the treatment of alcohol use disorders. Topiramate has been successful in reducing alcohol consumption in a large subset of patients. Surprisingly, Topiramate treatment also reduced smoking behaviors in these same patients, highlighting a possible use for the drug for nicotine cessation. GluK1-containing kainate receptors (GluK1*KARs) are non-selectively inhibited by Topiramate and genetic association studies suggest that this receptor system could be targeted to reduce drinking in AUD patients. To date the connection between these two receptor types has not been explored. The goal of this proposal is to gather data to support the use of selective GluK1*KARs antagonists as viable nicotine cessation aids. To start to understand the role of GluK1*KARS we tested the ability of Topiramate to alter physical symptoms of nicotine withdrawal. For our pilot experiment, mice were treated with nicotine for a minimum of 6 weeks via the drinking water, vehicle control groups were also used. On test day control treated, nicotine satiated and nicotine withdrawal mice were treated with Topiramate and physical signs were recorded. Similar to our previous studies in alcohol, Topiramate was able to precipitate physical symptoms in nicotine satiated mice. Unlike our previous results, Topiramate did not reduce withdrawal symptoms but accentuated them. Our results suggest that Topiramate treatment does not alter nicotine-induced behaviors, however it is distinct than what has been observed with ethanol. These results do support the continued study using more selective antagonist to understand the connections between GluK1*KARS and nicotine withdrawal.

Poster Session Abstracts

ID 43 Biochemical Characterization of Anticancer Alkaloid Methyltransferases in Medicinal Plant Camptotheca acuminata

I, Rm 25 Ms. Stephanie Provenzano, Ryan Miller, Paul Erba, Pearl Merry, Vonny Salim

Louisiana State University Shreveport, Louisiana State University in Shreveport

Camptotheca acuminata produces the anticancer monoterpene indole alkaloid camptothecin, antioxidant flavonoids, and other specialized metabolites. Despite wide clinical applications of camptothecin, the isolation of this high-value compound depends on low-yield extraction from plants. To increase the biosynthetic capacities of the plants, understanding the functions of biosynthetic genes is necessary for further genetic manipulations. Important biosynthetic steps in monoterpene indole alkaloid pathways include O-methylation reactions. Previously, 10-hydroxycamptothecin O-methyltransferase was reported as an active alkaloid methyltransferase with broader substrate specificities toward flavonoids and phenolic compounds. Many *C. acuminata* O-methyltransferases have yet to be biochemically characterized. Here, we selected four O-methyltransferases that were recombinantly expressed in *Escherichia coli* to test toward flavonoids, resveratrol, and caffeic acid. The O-methyltransferase activities revealed in this study contribute to the understanding of monoterpene indole alkaloids and the biosynthetic pathways of specialized metabolites in *C. acuminata*. The functional characterization of these methyltransferases provides a potential avenue for future development of enzyme engineering to modulate the substrate specificity, and therefore increase the diversity of plant metabolites with anticancer properties.

ID 44 Improving Patient Outcomes for Inflammatory Bowel Disease through Physician Interactions during Infusion Treatment : Symptomatic Review of Biologic Therapy in IBD (STABILITY)

I, Rm 26 Ms. Prerana Ramesh, Kelli Morgan, Meher Sindhoora Mavuram, James Morris, Qiang Cai, Phillip Kilgore, Urska Cvek, Marjan Trutschl, J. Steven Alexander

LSU Health Shreveport, LSUHS (Molecular and Cellular Physiology, Gastroenterology and Hepatology), LSUS (Department of Computer Science)

Inflammatory Bowel Disease (IBD) includes Crohn's Disease (CD) and Ulcerative colitis (UC), both of which are characterized by chronic inflammation of the gastrointestinal (GI) tract and extra intestinal manifestations. IBD can be treated by 'biologics' (antibodies) administered via intravenous infusion at infusion clinics with periodic monitoring (colonoscopies and/or abdominal imaging) scheduled during separate clinical visits; based on such screening GI physicians can decide to implement changes in treatment. At LSUHSC-S, IBD patients who received biologic infusions did not routinely meet with a GI physician unless the patient requested this, or upon the infusion nurses' request if the patient was visibly ill. It was observed that many of the IBD patients who did not meet with a GI physician during their infusions would often be absent for their clinical visits. Consequently, these patients' disease progression could not be reliably traced, and alterations that needed to be made in their medication doses, treatment frequency, or therapy plans could go unnoticed. In order to combat this problem, the Department of Gastroenterology implemented patient meetings with GI physicians in the infusion clinics from January 2017 to August 2020 (termed 'STABILITY'). These patients were given anonymous surveys during their infusions to measure their understanding of their disease, how their symptoms had progressed during their treatment, and whether they would want to continue seeing a GI physician during their infusions. Clinical features such as disease severity and colonoscopic evaluations, levels of inflammatory biomarkers (e.g. C-reactive protein, disease activity, rate of hospitalization, etc.) was measured in 110 patients before and after STABILITY. Data analysis revealed significant reductions in disease severity, frequency of hospitalizations, and inflammatory biomarker levels in both CD and UC patients at the end of the treatment period.

Poster Session Abstracts

ID 45 Frequency domain approach for improvement of cochlear implant performance
II, Rm
24
Ms. Silvia Robert, Dr. Sanichiro Yoshida

Southeastern Louisiana University, Southeastern Louisiana University

A cochlear implant is a sensory-neural prosthetic electronic device that can help people with loss of hearing with a sense of hearing. The audio conversion process is studied continuously in the frequency domain, and with high respect to the development of technology, cochlear device sensitivity can improve. The challenge is to allocate the frequency spectral components properly to the limited number of electrodes and generate pulsed signals accordingly. The purpose of the research is to improve the generation of sound sensitivity by the implant by altering and allocating parameters within the spectral process.

ID 46 Elucidation of Anticancer Alkaloid Biosynthetic Pathways in Medicinal Plants: Improved Solutions for Drug Development
II, Rm
25
Dr. Vonny Salim, Vonny Salim, Ryan Miller, Paul Erba, Stephanie Provenzano, Pearl Merry, Keelin North, Shandrekia Robinson, Christopher Stratton, Elahe Mahdavian, Urska Cvek, Phillip Kilgore, and Shile Huang
Louisiana State University Shreveport, Louisiana State University Shreveport, Louisiana State University Health Sciences

Medicinal plants produce specialized metabolites with a diverse array of pharmaceutical properties, including as anticancer agents. Two plant species, *Catharanthus roseus* and *Camptotheca acuminata* produce alkaloids, known as vinblastine and camptothecin that have been extensively used in chemotherapy. Since these high-value compounds are produced in small amounts in plants, metabolic engineering efforts are pursued to enhance the production of anticancer alkaloid compounds by reconstituting the plant biosynthetic pathways in microbial systems. However, the comprehensive biochemical characterization of enzymes involved in the biosynthetic machineries is necessary to develop approaches that will allow further metabolic and enzyme engineering. We combine bioinformatic approaches in analyses of genomics, transcriptomics, and metabolomics to identify potential candidate biosynthetic genes, followed by biochemical characterizations and in-vivo reverse genetics approach to accelerate the elucidation process. Furthermore, molecular modeling of biosynthetic enzymes reveals the key amino acid residues that contribute to diversifying the alkaloids in *Camptotheca acuminata*, such as in the synthesis of central intermediate, known as strictosidinic acids and in deglycosylation steps. The functional characterization of key biosynthetic enzymes will open new doors in our efforts to modulate the substrate specificities and further genetic manipulations both in plant and microbial systems for increasing the diversity of alkaloids with therapeutic properties.

ID 47 Identifying Lethal Alleles in Human
II, Rm
26
Dr. Jeffry Shultz, Telfah, R., Abadie, W., Schluter, J., Hicks, C.
Louisiana Tech University, LSU-HSC

Lethal alleles have long been described as the lack of a living homozygous recessive offspring from two carrier parents. Because it is unethical to perform specific crosses in Human to identify which genes may be lethal, we seek to identify several analytical methods to identify a subset of Human gene mutations that could be lethal. Initially, we will eliminate genes associated with known recessive diseases, followed by analysis of genes that are highly conserved, integral to a required pathway, exhibit high transcription levels early in development or that are linked to increased non-disjunction. After the creation of subsets of Human polypeptide-encoding genes classified according to their likelihood of being a lethal allele (this project), we will test putative lethal alleles using an siRNA knockout approach (subsequent project).

Poster Session Abstracts

ID 48 Translation initiation factors from early-branching eukaryote Giardia lamblia can form multifactor complex in the absence of 40S ribosome in vitro

I, Rm 27 **Mr. Bryan Strong**, Zachary Wiggins, Francis Kwarteng, Zachary Shaw, Breanna Gottschalk, Srinivas Garlapati

University of Louisiana at Monroe, University of Louisiana at Monroe

The eukaryotic translation initiation process involves the binding of a pre-initiation complex to the 5' end of mRNA strands. This binding is mediated by protein-protein interactions between the 5' cap bound eIF4F complex and eIF3 (in mammals) or eIF5 (in yeast) of the pre-initiation complex. The scanning for a start codon placed in a proper sequence context (with a Kozak sequence) is mediated by several protein initiation factors: eIF1, eIF2, eIF3, eIF5, and eIF4G. It has also been demonstrated that initiation factors eIF1, eIF2, eIF3, and eIF5 can form a multifactor complex (MFC) in the absence of a 40S ribosome, indicating that these complexes act together to stabilize the pre-initiation complex formation and facilitate start codon selection. Giardia lamblia is an early-branching eukaryote that lacks eIF4G, a scaffold protein in the eIF4F complex. Giardia mRNAs have very short 5' untranslated regions (UTRs). Preliminary observations have suggested that the pre-initiation complexes are recruited to the initiation codon without a prior scanning mechanism in Giardia, apparently due to the short 5' UTRs. However, Giardia cells have all the initiation factors that are necessary for the scanning process. To determine whether the lack of a scanning mechanism is due to the absence of protein-protein interactions between initiation factors eIF1, eIF2, eIF3, and eIF5, yeast two-hybrid assays and GST-pull down assays were performed. These assays were used to not only determine interactions between these factors but also to detect MFC formation.

ID 49 Complex interplay between Hsp90 and Beclin-1 regulates TLR-4 mediated autophagy during Pentachlorophenol exposure-in vitro

II, Rm 27 **Mrs. Shilpa Thota**, Rizwana Begum, Dr. Waneene C Dorsey, Dr. Sanjay Batra

Southern University and A&M College, Southern University and A & M College, Grambling State University

Pentachlorophenol (PCP) was widely used organochlorine pesticide and wood preservative in the U.S. Due to its carcinogenic activity, the use of PCP was restricted by EPA. PCP is easily absorbed through the skin and lungs. Since it is an environmental toxicant, chronic exposure leads to severe lung and liver toxicity in humans. There are few reports which demonstrate PCP-mediated increase in inflammatory responses using murine and cellular study models. The role of autophagy in regulating inflammatory mediators including pattern recognition receptors, cytokines, and chemokines has been well studied. Earlier reports also demonstrate that Beclin-1 regulates TLR-4 mediated autophagy by directly binding to TLR-4 signaling complex; while Hsp90 maintains Beclin-1 homeostasis and participates in TLR-mediated autophagy. A significant increase in the production/transcription of chemokines (CXCL8, CCL2 and CCL5) and pro-inflammatory cytokines (IL-1B and IL-6) was observed in PCP-challenged human lung epithelial cells (A549). Our results show important role of transcription factor-NF-kB in PCP-induced inflammation. Besides regulating pro-inflammatory mediators, NF-kB has also been shown to regulate autophagy process in response to a wide variety of stimulants. We therefore hypothesized that autophagy mechanism plays important role in PCP-induced inflammation in A549 cells. Using PCP-challenged A549 cells we observed increase in the expression of several autophagy related proteins (LC3B, Beclin-1, ATG5, and ATG16). Further, PCP-mediated increased expression of heat shock protein (HSP)90 and TLR-4 demonstrate their role in inflammatory'autophagy process. Interestingly, siRNA mediated knockdown of Beclin-1 or HSP90 abrogated the expression of autophagy genes, TLR4 and the activation of NF-kB in PCP-challenged cells. Overall, our findings identified the importance of HSP90 and Beclin-1 in regulating autophagy process and inflammatory responses in PCP-challenged A549 cells.

Poster Session Abstracts

ID 50 Correlations Among Evaluator's Level of Training, Assigned HEART Scores, and Major Adverse Cardiac Events

II, Rm 28
Mr. Billy Tran, Philip Kilgore, Urska Cvek, Marjan Trutschl, David Janese, Danielle Handrop, John Felty
Louisiana State University Shreveport, LSUS (Department of Computer Science), LSUHS (Emergency Medicine)

Background: The HEART Score was developed to predict Major Adverse Cardiac Events (MACE) within 6 weeks of the patient's evaluation. We retrospectively reviewed 1,284 emergency room visits for chest pain between 9/1/2017 and 8/31/2018 at LSU Health Center Shreveport, an urban medical center. Evaluators' level of training varied from physician's assistant, off-service, attending physician, to resident. The average age of patients in the study was 51.9 y.o. and included MACE of 1 (major adverse cardiac event) and 2 (no cardiac event). This study's primary goal was to identify the correlations between various variables, the HEART score, and the subsequent occurrence or nonoccurrence of MACE . **Methods:** Patients' HEART score, level of training of the evaluator, age at discharge, gender, and occurrence of MACE were analyzed using statistical tests for distribution and correlation including Wilcoxon rank sum test, Spearman correlation, and Kruskal-Wallis test. **Results:** We observed a low correlation between the HEART score and the rate of MACE. Assigned HEART Scores did not appear to be affected by the level of training of the evaluator. Age has an expected moderate correlation with the HEART Score, but little to no correlation with MACE. Gender appears to have little to no correlation with the subsequent occurrence of MACE and HEART Score.

ID 51 Bioinformatics Analysis of Large-Scale Neoproteomic Data and Prediction of Neurovascular Change

I, Rm 28
Dr. Marjan Trutschl, Hyung Nam, Phillip Kilgore, Urška Cvek
Louisiana State University Shreveport, LSUHS (Departments of Pharmacology), LSUS (Department of Computer Science and Laboratory for Advanced Biomedical Informatics)

Advances in proteomics resulted in large-scale datasets that have driven the interest in data analysis, geared towards understanding biological systems. The integration of computational modeling and experimental results helps us predict and characterize the dynamic properties of biological systems. In this collaborative research, we applied bioinformatics to proteomic analysis to elucidate the disease-perturbed brain networks in transgenic mice model. The neurogranin gene (Nrgn) has been selectively depleted in the brain vasculature, increasing brain permeability. The brain tissue from the prefrontal cortex (PFC) and nucleus accumbens (NAc) was isolated. A large-scale proteomic approach using nanoLC-MS/MS resulted in ~4,000 protein profiles across the genotype (Nrgn vs. wild-type) and brain regions (PFC and NAc). Interestingly, a vascular-specific Nrgn knockout in the PFC increases the cluster of amyloid-beta processing, while vascular-specific Nrgn knockout in the NAc increase GABA neurotransmission. Utilizing bioinformatics, we further determined the molecular networking between PFC and NAC in response to Nrgn knockout in the brain vasculature. The Ingenuity Pathway Analysis has been utilized for mapping the biological processes regulated by the genotype and brain regions. Moreover, we applied visual mapping to establish a proteome network, and a self-organizing map to predict possible neurovascular change. Finally, our bioinformatics for proteomics analyses illustrate a potential molecular basis for the Nrgn-mediated brain damage, which provides a better understanding of the neurovascular disease.

ID 52 Construction of a model cell line to test DNA replacement catalyzed by tyrosine

Poster Session Abstracts

I, Rm 29 **recombinases**
Dr. Yuri Vozianov, Joe Dalton Williams and Yuri Vozianov
Louisiana Tech University, Louisiana Tech University

We recently developed a new genome engineering tool called TAL-fused tyrosine DNA recombinases, or TFRs. These hybrid DNA recombinases are composed of two functional modules, target specificity of which can be intentionally altered: a variant of the tyrosine recombinases Flp or Cre and the DNA binding domain of the transcription activator-like effector (TAL). TFRs are capable of targeting the desired sequences in the human genome opening an opportunity to advance the genome engineering field. The ultimate goal of our research is to adapt TFRs to efficiently replace mutated genomic fragments with the normal DNA thus paving way to correct genetic diseases. To optimize the parameters of the replacement reaction catalyzed by the hybrid DNA recombinases we created a model CHO cell line, functionality of which was successfully tested using Flp-TAL and Cre-TAL recombinase variants.

ID 53 Comparative transcriptomic analysis of GABAergic versus dopaminergic neuronal differentiation in mouse ES cells
II, Rm 29 **Mrs. Anna Wilson**, Anna Davis Wilson, Harpreet Kaur, Elia Brodsky, Eduardo Martinez-Ceballos
Southern University and A&M College, Southern University A&M - Baton Rouge, Pine Biotech, Pine Biotech. Southern University A&M - Baton Rouge

The ability of embryonic stem cells (ESCs) to differentiate into any cell type of the body presents an opportunity in regenerative medicine to obtain neuronal progenitors capable of repairing nervous tissues. Specifically, particular studies have focused on generating GABAergic neurons from ESCs as a method to replace damaged neurons due to their ability to release the GABA inhibitory neurotransmitter. In this regard, studies have shown the potential of neural stem cell (NSC) transplantation, but a major drawback of this approach is that NSCs produced from stem cells have the ability to cause allogeneic responses, which can lead to tumor formation due to the heterogeneity of the neuronal populations being produced during culture. Thus, because teratogenesis after transplantation is possible, a better understanding on the molecular mechanism of ESC to GABAergic neuronal differentiation is required. In this regard, we previously reported that mouse ESCs encapsulated in hydrogels and treated with all-trans-retinoid acid (RA) were able to generate GABAergic neurons with high efficiency. However, the molecular mechanism associated with GABAergic differentiation through this differentiation protocol is not well known. To address this gap in knowledge, we performed time-series transcriptome analyses on encapsulated vs standard 3D cell culture (embryoid bodies or EBs) of mouse ESCs treated with RA for two (2D-RA) or four days (4D-RA). Control cells were treated with vehicle only for two days. We found that genes expressed in excitatory pyramidal neurons, such as Nxf7, were differentially expressed in EBs as compared to encapsulated cells at 4 days of RA treatment, but not at 2 days. In contrast, genes such as Slit1, whose gene product is expressed in the ventral midline of the neural tube, and Tnip1, whose gene product is an inhibitor of the neuronal modulator NF- κ B, were upregulated in 4D-RA encapsulated cells versus EBs. Additional differentially expressed genes are desc

ID 54 Comparing Solubility of the catalytic mutant in the lyase-isomerases MpeQ and MpeZ from Synechococcus sp. A15-62 and RS 9916
I, Rm 3 **Ms. Julianna Berger**, Kes Lynn Joseph, Wendy M. Schluchter
University of New Orleans

Marine cyanobacteria contain a large proteinaceous structure called a phycobilisome (PBS). The ability to alter bilin molecules attached to pigmented phycobiliprotein (PBP), such as phycoerythrin II (PEII), has conferred ecological success of the genus *Synechococcus*. Some *Synechococcus* species are able to

Poster Session Abstracts

undergo Type IV chromatic acclimation by altering the ratio of green light absorbing phycoerythrobilin or blue light absorbing phycourobilin on PEII in response to the light environment. The ability to adapt to these light conditions is mediated by enzymes from the MpeQWYZ family of lyases and lyase-isomerases that attach bilin on Cys-83 of the PEII alpha subunit (MpeA). Members of this family, such as MpeQ and MpeZ, attach the bilin phycoerythrobilin and isomerize it to phycourobilin. Mutagenesis and heterologous recombinant expressions of MpeQ (Y318F), a mutant needed to trap intermediate phycourobilin in MpeA crystallization studies, demonstrated MpeQ's inability to attach bilin to MpeA. Results, however, were not conclusive for the continued ability of MpeQ to isomerize bilin due to low solubility of MpeQ. Therefore, the theoretically more soluble MpeZ was mutated at Tyr-318 into a phenylalanine using overlapping PCR. The solubility of hexa-histidine tagged wild type and mutant MpeQ and MpeZ were purified by Cobalt chromatography and compared using Coomassie stained SDS-PAGE after recombinant expression in E.coli. Our results suggest that both wild type and mutant MpeZ have a higher solubility than MpeQ. These studies will be used to study the biochemical mechanism of lyase-isomerase enzymes and can be applied to creating fluorescent fusion tags.

ID 55 Heterogeneous Cu@Hal catalyzed [3+2] cycloaddition reactions for the preparation of 1,2,3-triazoles

I, Rm 6 **Ms. Loandi Cruz**, Loandi E. Cruz, Brooke N. Diehl, Mark L. Trudell
University of New Orleans, Department of Chemistry, University of New Orleans

The copper catalyzed [3+2] cycloaddition of alkynes with alkyl azides has become a widely used and reliable synthetic method for the construction of 1,2,3-triazoles. These important heterocycles are often privileged structures and bioisosteres variety of medicinal chemistry applications. As part of broader program at UNO aimed at developing "green chemistry" for organic synthesis, conditions were developed for the preparation of 1, 2, 3-triazoles using a heterogenous copper catalyzed click [3 + 2] cycloaddition of alkynes with azides. The catalyst employed for these reactions was a nanocomposite material of copper nanoparticles encapsulated in the natural clay halloysite (Cu@Hal). The reactions were performed with several alkynes with in situ generation of the alkyl azides from the corresponding alkyl halide (Cl or Br) and sodium azide in water at 50-80°C. These conditions afforded good yields of the corresponding 1,5-disubstituted-1,2,3-triazoles. The scope and limitations of Cu@Hal catalyzed [3+2] cycloaddition reaction will be presented.

ID 56 Accurate identification of ncRNA-protein interactions using ensemble deep learning methods

II, Rm 1 **Dr. Duaa Alawad**, Md Tamjidul Hoque
University of New Orleans, University of New Orleans

Interactions between non-coding RNA (ncRNA) and proteins are crucial in various physiological and pathological processes. Using the *in vivo* experimental approaches for predicting ncRNA-protein interactions take a long time and need a lot of effort. As a result, computational approaches for reliably and effectively predicting ncRNA-protein interactions are in high demand. In this work, we describe an ensemble deep learning technique for predicting ncRNA-protein interactions utilizing a mix of multi-scale data, such as primary sequence features, secondary structure sequence features, and tertiary structure features. First, we used conjoint k-mer to extract protein/ncRNA sequence features, next we integrated the tertiary structure features, then fed them into an ensemble deep learning models to predict the interactions between ncRNA and protein.

ID 57 Growth inhibitory and apoptotic effects of Graviola (*Annona Muricata*) fractions in

Poster Session Abstracts

human melanoma and non-melanoma skin cancer in vitro

II, Rm 5 **Ms. Chelsea Bock**, RN Chamcheu¹, ST Boateng¹, T Roy¹, S Banang-Mbeumi¹, J Fotie² and JC Chamcheu¹
University of Louisiana at Monroe, College of Pharmacy, University of Louisiana at Monroe, LA and Department of Chemistry and Physics , Southeastern Louisiana University, LA.

The global increase in health awareness has propelled the chemopreventive utility of nutraceuticals especially as supplements, prophylaxis, and in treating chronic diseases. Graviola, or soursop, is an evergreen plant of the family Annonaceae, which has numerous reported therapeutic benefits in the control of various human diseases including cancer due to its multi-vested phytochemical make-up; tannins, flavonoids, saponins, alkaloids, steroids, acetogenins and polyphenols. These exert these beneficial effects while having minimal to no side-effects which could be exploited to serve this purpose. Skin cancer is the most common cancer in the United States and affects one-fifth of Americans in their lifetime accounting for an annual financial burden of over \$8.1 billion. In this project, macerated aerial parts of graviola was fractionated using soxhlet in 3 solvents namely, hexane, dichloromethane (DCM) and methanol and were used to test their differential cancer properties against melanoma (A375) and non-melanoma (A431) skin cancer cell-lines. DCM solvents extract had the most suitable pharmacological effect, as it exerted the most potent activity, hence the solvents were further fractionated using gradient elution to obtain 8 sub-fractions; GRMB (1-8) with varied polarity, which were subsequently characterized using the previous in-vitro model. It was observed that 3 fractions (GRMB-2, 3 and 4) and 2 other fractions (GRMB-7 and 8) exhibited significant and selective potency towards A375 and A431 cell-lines respectively. In summary, the preliminary data identifies the most effective solvent and supports this extraction pathway to be pursued for the isolation and characterization of the active phytochemical entities and family of molecule(s) accounting for these anti-skin cancer properties.

ID 58 Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females

II, Rm 7 **Mr. Eric Clifford**, Phillip Kilgore, Urska Cvek, Marjan Trutschl, Nadejda Korneeva, Steven A. Conrad, Thomas Arnold
Louisiana State University Shreveport, LSUS (Department of Computer Science and Laboratory for Advanced Biomedical Informatics), LSUHS (Department of Emergency Medicine)

LSU Health Sciences Center in Shreveport serves a largely minority-based, urban population. Prior analysis of emergency room urine drug screen results from 1998-2011 found that the African American population tested positive for cannabinoids, opiates, and cocaine at high rates, while the Caucasian population tested positive for cannabinoids, benzodiazepines, and opiates at high rates. The focus of this study was to determine connections between visit reasons and rates of positive drug screens, tracked by race and age, among 18-35 years old females during 2012-2019. Similar to the 1998-2011 general population study, Caucasian and African-American females tested positive mostly for cannabinoids and opiates during 2012-2019. Caucasian females also tested positive for amphetamines and benzodiazepines at higher rates than African American females. African American females tested positive for cannabinoids and cocaine at higher rates than Caucasian females. From 2012-2016, Caucasian females tested positive for opiates at higher rates. Beyond 2016, African American females tested positive for opiates at higher rates. Most visits in both populations were for pain, pregnancy, or psychiatric/neurologic reasons. About 30% of pregnancy and gynecologic visits were associated with cannabinoid use, followed by opiates. Gastroenterology patients tested positive for cannabinoids in over 40% of cases and for opiates in 20%. Psychiatric/neurologic patients tested positive mostly for cannabinoids and amphetamine (36% and 15%, respectively). Sickle Cell patients (all African American) tested positive for opiates at a rate of 72%. GatewayNet analysis indicated that cannabis use likely precedes cocaine, amphetamine, benzodiazepine, and opiate use. This work is supported by the

Poster Session Abstracts

2021 Summer Research Program of the Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P2O GM103424-19.

ID 59 HSP70 and proteasomes coalesce in lipid rafts to regulate E-cigarette Vapor condensate induced inflammation

II, Rm 4 **Dr. Rizwana Begum**, S. Thota, S. Batra, D. Kambiranda

Southern University and A&M College, 1 Laboratory of Pulmonary Immuno-toxicology, 1Department of Environmental Toxicology & 2 Southern University Agriculture Research and Extension Center, Southern University and A&M College

Electronic cigarettes (e-cigs) and other tobacco-based products are addictive. However, due to their projection as less harmful alternatives, electronic smoking devices or e-cigs gained popularity in the US markets rapidly. Earlier reports suggest that HSP70 interacted with the ubiquitin-proteasome system (UPS) to eliminate the damaged and malfunctioning proteins in the cell. In addition to protecting the cellular proteome, HSP70—the primary stress-inducible heat shock protein has been demonstrated to interact with lipids. In light of these facts, we hypothesized the important role of lipid rafts in-a) compartmentalization of HSP70 and proteasome/immunoproteasomes; and b) regulating inflammatory responses-in e-cig vapor condensate (tobacco flavor; TF-ECVC) challenged human lung epithelial cells (A549). Our experiments revealed TF-ECVC mediated increase in-1) transcription and translation of lipid raft-associated proteins (caveolin-1, flotillin-1, and flotillin-2); 2) inducible proteasome subunits (LMP7/PSMB8, LMP2/PSMB9, MECL-1/PSMB10); c) expression of NF- κ B and MAPK genes; d) transcription and extracellular accumulation of HSP70; and e) production of pro-inflammatory cytokines/chemokines in A549 cells. We also observed a decrease in the expression of constitutive proteasome subunits (β 1/PSMB6, β 2/PSMB7, and β 5/PSMB5). Also, the localization of HSP70, β 2/PSMB7, and LMP7/PSMB8 subunits was observed in lipid raft fractions of TF-ECVC challenged alveolar epithelial cells. Furthermore, using siRNA mediated approach, we observed a decrease in the expression of lipid rafts associated protein flotillin-1 and proteasome subunit β 1/PSMB6 in HSP70 knockdown A549 cells challenged with ECVC. Overall, our findings provide critical information about the role of lipid rafts and HSP70 in ECVC-induced inflammation. Studies are in progress to identify the detailed molecular mechanisms.

ID 60 Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells

I, Rm 24 **Dr. Nandini Bidarimath**, N. Bidarimath, S. Thota, S Batra

Southern University and A&M College, Laboratory of Pulmonary Immuno-toxicology, Department of Environmental Toxicology Southern University and A&M College

Pentachlorophenol (PCP), an anthropogenic chlorophenol compound, was primarily used as a wood preservative and in formulations of fungicides, insecticides, and herbicides. Household and occupational exposure to PCP via inhalation and/or ingestion has been associated with immune modulation in humans. However, the genetic and molecular mechanisms regulated during PCP exposure are still not completely understood. To cover the gap in our understanding, we conducted a high-throughput RNA sequencing for determining the potential molecular mechanisms associated with PCP-induced immune regulation. We exposed human lung (A549) and liver (HepG2) epithelial cells to PCP (10 μ M) for determining the effect on transcript abundance and transcriptomic profiles. Two independent RNA-sequencing pipelines were run for identifying differential gene expression (DGE), while Principal component analysis (PCA) was performed independently to understand the variation and pattern in each dataset. This was followed by Gene Set Enrichment analysis (GSEA), Gene ontology (GO) term, KEGG pathway and network/pathway (GAGE-Generally applicable gene set enrichment) analyses to assess the biological implications. The DGE analysis of HepG2 cells revealed 17 significantly upregulated and 49 downregulated genes, while A549 cells revealed 6 upregulated and

Poster Session Abstracts

16 downregulated genes following PCP-exposure in our preliminary studies. The GSEA and KEGG analysis on HepG2 cells yielded a distinct cluster of significantly expressed genes associated with hepatocellular carcinoma, MAPK signaling, xenobiotic metabolism and steroid hormone biosynthesis-highlighting altered biological mechanisms during PCP-exposure. While A549 cells showed altered VEGF signaling pathway, Hippo signaling pathway, oxidative phosphorylation, neutrophil extracellular trap formation-highlighting altered immune signaling. Further studies are in progress to determine the molecular mechanisms associated with PCP-induced immunotoxicity.

Oral Presentation Index

Dr. J. Steven Alexander (<i>Louisiana State University Health Shreveport</i>), Prerana Ramesh, Kelli Morgan, Meher Sindhoora Mavuram, James Morris, Qiang Cai, Phillip Kilgore, Urska Cvek, Marjan Trutschl, J. Steven Alexander “Improving Patient Outcomes for Inflammatory Bowel Disease through Physician Interactions during Infusion Treatment: Symptomatic Review of Biologic Therapy in IBD (STABILITY)”	Page 9
Dr. Nektarios Barabutis (<i>University of Louisiana at Monroe</i>), “Protective role of activating transcription factor 6 against endothelial barrier dysfunction”	Page 9
Dr. Jean Christopher Chamcheu (<i>University of Louisiana at Monroe</i>), Tithi Roy1, Sergette Banang-Mbeumi1, Samuel Boateng1, Stephane Esnault2, Roxane-Cherille Chamcheu1, Shile Huang3, Kousoulas Gus Konstantin4 and Jean Christopher Chamcheu1 “Developing fisetin, a polyphenolic ingredient co-targeting the central mTOR pathway and IL-17A for Treating Psoriasis”	Page 10
Dr. George Matthaiolampakis (<i>University of Louisiana at Monroe</i>), “micro-RNA therapy against cell cycle progression for Lung Cancer treatment”	Page 10
Dr. Siva Murru (<i>University of Louisiana at Monroe</i>), Prof. Seetharama Jois, Dr. JeanChristophe Chamcheu, Dr. Jayalakshmi Sridhar “Design, Synthesis and Evaluation of Pyrazole Derivatives as Potential Anti-Cancer Agents”	Page 11
Dr. Devaiah Kambiranda (<i>Southern University and A&M College</i>), Rizwana Begum, Shilpa Thota, Lauryn Langley, Sanjay Batra “Proteasomes/immunoproteasomes: Role of lipid rafts in compartmentalization/ activation in e-cigarettes vapor exposed lung epithelial cells”	Page 11
Dr. Kyle Piller (<i>Southeastern Louisiana University</i>), “Life in the fastlane: Testing for congruence among transcriptomic signatures in model organisms”	Page 12
Dr. Rizwana Begum (<i>Southern University and A&M College</i>), S. Thota1, S. Batral and D. Kambiranda2 “HSP70 and proteasomes coalesce in lipid rafts to regulate E-cigarette Vapor condensate induced inflammation”	Page 12

Oral Presentation Index

Dr. Nandini Bidarimath (<i>Southern University and A&M College</i>), N. Bidarimath, S. Thota and S Batra “Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells”	Page 13
Mr. Eric Clifford (<i>Louisiana State University Shreveport</i>), Phillip Kilgore, Urska Cvek, Marjan Trutschl, Nadejda Korneeva, Steven A. Conrad, Thomas Arnold “Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females”	Page 14
Mr. Denzel El Hage (<i>University of Louisiana at Monroe</i>), Jafrin Jobayer Sonju, Prof. Seetharama Jois, Dr. Siva Murru “Development of a pH-sensitive liposome formulation for targeted delivery of anticancer pyrazolones in lung cancer cells”	Page 14
Ms. Tithi Roy (<i>University of Louisiana at Monroe</i>), Tithi Roy ¹ , Sergette Banang-Mbeumi ¹ , Samuel Boateng ¹ , Stephane Esnault, Roxane-Cherille Chamcheu ¹ , Kousoulas Gus Konstantin and Jean Christopher Chamcheu ¹ “The dietary antioxidant Fisetin suppresses Psoriasis-like characteristics in vitro and in vivo in an imiquimod-induced dermatitis in Balb/c mice: Involvement of the central mTOR signaling pathway”	Page 15
Dr. April Wright (<i>Southeastern Louisiana University</i>), Jeremy Brown “Evaluating model selection frameworks for complex hierarchical models”	Page 15
Dr. Srinivas Garlapati (<i>University of Louisiana at Monroe</i>), Dr. Yong-Hwan Lee “Mechanism of Translation initiation in the protozoan parasite Giardia lamblia”	Page 16
Dr. Vonny Salim (<i>Louisiana State University Shreveport</i>), Ryan Miller, Paul Erba, Stephanie Provenzano, Pearl Merry, Keelin North, Shandrekia Robinson, Christopher Stratton, Elahe Mahdavian, Urska Cvek, Phillip Kilgore, Shile Huang “Elucidation of Plant-Derived Anticancer Alkaloid Biosynthetic Pathways”	Page 16

Poster Session Abstracts Index

ID #1	Mr. Abubakar Abdulkadir (SUBR) , Dr. Sanjay Batra “Comparative Bioinformatics and Conventional approach reveal some common signaling mediators in DE-particulate exposed A549 and BEAS-2B cells”	Page 18
ID #2	Mr. Mohammad Shohel Akhter (ULM) , Mohammad Shohel Akhter, Antoinette Jaci Leo, Khadeja-Tul Kubra, Nektarios Barabutis “Growth Hormone Releasing Hormone Antagonists Protect Against LPS-Induced Endothelial Hyperpermeability”	Page 18
ID #4	Ms. Alexis Bardwell (LATECH) , M. Bowles, R. Giorno “Identification of Spore-Forming Bacteria in a Louisiana Salt Marsh”	Page 19
ID #5	Mr. David Basnet (ULM) , Siva Murru “N-Boc-hydroxylamine as a Boc-donor Agent for the Catalytic N-tert-Butoxycarbonylation of Pyrazoles and Indazoles”	Page 19
ID #6	Mr. Samuel Boateng (ULM) , T Roy, S Banang-Mbeumi, RN Chamcheu, Mercy E. Agbo, J Fotie, JC Chamcheu “Biological evaluation, in silico molecular docking and ADMET screening of a small library of phenolic compounds identified novel anti-skin cancer agents”	Page 19
ID #7	Dr. Mary Calderera-Moore (LATECH) , Claire Colley, Tyler Priddy-Arrington, Mary Calderera-Moore “Assessment of injectable chitosan-genipin hydrogels biomaterial biocompatibility”	Page 20
ID #8	Dr. Joseph Chaney (XULA) , Amaya Sanders (1), Thandiwe Bush (1), Alyria Terry (1), Carolyn Scruggs-Webster (1), Nelson Brown, Kennedy Drake (1), Jada Montley (1), Micquel Downs (2), Edward Wojcik (2), Joseph Chaney (1) “Applying the Brakes: Understanding the Role of the Conformational Changes in the Kinesin-5 on Processivity and Inhibition”	Page 21
ID #9	Ms. Karli Clifton (ULM) , Dr. Siva Murru “Electro-chemical Cyclization of Hydroxychalcones for the Synthesis of Flavonoids”	Page 21
ID #10	Dr. Urska Cvek (LSUS) , Urska Cvek, Phillip Kilgore, Eric Clifford, Marjan Trutschl, Tingting Li, Lauren S. Maniscalco, Jane Gulick Sugar, Terry C. Lairmore “Disparities in Breast Cancer Treatment Outcomes: Improving Access with Health Informatics”	Page 21
ID #11	Ms. Devika Dua (CCS (HS)) , Devika Dua, Dr. Norman John Mapes “Investigating Key COVID-19 Questions by Using Natural Language Processing on Scientific Publications”	Page 22
ID #12	Dr. Samrat Dutta (XULA) , Dr. Thomas Wiese, Mentor “Diagnostic Cancer Imaging In the Mid-Infrared Using Novel Contrast Agents”	Page 22

Poster Session Abstracts Index

ID #13	Mr. PJ Erba (LSUS) , Paul Erba, Ryan Miller, Stephanie Provenzano, Pearl Merry, and Vonny Salim “Development of Methodology in Microbial DNA Isolation for Characterization of Soil Microbiome”	Page 23
ID #14	Mr. Anup Ghimire (SELU) , Kazim Sekeroglu, Max Cole “EEG Based Motor Imagery Task Classification Utilizing Spatiotemporal Deep Learning for BCI Applications”	Page 23
ID #15	Dr. Matthew Hayes (XULA) , Derrick Mullins, Angela Nguyen “Complex Germline Structural Variant Discovery Via Discordant Cluster Normalization”	Page 24
ID #16	Mr. Bennett Hibner (SELU) , William A. Parkinson, Bennett K. Hibner “Computational Investigations Of Stereospecificity In Concerted Electrocyclic Reactions”	Page 24
ID #17	Mr. Hunter Hollie (SELU) , Patrick Moyer (faculty advisor) “Design and Development of a Low-Cost High-performance Atomic Force Microscope (AFM)”	Page 24
ID #18	Dr. Moses Ihachi (SELU) , Dr. Vicente (Mentor) “Aryl-fused (Imidazole, Pyrazine and Pyrrole) Boronated Dye Derivatives”	Page 25
ID #19	Ms. Chelsey Jordan (LSUS) , Chelsey Jordan, Avery Christensen, Brian A. Salvatore, and Elahe Mahdavian “Assessment of student appreciation for applied bioinformatics and computational drug discovery methods in a project-based course”	Page 25
ID #20	Ms. Supriya Karki (LSUS) , Kathryn Hamilton, Stephanie Villalba “Developmental Stages of Olfactory Sensory Neurons in Neonatal Life vs. Adulthood”	Page 26
ID #21	Mr. Waheed Khan (LSUS) , Elahe Mahdavian “Using computational drug repurposing methodology to identify promising bictegavir-based drug candidates for COVID-19”	Page 26
ID #22	Mr. Phillip Kilgore (LSUS) , Phillip C.S.R. Kilgore, David Janese, Jenny Jones, Kasi Addison, Raymond Kessler, Rachel Waesche, Mary Ann Edens, Angela Cornelius, Marjan Trutschl, Urska Cvek “Racial Disparities in COVID-19 Symptoms in Northern Louisiana”	Page 26
ID #23	Dr. Vladimir Kolesnichenko (XULA) , Galina Goloverda, Quincy J. Brown, Thomas Wiese “Cancer-Specific Magnetic Imaging Agent”	Page 27

Poster Session Abstracts Index

ID #24	Mrs. Khadeja-Tul Kubra (ULM) , Khadeja-Tul Kubra, Mohammad S. Akhter, Yogesh Saini, Konstantin G. Kousoulas, Nektarios Barabutis “Activating transcription factor 6 modulates endothelial barrier function.”	Page 27
ID #25	Mr. James Lee (SELU) , Matthew Giblin, Dr. Teague O'Mara “Heart rate variability and novel torpor states in tent-making bats”	Page 28
ID #26	Ms. Laura Lee (LATECH) , Laura Lee, Michael Foster, Paul Austin, Tom Bishop, Paul Kim, Jamie Newman “Wastewater Analysis and Genomic Sequencing of SARS-CoV-2 Benefit COVID-19 Surveillance”	Page 28
ID #27	Mr. Chi Jing Leow (SELU) , Chi Jing Leow and Kyle R. Piller “Accessing the congruency of DNA repair genes among killifishes with different life histories using QuantSeq”	Page 29
ID #28	Mr. Raj Letchuman (CPM (HS)) , Elahe Mahdavian, Christopher Stratton “Identifying Promising Drug Candidates Against SARS-CoV-2 Using Computational Drug Repurposing Methodology”	Page 29
ID #29	Dr. Elahe Mahdavian (LSUS) , “An interdisciplinary course on computer-aided drug discovery to broaden student participation in original research”	Page 30
ID #30	Mr. Ethan Manco (LSUS) , Co-author: Dr. Subhajit Chakrabarty “Patterns in Electroencephalograms during Meditation”	Page 30
ID #31	Ms. Pearl Merry (LSUS) , Paul Erba, Ryan Miller, Stephanie Provenzano, Vonny Salim “Virus-Induced Gene Silencing: In-Vivo Characterization of Anticancer Alkaloid Biosynthetic Genes in Medicinal Plants”	Page 31
ID #32	Mr. Ryan Miller (LSUS) , Vonny Salim, Paul Erba, Stephanie Provenzano, Pearl Merry “Whole Cell Biotransformation for Central Intermediate Formation in Anticancer Monoterpene Indole Alkaloid Biosynthetic Pathways”	Page 31
ID #33	Mr. Joseph Mondello (LSUS) , Tauhidul Alam “Computing Representative Protein Conformations from Molecular Dynamics Simulations”	Page 32
ID #34	Ms. Savannah Montgomery (XULA) , Angela Nguyen, Dr. Hayes “Identifying Double Minutes Chromosomes within Hi-C and Deletion-Episomes”	Page 32
ID #35	Mr. Derrick Mullins (XULA) , Derrick Mullins, Zoe Mitchell, Matthew Hayes “Simulating Double Minute Chromosome and Phylogenetic Tree Evolution using Java”	Page 32

Poster Session Abstracts Index

ID #36	Dr. Christopher Murray (SELU) , Tristan Herod, Jorge Lopez-Perez, Karen Maruska “Alligators as Models for Human Pathology: Neuroendocrine Effects of Methyltestosterone Exposure”	Page 33
ID #37	Ms. Kalani Myles (LSUS) , Elahe Mahdavian “Computer-aided drug discovery for COVID-19 using virtual screening and molecular docking”	Page 33
ID #38	Dr. Jamie Newman (LATECH) , Taylor Teach “Canonical and Noncanonical Notch Signaling Regulates Adult Stem Cell State”	Page 34
ID #39	Ms. Keelin North (LSUS) , Ryan Miller, Paul Erba, Stephanie Provenzano, Pearl Merry, Vonny Salim “Metagenomic Profiling of Soil Microbiome from Anticancer Compound-Producing Plants”	Page 34
ID #41	Ms. Uchechi Owunna (ULM) , Uchechi Owunna ¹ , Ramesh Bista ¹ , Samuel Boateng ² , Tithi Roy ² , Jean Christopher Chamcheu ² , Siva Murru ^{1,*} “Synthesis and Biological Evaluation of 1,3-Diarylpyrazoles: in vitro Cytotoxicity Studies on Human Melanoma and Non-melanoma Cancer Cells”	Page 35
ID #42	Dr. Erika Perez (XULA) , “Topiramate treatment precipitates and accentuates physical symptoms of nicotine withdrawal in mice.”	Page 35
ID #43	Ms. Stephanie Provenzano (LSUS) , Ryan Miller, Paul Erba, Pearl Merry, Vonny Salim “Biochemical Characterization of Anticancer Alkaloid Methyltransferases in Medicinal Plant Camptotheca acuminata”	Page 36
ID #44	Ms. Prerana Ramesh (LSUHS) , Prerana Ramesh, Kelli Morgan, Meher Sindhoora Mavuram, James Morris, Qiang Cai, Phillip Kilgore, Urska Cvek, Marjan Trutschl, J. Steven Alexander “Improving Patient Outcomes for Inflammatory Bowel Disease through Physician Interactions during Infusion Treatment : Symptomatic Review of Biologic Therapy in IBD (STABILITY)”	Page 36
ID #45	Ms. Silvia Robert (SELU) , Dr. Sanichiro Yoshida “Frequency domain approach for improvement of cochlear implant performance”	Page 37
ID #46	Dr. Vonny Salim (LSUS) , Vonny Salim, Ryan Miller, Paul Erba, Stephanie Provenzano, Pearl Merry, Keelin North, Shandrekia Robinson, Christopher Stratton, Elahe Mahdavian, Urska Cvek, Phillip Kilgore, and Shile Huang “Elucidation of Anticancer Alkaloid Biosynthetic Pathways in Medicinal Plants: Improved Solutions for Drug Development”	Page 37
ID #47	Dr. Jeffry Shultz (LATECH) , Telfah, R., Abadie, W., Schluter, J., Hicks, C. “Identifying	Page 37

Poster Session Abstracts Index

Lethal Alleles in Human”

ID #48	Mr. Bryan Strong (ULM) , Bryan Strong, Zachary Wiggins, Francis Kwarteng, Zachary Shaw, Breanna Gottschalk, Srinivas Garlapati “Translation initiation factors from early-branching eukaryote Giardia lamblia can form multifactor complex in the absence of 40S ribosome in vitro”	Page 38
ID #49	Mrs. Shilpa Thota (SUBR) , Rizwana Begum, Dr. Waneene C Dorsey, Dr. Sanjay Batra “Complex interplay between Hsp90 and Beclin-1 regulates TLR-4 mediated autophagy during Pentachlorophenol exposure-in vitro”	Page 38
ID #50	Mr. Billy Tran (LSUS) , Billy A. Tran, Philip Kilgore, Urska Cvek, Marjan Trutschl, David Janese, Danielle Handrop, John Felty “Correlations Among Evaluator's Level of Training, Assigned HEART Scores, and Major Adverse Cardiac Events”	Page 39
ID #51	Dr. Marjan Trutschl (LSUS) , Hyung Nam, Phillip Kilgore, Marjan Trutschl, Urška Cvek “Bioinformatics Analysis of Large-Scale Neuroproteomic Data and Prediction of Neurovascular Change”	Page 39
ID #52	Dr. Yuri Voziyanov (LATECH) , Joe Dalton Williams and Yuri Voziyanov “Construction of a model cell line to test DNA replacement catalyzed by tyrosine recombinases”	Page 40
ID #53	Mrs. Anna Wilson (SUBR) , Anna Davis Wilson, Harpreet Kaur, Elia Brodsky, Eduardo Martinez-Ceballos “Comparative transcriptomic analysis of GABAergic versus dopaminergic neuronal differentiation in mouse ES cells”	Page 40
ID #54	Ms. Julianna Berger (UNO) , Kes Lynn Joseph, Wendy M. Schluchter “Comparing Solubility of the catalytic mutant in the lyase-isomerases MpeQ and MpeZ from Synechococcus sp. A15-62 and RS 9916”	Page 40
ID #55	Ms. Loandi Cruz (UNO) , Loandi E. Cruz, Brooke N. Diehl, Mark L. Trudell “Heterogeneous Cu@Hal catalyzed [3+2] cycloaddition reactions for the preparation of 1,2,3-triazoles”	Page 41
ID #56	Dr. Duaa Alawad (UNO) , Md Tamjidul Hoque “Accurate identification of ncRNA-protein interactions using ensemble deep learning methods”	Page 41
ID #57	Ms. Chelsea Bock (ULM) , RN Chamcheul, ST Boateng1, T Roy1, S Banang-Mbeumi1, J Fotie2 and JC Chamcheul “Growth inhibitory and apoptotic effects of Graviola (<i>Annona Muricata</i>) fractions in human melanoma and non-melanoma skin cancer in vitro”	Page 42
ID #58	Mr. Eric Clifford (LSUS) , Phillip Kilgore, Urska Cvek, Marjan Trutschl, Nadejda Korneeva, Steven A. Conrad, Thomas Arnold “Drug Screen Trends in Emergency Rooms	Page 42

Poster Session Abstracts Index

Among Childbearing-Aged Females”

- ID #59 **Dr. Rizwana Begum** (*SUBR*), S. Thota, S. Batra, D. Kambiranda “HSP70 and proteasomes coalesce in lipid rafts to regulate E-cigarette Vapor condensate induced inflammation” Page 43
- ID #60 **Dr. Nandini Bidarimath** (*SUBR*), N. Bidarimath, S. Thota, S Batra “Pentachlorophenol induced transcriptome dynamics in human lung and liver Cells” Page 43

Core Structures and Committees

Administrative Core

The Administrative Core (AC) of the Louisiana Biomedical Research Network (LBRN) provides the project with its overall leadership, day-to-day management, evaluation of all of its component parts, and communication with NIH staff. The AC is led by the Principal Investigator in close consultation with the Program Coordinator, as well as the Steering Committee and External Advisory Committee.

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Core Structures and Committees

Bioinformatics, Biostatistics, and Computational Core

The Bioinformatics, Biostatistics, and Computational Biology Core (BBCC) of the Louisiana Biomedical Research Network (LBRN) serves to train and support project investigators and their teams across Louisiana, and to lead and support translational research activities at the frontiers of biomedical science. Its team uses both established and custom computational tools, operating at computational scales ranging from the mundane to analyses engaging many hundreds of compute cores.

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Core Structures and Committees

Molecular and Cell Biology Resources Core

Molecular and cell biology provide an essential linkage among important basic fields of biomedical science, such as genetics, developmental biology, structural biology, immunology, neurobiology, and cancer biology. The MCBRC takes advantage of existing highly organized, centralized services and equipment facilities located primarily at the LSU flagship institution in Baton Rouge, effectively uniting these units toward the common goal of supporting biomedical research performed by PUI investigators. The MCBRC will provide technical and logistical support, enabling the ready exchange of information, ideas, technology, and research capabilities among PUI investigators. MCBRC will ensure that PUI researchers have full access to state-of-the-art equipment and modern research techniques and services.

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Core Structures and Committees

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