



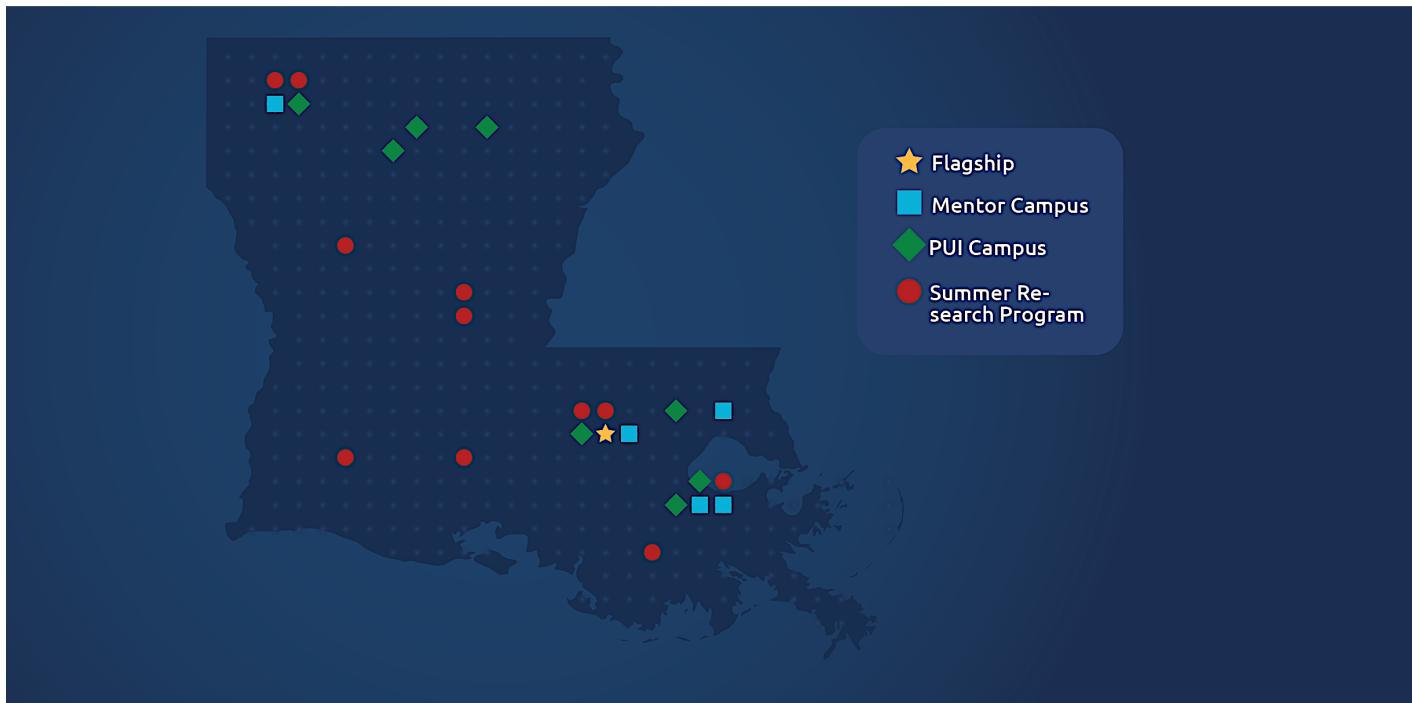
LBRN

**Louisiana Biomedical
Research Network**

Louisiana Biomedical Research Network

19th Annual Meeting

February 12 – 13, 2021



**Louisiana State University
Virtual Event
Baton Rouge, LA**

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LBRN 19th Annual Meeting
Louisiana State University
Via Zoom
February 12 & 13, 2021

| Day 1, Friday | | |
|------------------------|------------------|--|
| Time Begin | Time Ends | Event |
| 11:30 AM | Open | <i>Registration (login check)</i> |
| 11:45 AM | 12:00 PM | <i>Introduction</i> |
| 12:00 PM | 12:30 PM | AREA – R15 Overview, Dr. Alexandra Ainsztein, NIH |
| 12:30 PM | 1:30 PM | AREA - R15 Grants Panel discussion – Panel Members: Dr. Alexandra Ainsztein, NIH Dr. Eduardo Martinez-Ceballos, SUBR Dr. Hector Biliran, XULA Dr. Kevin E. Riley, XULA Dr. Sanjay Batra, SUBR Dr. Seetharama Jois, ULM Chair: Dr. Samithamby Jeyaseelan (Jey), LSU |
| 1:30 PM | 1:40 PM | Introductory Remarks, Dr. Krishan Arora, NIGMS/NIH |
| 1:40 PM | 1:55 PM | Drs. Trutschl / Nam - INBRE / COBRE Supplement, LSU-S/LSUHSC-S |
| 1:55 PM | 2:10 PM | Dr. David Mills Translational Project, LATECH |
| 2:10 PM | 2:25 PM | Dr. Jamie Newman Translational Project, LATECH |
| 2:25 PM | 2:40 PM | Dr. Seetharama Jois Translational Project, ULM, |
| 2:40 PM | 2:55 PM | Drs. Cvek/Nadejda - Maternal Health Supplement, LSU-S |
| 2:55 PM | 3:00 PM | BREAK |
| 3:00 PM | 3:30 PM | Bioinformatics Core Presentation (Christopher Taylor) |
| 3:30 PM | 4:00 PM | Molecular Biology Core Presentation (Yong-Hwan Lee) |
| 4:00 PM | 4:05 PM | Closing remarks for Day 1 |
| Day 2, Saturday | | |
| Time Begin | Time Ends | Event |
| 7:30 AM | Open | <i>Registration (Conference)</i> |
| 8:15 AM | 8:30 AM | <i>Introduction</i> |
| 8:30 AM | 9:30 AM | Keynote Talk - Dr. Ram Samudrala, Univ. at Buffalo |
| 9:30 AM | 9:50 AM | Dr. Garlapati Srinivas Full Project, ULM |
| 9:50 AM | 10:00 AM | BREAK |
| 10:00 AM | 10:20 AM | Dr. April Wright Full Project, SELU |
| 10:20 AM | 10:40 AM | Dr. Xiaoping Yi Full Project, SUBR |
| 10:40 AM | 11:00 AM | Dr. Paul Kim Full Project, GSU |
| 11:00 AM | 11:20 AM | Dr. Anup Kundu Full Project, XULA |
| 11:20 AM | 11:40 AM | Dr. Karen Zhang Full Project, XULA |
| 11:40 AM | 12:00 PM | Dr. Waneene Dorsey Full Project, GSU |
| 12:00 PM | 1:00 PM | LUNCH |
| 1:05 PM | 1:30 PM | Graduate Student Flash Talks 4 minutes each Rizwana Begum, SUBR Anne Hancock/John Neal, ULM Jolin Rodrigues, LATECH Shilpa Thota, SUBR |
| 1:40 PM | 2:25 PM | Poster Session 1, Breakout Rooms (see page 2) |
| 2:30 PM | 3:15 PM | Poster Session 2, Breakout Rooms (see page 2) |
| 3:15 PM | 3:35 PM | BREAK |
| 3:35 PM | 3:50 PM | AWARDS |
| 4:00 PM | 4:40 PM | EAC, SC, Core Directors, & Admin Mtg |

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LBRN Annual Meeting Poster Summary – iPosterSession Gallery https://lbrn2021am-lsu.ipostersessions.com/Default.aspx?s=lbrn_2021_gallery

| ID# | Sess/Rm | Name | iPoster Title | Institution |
|-----|----------|---------------------------|---|---------------|
| 1 | 1, Rm 1 | Sagun Poudel | Novel polymeric nanocarrier for oral administration of nucleic acids against colon cancer | ULM |
| 2 | 1, Rm 2 | Shilpa Thota | Pentachlorophenol mediated regulation of cannabinoid receptor-mediated signaling (in vitro) | SUBR |
| 3 | 1, Rm 3 | Rizwana Begum | Urolithins rescue e-cigarette vapor condensate induced distinct histone signatures-in vitro study | SUBR |
| 4 | 1, Rm 4 | Omer Soysal | Development of a proto-type fNIR system for measuring brain hemodynamic | SELU |
| 5 | 1, Rm 5 | Nandini Bidarimath | Molecular Chaperones and Caspase family proteins: Role and Regulation in Diesel Particulate Extract challenged cells | SUBR |
| 6 | 1, Rm 6 | Samuel Boateng | Maximizing the medicinal value of Graviola (<i>Annona Muricata</i>) in skin cancer management | ULM |
| 7 | 1, Rm 7 | Xiaoping Yi | A genome scale screen reveals differential transcription of cancer relative genes induced by FBD in prostate cancer cells | SUBR |
| 8 | 1, Rm 8 | Samuel Hickey | Hierarchical Deep-Fusion Learning for Computer Aided Detection of Tumors | SELU |
| 9 | 1, Rm 9 | Mohammad Shohel Akhter | Involvement of the unfolded protein response in the protective effects of growth hormone releasing hormone antagonists in the lungs. | ULM |
| 10 | 1, Rm 10 | Khadeja-Tul Kubra | Luminespib counteracts the Kifunensine-induced lung endothelial barrier dysfunction | ULM |
| 11 | 1, Rm 11 | Mohammad Afaz Uddin | Hsp90 inhibition protects the brain microvascular endothelium against oxidative stress | ULM |
| 12 | 1, Rm 12 | Homyra Tasnim | Investigating the FMN binding site in the mitochondrial outer membrane protein mitoNEET with FMN analogs | LSU |
| 13 | 1, Rm 13 | Kun Zhang | Effective Cancer Subtype and Stage Prediction via Dropfeature-DNNs | XULA |
| 14 | 1, Rm 14 | Phillip Kilgore | Establishing a Protocol for Activating the Massive Transfusion Protocol for Air Medical Service Trauma Patients | LSU-S |
| 15 | 1, Rm 15 | Anusha Elumalai | Making Strontium-Coated Clay Nanoparticles For Bone Regeneration | LATECH |
| 16 | 1, Rm 16 | Marjan Trutschl | Pharmacometabolomics and Pharmacoproteomics Analysis for Cardiovascular Disease | LSU-S |
| 17 | 1, Rm 17 | Camaray Rouse | Computational Binding Analysis of Human Serum Albumin with Antiviral Compound Umifenovir (Arbidol) 1,3-Diarylpyrazol-5-ones as Potential Anticancer Agents for Non Small Cell Lung Cancer: Synthesis and Cytotoxic Evaluation | LSU-S |
| 18 | 1, Rm 18 | Siva Murru | | ULM |
| 19 | 1, Rm 19 | Matthew Hayes | Unambiguous Computational Prediction of eccDNA in Cancer Genomes | XULA |
| 20 | 1, Rm 20 | Urska Cvek | Substance Abuse Trends in North Louisiana Young Women of Child Birth Age and Children | LSU-S |
| 21 | 1, Rm 21 | Anne Hancock | Functional Annotation and Comparative Analysis of Two <i>Gordonia terrae</i> Phages - Dexdert (Cluster DE3) and Schwartz33 (Cluster DJ) | ULM |
| 22 | 1, Rm 22 | Duaa Alawad | Reconstructing gene regulatory network for the differentiation of hematopoietic stem cells | UNO |
| 23 | 1, Rm 23 | Emily Meaney | The Influence of MED12 Knockdown on Adipogenesis | LATECH |
| 24 | 1, Rm 24 | Md Wasi Ul Kabir | An Improved Machine Learning Method to Predict the Backbone Torsion Angle Fluctuations from a Protein Sequence | UNO |
| 25 | 2, Rm 1 | Tithi Roy | Data-Driven Evaluation of New Synthetic Fisetin Analogs Identify Kinase Inhibitors with Anti-Skin Cancer Activities | ULM |
| 26 | 2, Rm 2 | Caryn Butler | Quantification of Double Minute Chromosome Touch Patterns in Hi-C Sequencing Data | XULA |
| 27 | 2, Rm 3 | Remmington Bishop | Computational-Aided Drug Discovery of Anti-Viral Therapeutics for COVID-19 | LSU-S |
| 28 | 2, Rm 4 | Antwine McFarland | Design of a Novel Antimicrobial/Antiviral Filtration System | LATECH |
| 29 | 2, Rm 5 | John Cart | Notch Signaling Plays a Key Role in Regulating Adult Stem Cell Osteogenic Differentiation | LATECH |
| 30 | 2, Rm 6 | Lauren Griffin-Scudari | Expression vectors for expression of Human HPRT and LDH variant in recombinant E. coli | SELU |
| 31 | 2, Rm 7 | Anup Kundu | Targeted Delivery of Doxorubicin Liposomes for Her-2+ Breast Cancer Treatment | XULA |
| 32 | 2, Rm 8 | Abubakar Abdulkadir | Diesel Particulate Extract induces Cannabinoid Receptors mediated Signaling: an in silico and in vitro study | SUBR |
| 33 | 2, Rm 9 | April Wright | RevKnitR: An integration of Bayesian phylogenetics with the R programming environment | SELU |
| 34 | 2, Rm 10 | William Yu | Surface Enhanced Fluorescence of Metal Nanostructures | LSU-S |
| 35 | 2, Rm 11 | Vonny Salim | In-Silico Analysis for Characterization of Biosynthetic Genes from Anticancer Alkaloid-producing Medicinal Plants | LSU-S |
| 36 | 2, Rm 12 | Jean Christopher Chamcheu | Topically applied fisetin ameliorates psoriasisform dermatitis in Balb/c mice | ULM |
| 37 | 2, Rm 13 | Achyut Dahal | Conformationally Constrained Multicyclic Grafted Peptidomimetic as an Immunomodulator in Rheumatoid Arthritis | ULM |
| 38 | 2, Rm 14 | Matthew Overturf | Autism Spectrum Disorder in Zebrafish (<i>Danio rerio</i>) after Exposure to Four Organophosphate Pesticides | ULM |
| 39 | 2, Rm 15 | Paul Kim | TTR overexpression in HepG2 cells: secretion vs retention? | GSU |
| 40 | 2, Rm 16 | Jafrin Jobayer | Novel pH-Sensitive Liposome Formulation of Peptidomimetic-Doxorubicin Conjugate for Enhanced, Site Specific and Targeted Delivery of Anticancer Conjugate on HER2 Positive Lung and Breast Cancer | ULM |
| 41 | 2, Rm 17 | Emmanuel Williams | Elevated Oxygen Consumption Rate in Response to Acute Low-Glucose Stress: Metformin Restores Rate | SUBR |
| 42 | 2, Rm 18 | Rami Al-Horani | Inhibition of FXIIIa by Sulfonated Molecules as Potential Avenue to Novel Anticoagulants | XULA |
| 43 | 2, Rm 19 | Joseph Chaney | Understanding the Role of the Conformational Changes in the Kinesin-5 on Processivity and Inhibition | XULA |
| 44 | 2, Rm 20 | Taylor Austin | Comparison of Differential Gene Expression in Cultured Human Tissue exposed to Human Rhinovirus 16 and Carbamate/Organophosphate Pesticides | GSU |
| 45 | 2, Rm 21 | Derrick Mullins | Simulating Double Minute Chromosomes using Java | XULA |
| 46 | 2, Rm 22 | Devika Dua | Using Machine Learning to Discover Factors Impacting Healthcare Insurance Coverage | CCHS - Ruston |
| 47 | 2, Rm 23 | Jolin Rodrigues | Design of an Arbidol-based antiviral compound library for virtual screening against SARS-CoV-2 | LATECH |

LBRN 19th Annual Meeting



Alexandra Ainsztein, Ph.D. Program Director at The National Institutes of Health

Alexandra Ainsztein, Ph.D., is a program director in the Division of Genetics and Molecular, Cellular, and Developmental Biology. She administers research grants in the areas of the cytoskeleton, and membrane trafficking. She is the NIGMS point of contact for the Academic Research Enhancement Awards (AREA) (R15) program, and the Collaborative Program Grant for Multidisciplinary Teams (RM1).

Ainsztein is a biochemist and cell biologist whose research focused on the microtubule cytoskeleton, centromeres, and cytokinesis. Prior to joining NIGMS, she served as a scientific review officer in the NIH Center for Scientific Review from 2001-2010. At NIGMS she has managed a portfolio on membrane trafficking and organelle biogenesis; she was both the program director and scientific liaison for several grants in the NIGMS Protein Structure Initiative; and has managed the Research Initiative for Scientific Enhancement (RISE program). Ainsztein earned a B.A. in biochemistry from Brandeis University and a Ph.D. in biochemistry and molecular biology from the University of Florida. She conducted postdoctoral research at Johns Hopkins University, the University of Edinburgh, and NIH's National Institute of Child Health and Human Development.

To contact Ainsztein, send email to ainsztea@mail.nih.gov or call 301-594-0943.

NIH AREA R15 grant Overview
Friday February 12th, 2021 - 12:00 pm (Central Time)



Virtual Meeting
February 12-13, 2021

Panel Discussion : NIH AREA R15 grant

Friday February 12th, 2021 - 12:30 pm (Central Time)

Panel Members:

- Dr. Alexandra Ainsztein
- Dr. Eduardo Martinez-Ceballos
- Dr. Hector Biliran
- Dr. Kevin E. Riley
- Dr. Sanjay Batra
- Dr. Seetharama Jois

Session Chair:

- Dr. Samithamby Jeyaseelan (Jey)



Panel Discussion : NIH AREA R15 grant

Friday February 12th
2021 - 12:00 pm (Central Time)

Alexandra Ainsztein, Ph.D. Program Director at The National Institutes of Health



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Panel Discussion : NIH AREA R15 grant

Friday February 12th
2021 - 12:00 pm (Central Time)



Dr. Eduardo Martinez-Ceballos is a Professor in the Department of Biological Sciences and Chemistry at Southern University, Baton Rouge. He received his Ph.D. in Cell and Molecular Biology in 2001 from Tulane University. After obtaining his degree, he worked as a Postdoctoral Researcher in the laboratory of Dr. Lorraine Gudas at the Weill Cornell Medical College in New York City. Dr. Martinez-Ceballos joined the Biology Program at Southern University in August 2007. In 2012, he became a tenured Associate Professor and was promoted to Full Professor in 2017. Since joining Southern University, Dr. Martinez-Ceballos has been fully engaged in research and has received funding from both the NIH (R15) and NSF. Currently, the main project in his laboratory focuses on the role of the Hoxa1 transcription factor on the differentiation of mouse Embryonic Stem (ES) cells along a neuroectodermal pathway. In humans, this transcription factor has been found to promote cancer progression. Thus, the long-term goal of Dr. Martinez-Ceballos' research is to elucidate and characterize the molecular mechanisms by which the Hoxa1 transcription factor exerts its function in both mouse ES cells and human cancer cells. This project is currently funded by the NSF through an Excellence in Research (EiR) grant until July of 2022. At Southern, Dr. Martinez-Ceballos has trained a number of graduate and undergraduate students in the areas of Stem Cell and Cancer research. To date, five PhD students, five Masters, and five undergraduate students have completed their thesis dissertations working under his direction. Currently, four students (graduate and undergraduate) work on different projects in his laboratory. Dr. Martinez-Ceballos expects that the results from his research will lead to a better understanding on the dual role played by Hoxa1 as director of both embryonic differentiation and cancer progression.



Panel Discussion : NIH AREA R15 grant

Friday February 12th
2021 - 12:00 pm (Central Time)

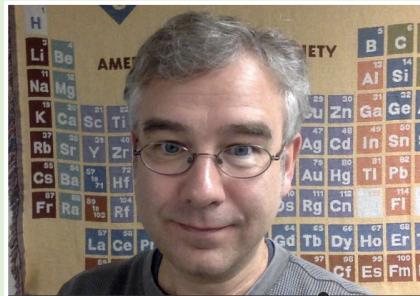


Dr. Hector Biliran is a Professor, Department of Biology, Xavier University of Louisiana, New Orleans, LA. He received his Ph.D. in the Molecular and Cellular Pathobiology program of Wayne State University, Department of Pathology, Detroit, MI in Dec., 2007. Following his graduate work, he focused on establishing his cancer research expertise on the molecular mechanisms and regulators of cancer cell survival and apoptosis. He did his post-doctoral research work in the laboratory of Dr. Erkki Ruoslahti at the NCI-designated Cancer Center, Sanford-Burnham Medical Research Institute, examining the novel Bcl2-inhibitor of transcription (Bit1) caspase-independent apoptotic pathway. Hector Biliran is an associate member of the Associate Member, American Association for Cancer Research (AACR) and Louisiana Cancer Research Consortium (LCRC). R15 CA158677-02, National Cancer Institute (NCI) - The major goal of this study is to elucidate the role of the Bit1 cell death machinery in the initiation and progression of NSCLC and as a molecular therapeutic target in lung cancer therapy. R15 CA158677-01A1, National Cancer Institute (NCI) - The goal of this project is to examine the role of Bit1 in the apoptosis resistance and survival of NSCLC cells and its potential use as a therapeutic target in alleviating NSCLC chemoresistance.



Panel Discussion : NIH AREA R15 grant

Friday February 12th
2021 - 12:00 pm (Central Time)



Dr. Kevin E. Riley is a Associate Professor of Chemistry at Xavier University of Louisiana. Dr. Riley's research is all based on computational chemistry techniques and is mainly focused on the treatment of noncovalent interactions. Noncovalent interactions play critical roles throughout Chemistry and are extremely important in protein structure, the interactions of ligands with proteins, material science, and fluid dynamics. The main focus of Dr. Riley's research is in the application of computational methods to treat noncovalent interactions in biological systems, including nucleic acids (DNA/RNA), proteins, and (especially) protein-ligand complexes. Dr. Riley is particularly interested in halogen bonds and the roles that they play in protein-ligand bonding.
1R15GM113193-01 - National Institute of General Medical Sciences (NIGMS) - The LXR α s are a nuclear receptor, exhibiting two isoforms (LXR α and LXR β) that have been demonstrated to be important mediators in a number of human diseases, including atherosclerosis, diabetes, cardiovascular disease, autoimmune disorders, Alzheimer's disease, and several types of cancer. The main goal was to conduct research, using modern computational and chemical synthetic techniques, that will lead to the development of new isoform-specific LXR agonists that selectively bind LXR β .



Panel Discussion : NIH AREA R15 grant

Friday February 12th
2021 - 12:00 pm (Central Time)



Dr. Sanjay Batra is a Professor of Environmental Toxicology at the Southern University-Baton Rouge (SUBR). Dr. Batra obtained his Ph.D. from Central Drug Research Institute, Lucknow and Kanpur University, Kanpur, India in 1993. He was selected through Union Public Service Commission of India as a Biochemist/In-charge of Clinical Biochemistry Department at Kalawati Saran Children's Hospital, New Delhi, India in 1992. In 2002, Dr. Batra came to US as a visiting scientist to work in the field of cancer and immunology at The Ohio State University, Columbus, OH. Subsequently Dr. Batra migrated to US in 2006 to pursue his advanced research career at The Ohio State University. He later worked at Texas Tech University, Amarillo, TX and Louisiana State University, Baton Rouge as a postdoctoral researcher, Senior Research Associate and as Assistant Professor (Research), respectively. Dr. Batra joined Southern University and A&M College in 2014 as an Associate Professor of Environmental Toxicology, and is currently serving as a Professor and Chair of the Department. Dr. Batra was able to secure funding from NIH (R15), Flight Attendant Medical Research Institute (FAMRI), Louisiana Biomedical Research Network and Southern University System Foundation during this period. His projects focus to determine the role and epigenetic regulation of autophagy mechanism, immunoproteasomes and lipid rafts during exposure to environmental pollutants. Dr. Batra has trained numerous undergraduate and graduate students, postdoctoral fellows and clinical residents. He has published over 65 original research/review articles in peer-reviewed journals. Dr. Batra has served on the review panels or as a grant reviewer for several national and international funding agencies including NIH, FAMRI, French National Cancer Institute; American University of Beirut; UK Research and Innovation (Future Leaders Fellowships), to name few.



Panel Discussion : NIH AREA R15 grant

**Friday February 12th
2021 - 12:00 pm (Central Time)**



Seetharama Jois is a Professor at the School Basic Pharm & Toxicol Sci – ULM.

Dr. Jois' research interest is to modulate the protein-protein interactions (PPI) using peptides and peptidomimetics. He has worked extensively on the design of peptide/peptidomimetic molecules to target proteins important in human diseases such as cancer and rheumatoid arthritis using computational and experimental methods. His research group is interested in structural aspects of epidermal growth factor receptor (EGFR) extracellular domains, which have important implications in cancer. He has designed novel peptidomimetics that target human epidermal growth factor receptors (EGFRs) and inhibit the dimerization of HER2 with other receptors such as EGFR and HER3. This research was supported by NCI (R15 CA188225-01A1, 2015-2019). In this project, Dr. Jois and his group investigate the molecular mechanism of inhibition of dimerization of peptides using in vitro and in vivo models of non-small cell lung cancer. Recently, he designed grafted peptides of these peptidomimetics using sunflower-trypsin inhibitors as a template to inhibit the PPI of EGFRs.

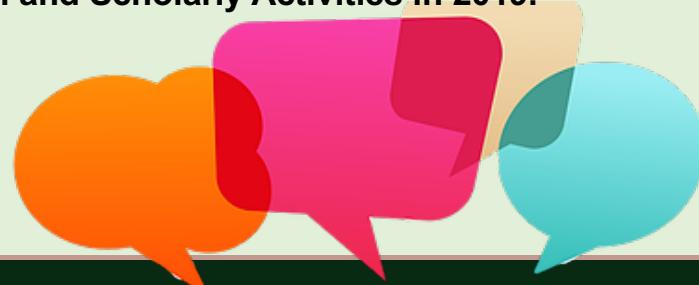


Panel Discussion : NIH AREA R15 grant

**Friday February 12th
2021 - 12:00 pm (Central Time)**



Dr. Samithamby Jeyaseelan (Jey) is the Dr. William L. Jenkins Endowed Professor and Director of COBRE Center for Lung Biology and Disease at LSU School of Veterinary Medicine (SVM). His laboratory is interested in delineating the regulatory networks in innate immunity with regard to pattern recognition receptors, transcription factors, and cytokines to determine their therapeutic potential for pharmacological intervention in the areas of lung injury and sepsis. As Principal Investigator, he has obtained funding from the NIH/NIGMS for the establishment of the Center for Lung Biology and Disease at LSU. In addition, his laboratory is continuously funded by NIH grants, such as R01s and R21s and foundations, such as Flight Attendant Medical Research Institute (FAMRI). He has more than 50 publications in high impact journals and has made more than 50 invited presentations locally, nationally, and globally. He has advised 5 research-track faculty, 11 post-doctoral fellows, 11 graduate students, 10 undergraduates and 9 summer scholars of which several have progressed to become tenure-track or tenured faculty members, pathologists, or MD/PhD students. He had served on more than 60 NIH study sections, including U19, R01, R21, P01, P42, F30, F31, F32, and R15 panels as a standing, *ad hoc* member or Co-Chair. He has appointed as the Academic Editor, Associate Editor, and Review Editor for several journals, has written more than 15 invited reviews, commentaries, and editorials, and he acts as an occasional reviewer for several top-flight journals, including *Science Translational Medicine*, *Immunity*, and *Blood*. He has been recognized as an LSU Rainmaker (Senior Scholar) for **exceptional accomplishment in Research and Scholarly Activities in 2019**.



Project Oral Presentations & Graduate Student Presentations Abstracts

Oral Presentation Abstracts

1:40 PM - 1:55 PM / Friday

Pharmacometabolomics and pharmacoproteomics analysis for cardiovascular disease

Dr. Marjan Trutschl, Marjan Trutschl, Hyung W. Nam

Louisiana State University Shreveport, Louisiana State University Shreveport and LSU Health Shreveport

Pharmaco-omics, including pharmacoproteomics and pharmacometabolomics, is a general trend of contemporary pharmacological research suggesting the use of blood biomarkers for individualized medicine strategies. Recent advances in mass spectrometry methodologies serve as powerful platforms for hypothesis generation or discovery of novel targets involved in pharmacological actions. However, outcome measurement of pharmacological treatment in humans can be challenging, due to highly complex and interconnected heterogeneous cell populations, in addition to computing and validating the large amounts of data generated. Therefore, it is required to develop bioinformatics analyses to validate raw data quality and facilitate our understanding of the protein sets of interest generated by both metabolomics and proteomics approaches.

1:55 PM - 2:10 PM / Friday

3D Printed Nanoenhanced Medical Devices for Craniofacial Repair

Dr. David Mills, Jennifer Woerner

Louisiana Tech University, LSU Health Shreveport

Metallic biomaterials are used to hold bones together, strengthen tendons and ligaments and attach them to the bone. The most commonly used screws and plates over the last few decades have been made of metals and are permanently placed at the site of implantation. As with most commercially-used biomaterials, metals and metal alloys were initially developed for non-biomedical applications and only later adopted by biomedicine. 3D printing enables the production of customized devices with the optimal size, shape, and mechanical properties. Recent advances in our lab have led to developing a 3D printing technique able to fabricate an implantable medical device capable of delivering therapeutic drugs (antibiotics, chemotherapeutics, hormones, and steroids) directly to the intended target and then degrade safely in the body. The objective of this research is to fabricate a customized drug-eluting and biodegradable orthopedic implant (using 3D printing technology and metalized halloysite nanotubes (mHNTs). Our polymer nanocomposites will couple the treatment of bone injuries while simultaneously encouraging tissue regeneration. The nanocomposites will consist of a polycaprolactone and polyethylene oxide polymer blend and a calcium phosphate cement enhanced with mHNTs. All composites will have controlled degradation coupled with mHNTs-doped with antimicrobials osteoinductive/osteogenic agents or growth factors. When implanted/inserted into bone tissue, it will facilitate disease remediation, osteogenesis, matrix formation, mineralization, and biointegration. This project will produce novel, cost-effective, and customizable medical devices to treat developmental or traumatic craniomaxillofacial defects or injuries. This project led to new research endeavors that resulted in numerous publications, an invitation to two NASA Technology competitions, two invention reports, one US Air Force contract, and five state and federal grant applications.

Oral Presentation Abstracts

2:10 PM - 2:25 PM / Friday

Comparing Treatment of Adipose Stem Cells for the Differentiation of Clinically Relevant Cells

Dr. Jamie Newman, India Pursell, Haley Barnett, John Cart, Bruce Bunnell, Mary Caldorera-Moore

Louisiana Tech University, Louisiana Tech University and Tulane University

Human adipose-derived stem cells are the easiest adult stem cells to access, harvest, and isolate, providing the largest supply of autologous stem cells for clinical application. As stem cells, hASCs have the ability to self-renew, differentiate, and suppress inflammation. These cells are being used along with other components of the stromal vascular fraction (SVF) to treat autoimmune conditions, inflammatory diseases, and specific injuries. In clinical trials, these cells are being isolated and expanded to treat a similar set of health conditions with a more targeted interest in regeneration. With the interest in using isolated stem cells in cell-based treatments and in areas of tissue engineering and regenerative medicine it is critical that we find efficient and clinically relevant methods for maintaining and differentiating stem cells. To work towards creating cells that can be reliably used in the clinic and generate functional myogenic tissue we are assessing conditions of hASCs culture in physiologically relevant environments and assessing the influence of physiologically relevant environment on cellular memory. This understanding will aid in the development of clinically relevant methods to overcome limitations currently presented for long-term culture and therapeutic use of adipose-derived stem cells. Myogenic differentiation will be assessed by examining cell morphology and expression of myogenic markers under each of the culture conditions.

2:25 PM - 2:40 PM / Friday

Immunomodulation by plant-based grafted cyclic peptides: Implications in treating chronic inflammation

Dr. Seetharama Jois, Achyut Dahal, Konstantin G Kousoulas, Seetharama Jois

University of Louisiana Monroe, University of Louisiana Monroe and Louisiana State University

The long-term goal of this project is to understand the protein-protein interactions (PPI) of cell surface molecules and inhibit these PPI to modulate cell signaling in the inflammatory response using novel stable peptide molecules. The objective is to use the sunflower trypsin inhibitor (SFTI) template to design stable peptide molecules to modulate the PPI of CD2-CD58 (CD48 in mice) adhesion/costimulatory molecular interactions. Blocking of CD2-CD58 molecule interactions results in inhibiting co-stimulatory signals required for the generation of the immune response that ensures the production of pro-inflammatory cytokines and inflammation. A newly grafted peptidomimetic (SFTI-DBF) from the SFTI template has recently been generated to inhibit the PPI of CD2-CD58 interactions. The peptidomimetic exhibited cell adhesion inhibition activity between T-cells and HFLS-RA cells with an IC₅₀ value of 3 nM. The ability of SFTI-DBF to inhibit protein-protein interaction of CD2-CD58 was evaluated by proximity ligation assay. SFTI-DBF is shown to inhibit the PPI of CD2-CD58 in a concentration-dependent manner. The peptidomimetic was able to decrease the calcium flux in T cells, indicating the ability of SFTI-DBF to modulate the T- cell-mediated immune response. To evaluate the ability of the peptidomimetic to modulate the immune response in an animal model, Collagen Induced Arthritis (CIA) model in mice was used. SFTI-DBF was able to suppress rheumatoid arthritis (RA) in the CIA model. Pharmacokinetic studies of SFTI-DBF suggested that SFTI-DBF has a terminal elimination half-life of 27 h. These studies suggest that SFTI-DBF can be developed as a potential therapeutic agent to treat autoimmune diseases such as RA. This research was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under the grant number P20GM103424-18.

Oral Presentation Abstracts

2:40 PM - 2:55 PM / Friday

Substance Abuse Trends in North Louisiana Young Women of Child Birth Age and Children

Dr. Urska Cvek, Phillip C.S.R. Kilgore(1), Marjan Trutschl(1), Nadejda Korneeva(2), Steven Conrad(3), Thomas Arnold(4)

Louisiana State University Shreveport, Louisiana State University and LSU Health Shreveport

The Emergency Department (ED) at Louisiana State University Health Sciences Center in Shreveport (LSUHSC-S) serves a predominantly minority-based urban population with a large rural catchment area. This study focuses on the demographic variables in substance abuse trends in this region based on urine drug screen (UDS) results. Detection of substance abuse disorders among ED patients can serve as a first step in drug abuse intervention. High percentage of opiate-positive and cannabinoids-positive patients is alarming, considering the addictive nature of opiates and cannabinoids. Our results reflect a common trend nationwide and in the State of Louisiana. Between 2013 and 2017, Louisiana experienced a 36% increase in drug-related deaths, more than twice the national increase. The high percentage of children testing positive for benzodiazepines raises concerns due to the adverse effects of long-term exposure to these drugs, leading to physical dependence and withdrawal. We report on our analysis of 923,528 records of UDSs of 71,311 patients of all ages and both genders for the period of 1998-2011. We present preliminary results from our data for the period of 2012-2019. One of the goals of our study is to analyze pairwise data sets of children and their mothers and we predict that this will not only yield information concerning the substance use rates in the more recent time period, but also shed light on the parent-child relationships.

9:30 AM - 9:50 AM / Saturday

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

Dr. Srinivas Garlapati, Dr. Yong-Hwan Lee

University of Louisiana Monroe, Louisiana State University

Translation initiation factor eIF4F is essential for cap-dependent translation initiation in eukaryotes. eIF4F is a trimeric complex consisting of a scaffold protein eIF4G, cap-binding protein eIF4E and DEAD-box RNA helicase eIF4A. eIF4F binds to the 5' cap structure of the mRNA through eIF4E and facilitates the binding of the preinitiation complex (PIC) via protein-protein interactions of eIF4G with eIF3 in mammals or with eIF5 in yeast. 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 with the components of the PIC. The results show that GleIF4E2 can interact with the subunit of the initiation factor GleIF2, a component of the PIC. To further confirm these interaction, Proximity dependent Biotin ligation assay was performed by expressing GleIF4E2-BirA* fusion protein in Giardia cells. Since, GleIF2beta interacts with several other initiation factors, deletion analysis is carried out to map the location of GleIF4E2 binding. The role of GleIF4A in translation initiation in Giardia is not clearly understood. Interestingly, Pateamine A, a specific inhibitor of human eIF4A, inhibited the growth of Giardia in a dose-dependent manner, suggesting that the activity of GleIF4A is probably required for translation. We further confirmed this observation using anti-sense morpholine oligos and CRISPRi. Using yeast two-hybrid assays, we have identified a novel interaction of GleIF4A with i subunit of the initiation factor GleIF3 (GleIF3i), another component of the PIC. Site-directed mutagenesis of ZDOCK predicted residues in N-terminal domain of GleIF4A disrupted its interaction with GleIF3i. To further confirm these interactions in Giardia cells, proximity dependent biotin ligation assay was performed by expressing GleIF4A-BirA* fusion protein.

Oral Presentation Abstracts

10:00 AM - 10:20 AM / Saturday

Extended models for divergence dating phylogenetic trees

Dr. April Wright, Jeremy Brown

Southeastern Louisiana University, Louisiana State University

Understanding both the relationships on the tree of life and the timing of speciation events on the tree is critical to many fields of biology, medicine, and biochemistry. Accurately modeling biological evolution is an increasingly complex process, involving modeling how molecular and specimen age data change over time. I will share insights about how to best model their data to obtain an accurate picture of deep-time evolutionary dynamics. Recent advances in methods for inferring dated phylogenetic trees, such as the fossilized birth-death process (FBD), model the extant and extinct data together as part of the same process of diversification. The FBD is typically implemented as a hierarchical Bayesian model involving a model phylogenetic character evolution, a model describing how rates of evolution are distributed across the tree, and a model of how diversification has proceeded in the focal taxa. These methods offer many advantages over older methods, such as being able to place specimens known from heterogeneous data on the tree. Despite their mathematical elegance, these models are also complex, which can make it difficult for researchers to apply them to their datasets, and evaluate their performance. Results presented in this talk will provide guidance for how to assess if a complex phylogenetic model is adequately capturing the vagaries of empirical data.

10:20 AM - 10:40 AM / Saturday

Differential transcription of genes induced by RES and FBD in prostate cancer cells.

Dr. Xiaoping Yi, Eduardo Martinez-Ceballos¹ and Konstantin Kousoulas²

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

Prostate cancer is the most common cancer among American men. Although new treatments for prostate cancer continue to be investigated, no definitive cure has been found yet for the advanced aggressive stages. Since the process of tumorigenesis involves a number of genes and proteins altering various cell signaling pathways, single-target drugs show limited efficacy and may lead to drug resistance. Resveratrol (RES) is a component of Asian traditional medicine used to treat cardiovascular diseases and appears to have many anti-tumor effects on different cancer cell types. Fenbendazole as a benzimidazole compound, is a safe and inexpensive clinically approved anthelmintic drug possessing an efficient anti-proliferative activity. But the molecular basis of these effects needs to be extensively studied using a cell culture model that best resembles the tumor environment in the body. To identify FDB and RES target genes involved in the tumorigenesis pathways, we exposed DU145 cells to different concentrations of FBD and RES and performed transcriptome analyses by RNA seq. We identified a number of genes down-regulated or up- regulated at least twofold ($P < 0.05$) in response to FBD and its combination with RES in prostate cancer cells. Ingenuity pathway analysis is in progress. This will allow us to better understand its mechanism of action and its potential use as a coadjuvant drug for established cancer treatments.

Oral Presentation Abstracts

10:40 AM - 11:00 AM / Saturday

Fluorescent turn-on probe to sense protein folding status - not seeing 2020

Dr. Paul Kim, Jacqueline Stephens

Grambling State University, Pennington Biomedical Research Center

The presence of unfolded proteins in the endoplasmic reticulum (ER stress) activates an adaptive signaling network called the unfolded protein response (UPR). Persistent UPR activation is associated with many chronic diseases. Saturated fatty acids are well known to induce ER stress and this may represent one mechanistic link between obesity and metabolic disorders. The overall goal of this project has been to better understand the mechanisms of ER stress and UPR activation. We previously demonstrated that saturated fatty acids do not alter the rates of protein synthesis or degradation in-vitro or in-vivo, suggesting that protein folding may be impaired. To explore that hypothesis, we aimed to use a probe that would sense the folding status of a target protein traveling through the ER. The probe turns on fluorescence when it binds properly folded and assembled transthyretin, a transport protein secreted by liver cells. Progress on this aim was significantly hindered by the COVID-19 pandemic, but this talk will present what work was possible.

11:00 AM - 11:20 AM / Saturday

Targeted delivery of doxorubicin liposomes for the treatment of chemoresistant breast cancer

Dr. Anup Kundu, Anup K. Kundu

Xavier University of Louisiana, Xavier University of Louisiana

The development of multidrug resistance (MDR) in cancer cells is of grave concern, limiting the efficacy of anticancer agents and, hence, the failure of breast cancer therapy. The greater potential of using doxorubicin as anticancer therapeutic depends on the availability of a targeted delivery vehicle. The goal of this study is to enhance the delivery of doxorubicin by formulating an aptamer-labeled liposomal nanoparticle delivery system that will carry and deliver doxorubicin specifically into chemoresistant Her-2+ breast cancer cells. We have recently reported that down regulating nuclear expression of MDR1 P-gp (ABCB1 gene) by P-gp specific siRNA carried by aptamer-labeled nanoparticles could increase the delivery of doxorubicin to doxorubicin resistant breast cancer cells. However, since the Dox was delivered as a free drug solution without encapsulating it into a particle for targeted delivery, it still caused toxicity to other non-cancerous cells. To address this, a targeted delivery system for doxorubicin will be developed which would enhance the killing of cancer cells as well as minimizing off-target toxicity. And a strategy needs to be in place to determine whether the targeted nanoparticles will carry both doxorubicin and siRNA within the same particles or in different particles to get the best results preventing chemoresistance and limiting off-target toxicity. Our hypothesis is that delivering doxorubicin and MDR-silencing siRNAs separately by targeted nanoparticle system will enhance the cellular toxicity and antitumor effects as compared to a targeted nanoparticle system that delivers the drug and siRNA simultaneously. The precise control of the timing of the siRNA delivery to knockdown chemoresistant genes as well as doxorubicin delivery into the chemoresistant breast cancer cells will provide invaluable findings of a co-operative effects of both siRNA and Dox delivery on chemoresistant breast cancer treatment.

Oral Presentation Abstracts

11:20 AM - 11:40 AM / Saturday

Detecting Race-Relevant Molecular Biomarkers with Clinical Utilities using Multi-omics Data across Tumor Types

Dr. Kun Zhang, Wensheng Zhang, Zhong Chen, Erik Flemington

Xavier University of Louisiana, Xavier University of Louisiana, Tulane University

Significant progress has been made in our understanding of the role of socioeconomic factors in cancer racial disparities. Increasing evidence now suggests that a number of intrinsic molecular factors specific to malignant cells must also partly account for the observed health inequalities. Although research has begun to explore the biological basis of cancer disparities, most existing work is limited to several common cancer types and does not methodically explore whether the observed genetic and molecular differences represent the clinically-meaningful racial disparities in other fatal human cancers. Moreover, massive amounts of multi-faceted omics data generated by high-throughput technologies have not been fully utilized and well integrated with clinical data to search for race-specific molecular characteristics, biomarkers or potential drug targets. The goal of this LBRN research project is to address these significant limitations by performing a data-driven, pan-cancer study to investigate the cancer-specific mutome, epigenome, and RNA-Seq transcriptome differences in different racial groups. The proposed study focuses on the eight TCGA cancer types, with pertinent cancer data from other sources being systematically utilized for methodology development and/or empirical validation throughout the entire project. For a specific cancer, in connection with clinical data, we develop new bioinformatics algorithms and pipelines to analyze these multiple types of omics data individually. As such, we establish a pan-cancer, race-relevant assemblage of coherent genes, modules and biological pathways, some of which hold significance and promise for clinical use. This study provides large-scale direct molecular-level evidence for the biological mechanism underlying racial disparities in cancer, which is practically impossible using the approaches of *in vitro*, *in vivo* and/or population follow-up. Progress made in the past year will be presented at the annual meeting.

11:40 AM - 12:00 PM / Saturday

Epigenetic Inflammatory Responses in A549 Alveolar Epithelial and HEPG2 Cells Exposed to Pentachlorophenol

Dr. Waneene Dorsey, Shilpa Thota, Sanjay Batra

Grambling State University, Southern University A&M College

Epigenetic modifications are involved in immune cell differentiation which is a primary component of the inflammatory response. Moreover, epigenetic modifications serve as conduits through which toxins or infectious agents can trigger the onset of cytokines, regulatory mediators, and specialized leukocytes. Cumulative studies have shown that pesticide exposure aggravates the immune system and augments proinflammatory cytokine activity. In this study, we used pentachlorophenol (PCP), an organochlorine pesticide, to engage the inflammatory response. PCP is a prevalent environmental contaminant because of the historical manufacturing in wood treatment plants. The risk of exposure to PCP compromises human health due the prevalence of contaminated wood treatment waste sites. We hypothesized that PCP could change epigenetic marks and mediate inflammatory responses in PCP-challenged A549 alveolar- and HepG2 cells. Data from our experiments demonstrated an increased expression of transcription factor NF- κ B and production of pro-inflammatory cytokines in HepG2 and/or A549 cells. Our results also showed that under epigenetic influence, PCP regulates histone 3 acetylation at Lys 9 and Tri-methylation at Lys 4 in A549 cells. We have shown that during DNA methylation, methyl groups can attach themselves to DNA and facilitate the activation of gene expression. Research reported in this publication was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103424-19.

Graduate Student Presentations

Urolithins rescue e-cigarette vapor condensate induced distinct histone signatures-in vitro study

Ms. Rizwana Begum, Elahe Mahdavian

Southern University, Louisiana State University Shreveport

In the last decade, the popularity of e-cigarettes (e-cigs) has exploded exponentially. A recent outbreak of vaping-related hospitalization and deaths in several US states has resulted in controversy about the earlier belief that e-cigs are safer alternates to conventional smoking. While the role of epigenetics in cigarette smoke-induced inflammation and pathologies have been reported in earlier studies, its role in regulating e-cigs vapor induced inflammation has not been explored in detail yet. In this regard, chemical modification of histone (H) proteins-particularly acetylation (ac) or methylation (me)- has been shown to play important role in several biological processes. We, therefore, hypothesized the important role of histone modifications in TF-ECVC induced inflammation. Our results showed a significant increase in cytokine/chemokine production in e-cigs vapor condensate (tobacco flavor; TF-ECVC-1%) challenged human lung adenocarcinoma cells with type II epithelial characteristics (A549). A decrease in cell viability was also observed in A549 cells challenged with TF-ECVC (>2%). Regarding epigenetic signatures, we observed an increase in histone 3-modifications (H3K9ac and H3K4me3) in our experimental groups when compared to the controls. Additionally, the analysis of transcriptional levels of associated histone acetyltransferase (PCAF) and methyltransferase (SET1) showed an increase in the later, but not the former in TF-ECVC-challenged cells. In terms of nutrvention, cells pretreated with 5 or 10 µM concentrations of ellagic acid metabolites- Urolithin A (Uro-A) or Uro-C showed significant rescue of TF-ECVC-induced histone modifications and inflammatory responses observed in our study. Overall, our findings demonstrate the possibility of epigenetically regulated inflammatory responses in TF-ECVC challenged cells which can be rescued by ellagic acid metabolites.

Functional Annotation and Comparative Analysis of Two *Gordonia terrae* Phages - Dexdert (Cluster DE3) and Schwartz33 (Cluster DJ)

Ms. Anne Hancock, John Neal, Ann M. Findley

University of Louisiana Monroe, University of Louisiana Monroe

We have successfully annotated two bacteriophages that infect the *Gordonia terrae* host. *Gordonia* phage Dexdert is a member of the DE3 cluster, has a circularly permuted genome with 55,006 bp, 82 open reading frames, and a GC content of 67.5%. Schwartz33 has 59,457 bp with a 3' sticky overhang of nine bases, 82 open reading frames, and a GC content of 67.5%. Twenty-five of the open reading frames in Dexdert code for recognizable protein gene products while the Schwartz33 genome has only twenty-three functional calls. The pBLAST analyses of the remainder of the open reading frames of both phages provide no matches to any known protein product. We provide functional annotations of these phage genomes and explore their relationship to other *Gordonia* phage clusters using pBLAST and the Phamerator visualization tool. Such analyses provide insight not only into the relationship between the *Gordonia terrae* phages but can point to extended comparisons between other Actinobacter phage group isolates.

Graduate Student Presentations

Using Computer-Aided Drug Discovery to Identify Antiviral Therapeutic Compounds Against SARS-CoV-2 - An Overview

Ms. Jolin Rodrigues, Elahe Mahdavian

Louisiana Tech University, Louisiana State University Shreveport

There is an unmet need for effective COVID19 therapeutics. In this project, we used an efficient computational aided drug discovery (CADD) methodology to identify promising drugs for COVID-19. A high resolution X-ray structural model of the spike protein-ACE-2 (6M0J) was used to identify compounds that bind to the receptor binding domain (RBD), disrupting interactions with ACE-2 and thus blocking viral entry into the human host. We also built a compound library based on arbidol, a broad-spectrum antiviral drug that functions as a viral entry inhibitor. Various computational modelling tools, including Swiss Similarity and Swiss Bioisostere, were used to identify analogs that share significant structural similarity with arbidol. We filtered out compounds with undesirable drug-like properties and those that are over-promiscuous and frequent hitters (tools: SWISS-ADME, PAINS, TEST). The compounds with the best ADMET properties were selected for virtual molecular docking experiments. Future work will include the analysis of binding modes in compound-6M0J complexes and their binding affinities to prioritize compounds for in-vitro validation. The goal to is select compounds that can serve as inhibitors of the SARS-CoV-2 viral infectivity mechanism.

Pentachlorophenol mediated regulation of cannabinoid receptor-mediated signaling (in vitro)

Ms. Shilpa Thota, Elahe Mahdavian

Southern University, Louisiana State University Shreveport

Pentachlorophenol (PCP), a restricted-use organochlorine pesticide, has been established as an environmental toxicant and Group B2 carcinogen by the United States Environmental Protection Agency. PCP is globally known for its wide-spread use in domestic, industrial, and agricultural applications. It can impact human health when inhaled, ingested, or absorbed through dermal contact. Earlier reports demonstrate that PCP-exposure results in aggravated immune responses in animal and cellular study models. Despite the available information about PCP-mediated toxicity, the molecular mechanisms have not been explored in detail. However, the role of organochlorine pesticides in disrupting endocannabinoid metabolism has been reported earlier, using DDT. This gave us the impetus to use PCP in our present study. The endocannabinoid system (ECS)-containing distinct G protein-coupled cannabinoid type 1 (CB1) and type 2 (CB2) receptors (CBR) has been implicated in regulating a wide range of cellular physiological processes, including homeostasis. The essential role of heat shock protein (HSP)90 as a molecular chaperone during CB2-mediated ERK1/2 activation; and ECS-mediated regulation of redox homeostasis has been reported in earlier studies. Therefore, we hypothesized that ECS and the downstream signaling pathways in PCP treated cells would cause an inflammatory response. Interestingly, our findings revealed transcriptional induction of CB1 and CB2 receptors in PCP-challenged human lung epithelial (A549) and human liver carcinoma (HepG2) cells. We also observed increased transcription and translation of HSP90, a molecular chaperone reported for CB2 signaling-in our study models. Regarding the downstream signaling events associated with CBR-mediated signaling, we observed PCP-mediated induction of a) MAPKs including ERK1/2; b) NADPH oxidase subunits-NCF-1 and NCF-2; and c) antioxidant enzymes-superoxide dismutase, catalase, and glutathione peroxidase in PCP-challenged cells.

Poster Session Abstracts

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1 Novel polymeric nanocarrier for oral administration of nucleic acids against colon cancer

Ms. Sagun Poudel, Seetharama Jois, George Mattheolabakis

University of Louisiana Monroe, University of Louisiana Monroe

Oral delivery of nucleic acids is challenging due to unfavorable physiological factors at the gastrointestinal tract. Some of the barriers for nucleic acid (NA) oral delivery are the acidic gastric environment, strong enzymatic activity in the intestines, and the mucus presence that make NA unable to transport and efficiently penetrate and reach the intestinal epithelial wall. We developed a novel NA nanodelivery system complexed with mannosylated PEI (Man-PEI) encapsulated in PEG-PCL matrix. We synthesized the Man-PEI to target colon cancer cells, which overexpress mannose receptors, and complexed a model NA, the pGL-3 luciferase-expressing plasmid, with Man-PEI at different N/P ratios. We transfected cancer cells *in vitro* and analyzed the luciferase expression, and analyzed the cytotoxicity of PCL-PEG nanoparticles containing Man-PEI/pGL-3 complexes, as well as the nanoparticles' capacity to protect and release NA. Man-PEI successfully complexed with the plasmid, protecting them from degradation against nucleases. Man-PEI/pGL-3 complexes transfected colon cancer cells optimally at the N/P ratio of 20:1, and the luciferase expression was significantly higher when compared to PEI alone, at 24 and 48 h. The complexes were taken up by cell lines in a time-dependent manner. Competitive transfection assay with free mannose confirmed the receptor-mediated uptake caused by targeting the mannose receptors. The PCL-PEG nanoparticles with Man-PEI/pGL-3 complexes had limited cytotoxicity. The carrier successfully protected the Man-PEI/pGL-3 complexes in a simulated gastric fluid environment and released them in a simulated intestinal fluid environment, enhanced by the presence of lipases. Such behavior would indicate a passive targeting to the small and large intestines. Hence, we can conclude that the formulated nanoparticles successfully protected the nucleic acids and can target the intestinal area and colon cancer cells.

2 Pentachlorophenol mediated regulation of cannabinoid receptor-mediated signaling (*in vitro*)

Ms. Shilpa Thota, Rizwana Begum, Waneene C Dorsey, Sanjay Batra

Southern University, Southern University, Grambling State University

Pentachlorophenol (PCP), a restricted-use organochlorine pesticide, has been established as an environmental toxicant and Group B2 carcinogen by the United States Environmental Protection Agency. PCP is globally known for its wide-spread use in domestic, industrial, and agricultural applications. It can impact human health when inhaled, ingested, or absorbed through dermal contact. Earlier reports demonstrate that PCP-exposure results in aggravated immune responses in animal and cellular study models. Despite the available information about PCP-mediated toxicity, the molecular mechanisms have not been explored in detail. However, the role of organochlorine pesticides in disrupting endocannabinoid metabolism has been reported earlier, using DDT. This gave us the impetus to use PCP in our present study. The endocannabinoid system (ECS)-containing distinct G protein-coupled cannabinoid type 1 (CB1) and type 2 (CB2) receptors (CBR) has been implicated in regulating a wide range of cellular physiological processes, including homeostasis. The essential role of heat shock protein (HSP)90 as a molecular chaperone during CB2-mediated ERK1/2 activation; and ECS-mediated regulation of redox homeostasis has been reported in earlier studies. Therefore, we hypothesized that ECS and the downstream signaling pathways in PCP treated cells would cause an inflammatory response. Interestingly, our findings revealed transcriptional induction of CB1 and CB2 receptors in PCP-challenged human lung epithelial (A549) and human liver carcinoma (HepG2) cells. We also observed increased transcription and translation of HSP90, a molecular chaperone reported for CB2 signaling-in our study models. Regarding the downstream signaling events associated with CBR-mediated signaling, we observed PCP-mediated induction of a) MAPKs including ERK1/2; b) NADPH oxidase subunits-NCF-1 and NCF-2; and c) antioxidant enzymes-superoxide dismutase, catalase, and glutathione peroxidase.

3 Urolithins rescue e-cigarette vapor condensate induced distinct histone signatures-in

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vitro study

Ms. Rizwana Begum, S. Thota, D. Kambiranda, S. Batra
Southern University, Southern University

In the last decade, the popularity of e-cigarettes (e-cigs) has exploded exponentially. A recent outbreak of vaping-related hospitalization and deaths in several US states has resulted in controversy about the earlier belief that e-cigs are safer alternates to conventional smoking. While the role of epigenetics in cigarette smoke-induced inflammation and pathologies have been reported in earlier studies, its role in regulating e-cigs vapor induced inflammation has not been explored in detail yet. In this regard, chemical modification of histone (H) proteins-particularly acetylation (ac) or methylation (me)- has been shown to play important role in several biological processes. We, therefore, hypothesized the important role of histone modifications in TF-ECVC induced inflammation. Our results showed a significant increase in cytokine/chemokine production in e-cigs vapor condensate (tobacco flavor; TF-ECVC-1%) challenged human lung adenocarcinoma cells with type II epithelial characteristics (A549). A decrease in cell viability was also observed in A549 cells challenged with TF-ECVC (>2%). Regarding epigenetic signatures, we observed an increase in histone 3-modifications (H3K9ac and H3K4me3) in our experimental groups when compared to the controls. Additionally, the analysis of transcriptional levels of associated histone acetyltransferase (PCAF) and methyltransferase (SET1) showed an increase in the later, but not the former in TF-ECVC-challenged cells. In terms of nutrvention, cells pretreated with 5 or 10 μ M concentrations of ellagic acid metabolites- Urolithin A (Uro-A) or Uro-C showed significant rescue of TF-ECVC-induced histone modifications and inflammatory responses observed in our study. Overall, our findings demonstrate the possibility of epigenetically regulated inflammatory responses in TF-ECVC challenged cells which can be rescued by ellagic acid metabolites.

4

Development of a proto-type fNIR system for measuring brain hemodynamic
Dr. Omer Soysal, Murtaza Aslam, William Brown, Samuel Hickey, Max Cole, Benjamin Cassel, David Shockley
Southeastern Louisiana University, Southeastern Louisiana University, Louisiana State University

Understanding the link between brain function and behavior is crucial to addressing neurological disorders. In this respect, developing tools that can measure the dynamics of the brain's activities plays an important role. In this study, we aim to build an fNIR (functional near infrared) signal detection and recording system to be used for brain activity recognition. First, we develop a simulator to measure effectiveness of the system. The system is composed of a pump to circulate the fluid at a specified rate, the pipes to mimic vessels, the dye capsules which are sensitive to a certain wavelength, the NIR light source, and optical detector. The system is to be shown effective if it detects a chain of the capsules filled with different die combinations. We tested the effectiveness of the system at different depth and flow rates using different optical detectors.

5

Molecular Chaperones and Caspase family proteins: Role and Regulation in Diesel Particulate Extract challenged cells
Ms. Nandini Bidarimath, Bidarimath, N., A.S Abdulkadir, S. Thota, R. Begum, S. Batra
Southern University, Southern University

An extensive exposure to the emissions from the diesel engine motors, non-road equipment in agriculture and industrial center is posing major threat to pulmonary health. These emissions include benzene, chrysene formaldehyde, nitrous oxide, and several other organic and inorganic chemical substances. Diesel particulate matter/extract (DPM/DPE) can cause immunomodulatory effects, leading to major health hazard. However, as per our literature review, only scant information is available regarding the characterization and the role of diesel particulate matter components and their deleterious effects on lung. Earlier studies suggest important role of heat shock proteins (HSPs; molecular chaperones) in maintaining cellular protein homeostasis/cell viability in response to wide array of stimulants. In this regard, HSP27 has been shown to regulate caspase-3 activation in human monocytes.

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We, therefore, hypothesize important role of HSP family proteins in DPE-mediated inflammation and apoptosis. We are focusing to investigate the role of HSPs in regulating caspase family proteins and inflammatory mediators in DPE-challenged cells using *in situ* and *in vitro* approach. Using *in situ* approach, we observed a possible crosstalk between HSP90, caspase-8 and caspase 3-in presence of DPE-components chrysene and benzene. Our *in vitro* experiments provide evidence about the possible induction of HSP90, caspase-8 and caspase-3 at transcriptional and/or translational level in DPE-challenged alveolar epithelial cells with type -II characteristics (A549). Further studies are in progress to determine translational and post-translational regulation of molecular chaperones and caspase-family proteins; and possible molecular interactions between the members of two protein families-in DPE-challenged cells. In brief, our findings will be helpful in identifying specific biomarkers to design future interventional strategies aimed at mitigating the harmful effects of environmental pollutants.

6 Maximizing the medicinal value of Graviola (*Annona Muricata*) in skin cancer management

Mr. Samuel Boateng, T Roy¹, RN Chamcheu¹, S Banang-Mbeumi¹, J Fotei², JC Chamcheu¹

University of Louisiana Monroe, University of Louisiana Monroe, Southeastern Louisiana University

Graviola, an evergreen plant of the Annonaceae family, is used both as food and in alternative medicine practice for the management several human disease including cancers, owing to the diversity of rich phytochemical agents like tannins, flavonoids, saponins, alkaloids, steroids, acetogenins, and polyphenols. Skin cancers is the most common cancers in the United States, reported to affect one fifth Americans in their lifetime with an annual financial burden of \$8.1 billion. These chronic ailments and the preeminent role their compelling trigger; UV or sunlight plays in the cosmos, precludes their one-time cure hence requires long-term treatment regime and monitoring. This makes the utility of agents that are available in plants with anticancer effects as alternative chemotherapies since nutraceuticals have minimal or no side-effects. Here in this project, the anti-proliferative properties of extracts derived from graviola plant material using soxhlet apparatus in 3 separate solvents namely, hexane, dichloromethane (DCM) and methanol were studied against melanoma (A375) and non-melanoma (A431) skin cancer cell-lines. The most pharmacologically active solvent extracts which was identified, DCM (GRMB), exerted potent anti-proliferative activity with an average IC₅₀ value of 38.46 μ g/ml \pm 1.58 and 49.68 μ g/ml \pm 7.74 for A431 and A375 respectively. Further fractionation using gradient elution with solvents of varied polarity on GRMB extracts to obtain 8 sub-fractions; GRMB (1-8), identified 3 very active fractions; GRMB-4(42.3 μ g/ml \pm 7.74), GRMB-5(40.2 μ g/ml \pm 7.64) and GRMB-6(43.1 μ g/ml \pm 4.00), and 2 others; GRMB-7(55.5 μ g/ml \pm 2.24) and GRMB-8(48.4 μ g/ml \pm 4.65), with selective potency towards A375 and A431 cell-lines respectively. In summary, these preliminary data suggest the most effective solvent extraction to pursue for the isolation and characterization of the exact active molecule(s) accounting for this anticancer property.

7 A genome scale screen reveals differential transcription of cancer relative genes induced by FBD in prostate cancer cells

Dr. Xiaoping Yi, Ira Baggett¹, Sugandhi Muthyalu¹, Eduardo Martinez-Ceballos¹, Konstantin Kousoulas²

Southern University, Southern University , Louisiana State University

Since the process of tumorigenesis involves a number of genes and proteins altering various cell signaling pathways. single-target drugs show limited efficacy and may lead to drug resistance. Prostate cancer is the most common cancer among American men. Although new treatments for prostate cancer continue to be investigated, no definitive cure has been found yet for the advanced aggressive stages. Fenbendazole as a benzimidazole compound, is a safe and inexpensive clinically approved anthelmintic drug possessing an efficient anti-proliferative activity. But the molecular basis of these effects needs to be extensively studied using a cell culture model that best resembles the tumor environment in the body. To identify FDB and target genes involved in the tumorigenesis pathways, we exposed DU145

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cells to different concentrations of and performed transcriptome analyses by RNA seq. We identified a number of genes down-regulated or up- regulated at least twofold ($P < 0.05$) in response to FBD in prostate cancer cells. This will allow us to better understand its mechanism of action and its potential use as a coadjuvant drug for established cancer treatments.

8 Hierarchical Deep-Fusion Learning for Computer Aided Detection of Tumors

Mr. Samuel Hickey, William Brown Jr., Max Cole, Omer Soysal

Southeastern Louisiana University, Southeastern Louisiana University

Lung cancer is the leading cause of mortality in men and women with cancer. Diagnosing this disease is no easy job, but with the help of computer aided detection (CAD), physicians can be confident in their decisions. The goal of this project is to create a framework which utilizes Hierarchical Deep-Fusion Learning for CAD of tumors in computed tomography (CT) scans. The model learns the parameters through supervised learning and is tested using data provided by the LIDC/IDRI database. A CT scan is observed and operated on from three perspectives, each consisting of two-dimensional images sliced from the volume of interest. By combining the decisions made on each image in a perspective, the model can determine an answer for that perspective. Through the combination of information from each perspective, the model formulates a final answer for the volume of interest.

9 Involvement of the unfolded protein response in the protective effects of growth hormone releasing hormone antagonists in the lungs.

Mr. Mohammad Shohel Akhter, Mohammad A. Uddin, Andrew V. Schally, Nektarios Barabutis

University of Louisiana Monroe, University of Louisiana Monroe, Veterans Affairs Medical Center Miami, University of Miami

Growth hormone releasing hormone (GHRH) antagonists enhance endothelial barrier function and counteract the LPS-induced lung endothelial hyper-permeability, the cardinal feature of the acute respiratory distress syndrome (ARDS). The unfolded protein response (UPR) is a multifaceted molecular mechanism, strongly involved in tissue defense against injury. The current study introduces the induction of UPR by GHRH antagonists, since those peptides induced several UPR activation markers, including the inositol-requiring enzyme-1 α (IRE1 α), the protein kinase RNA-like ER kinase (PERK), and the activating transcription factor 6 (ATF6). On the other hand, the GHRH agonist MR-409 exerted the opposite effects. Furthermore, GHRH antagonists counteracted the kifunensine (UPR suppressor)-induced lung endothelial barrier dysfunction. Our observations suggest that UPR mediates, at least in part, the protective effects of GHRH antagonists in the lung microvasculature. To the best of our knowledge; this is the first study to provide experimental evidence in support of the hypothesis that UPR induction is a novel mechanism by which GHRH antagonists oppose severe human disease, including ARDS. This study was supported by 1) R&D, Research Competitiveness Subprogram (RCS) of the Louisiana Board of Regents through the Board of Regents Support Fund (LEQSF(2019-22)-RD-A-26) (PI: N.B.), 2) The Faculty Research Support Program from the Dean's office (ULM) (PI: N.B.), and 3) The NIH/NIGMS (5 P20 GM103424-15, 3 P20 GM103424-15S1). AVS is supported by the Medical Research Service of the Department of Veterans Affairs, and University of Miami Miller School of Medicine.

10 Luminespib counteracts the Kifunensine-induced lung endothelial barrier dysfunction

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The Unfolded Protein Response (UPR) is consisted of the protein kinase RNA-like ER kinase, the activating transcription factor 6, and the inositol-requiring enzyme-1 α . It expands the endoplasmic reticulum capacity to support cellular function under stress conditions. UPR suppression by Kifunensine has been associated with lung hyperpermeability, the hallmark of Acute Respiratory Distress Syndrome (ARDS). On the other hand, heat shock protein 90 (Hsp90) inhibition triggers the

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activities of the unfolded protein response, which suggests that this molecular machinery contributes in the protective action of Hsp90 inhibitors in the lung microvasculature. We have shown that Hsp90 inhibitors suppress the LPS-induced P53 phosphorylation, protecting this transcription factor against degradation in bovine pulmonary arterial endothelial cells. Moreover, those anti-cancer compounds stabilize P53 by reducing both in vivo and in vitro MDM2 and MDM4 (P53 negative regulators). The present study investigates the effects of the Hsp90 inhibitor Luminespib (AUY-922) towards the Kifunensine-triggered lung endothelial dysfunction. Our results indicate that the UPR inducer Luminespib counteracts the effects of Kifunensine in both human and bovine lung endothelial cells. Hence, we suggest that mild UPR induction may serve as a promising therapeutic strategy against potentially lethal respiratory disorders, including the ARDS related to COVID-19.

11 Hsp90 inhibition protects the brain microvascular endothelium against oxidative stress

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The brain endothelium is an integral element of the blood-brain barrier (BBB). Dysfunction of this formation due to increased generation of reactive oxygen species (ROS) progresses the establishment of neurological disorders including stroke and traumatic brain injury. Heat shock protein 90 (Hsp90) inhibitors are anti-inflammatory agents, and their activities are mediated, at least in part, by P53. This is a tumor suppressor protein which regulates the opposing activities of Rac1 and RhoA in the cellular cytoskeleton. In the present study, we investigated the role of Hsp90 inhibitors in the H₂O₂-induced brain endothelium breakdown, by employing human cerebral microvascular endothelial cells (hCMEC/D3). Our findings suggest that H₂O₂ downregulates P53 by enhancing the P53 suppressor mouse double minute 2 homolog (MDM2), as well as by increasing the apyrimidinic endonuclease 1/redox factor 1 (APE1/Ref1). The H₂O₂-triggered violation of the brain endothelium barrier was reflected in measurements of transendothelial resistance, and the increased expression of the key cytoskeletal modulators cofilin and myosin light chain 2 (MLC2). Treatment of the hCMEC/D3 cells with Hsp90 inhibitors counteracted those events, and reduced the generation of the hydrogen peroxide-induced reactive oxygen species. Hence, our study suggests that Hsp90 inhibition supports the BBB integrity, and may represent a promising therapeutic approach for disorders associated with brain endothelium breakdown; including COVID-19. This study was supported by 1) The Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health (5 P20 GM103424-15 and 3 P20 GM103424-15S1) and 2) The R&D, Research Competitiveness Subprogram (RCS) of the Louisiana Board of Regents through the Board of Regents Support Fund (LEQSF(2019-22)-RD-A-26) to Nektarios Barabutis (PI).

12 Investigating the FMN binding site in the mitochondrial outer membrane protein mitoNEET with FMN analogs

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MitoNEET is a [2Fe-2S] cluster protein that inhabits the mitochondrial outer membrane and a key regulator of energy metabolism in human cells. In previous studies, we have demonstrated that the redox-active [2Fe-2S] clusters in the C terminal domain of mitoNEET can be reduced and oxidized by reduced flavin mononucleotide (FMNH₂) and oxygen/ubiquinone-2, respectively, implying that mitoNEET may be a novel redox enzyme catalyzing the transfer of electrons between FMNH₂ to oxygen/ubiquinone. In this study, we investigated the FMN binding site in MitoNEET utilizing FMN analogs: Lumichrome and Lumiflavin. Like FMN, lumiflavin has shown the ability to mediate redox reaction of the mitoNEET [2Fe-2S] clusters at a nanomolar concentration in the presence of flavin reductase and NADH under aerobic condition. In addition, electron paramagnetic resonance (EPR) experiments show that both lumiflavin and FMN can change the EPR spectrum of the reduced mitoNEET [2Fe-2S] clusters and form a covalently bound complex with mitoNEET under blue light

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exposure indicating specific interactions of FMN/lumiflavin with the [2Fe-2S] clusters in mitoNEET. On the other hand, lumichrome fails to mediate the redox reaction under the same experimental condition and does not affect the EPR spectrum of reduced mitoNEET [2Fe-2S] clusters on blue light; instead, it inhibits FMNH₂ mediated electron transfer via mitoNEET. Overall, these results suggest that lumichrome may act as a potential inhibitor to block the electron transfer activity of mitoNEET.

13 Effective Cancer Subtype and Stage Prediction via Dropfeature-DNNs

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Precise cancer subtype and/or stage prediction is instrumental for cancer diagnosis, treatment and management. However, most of the existing methods based on genomic profiles suffer from issues such as overfitting, high computational complexity and selected features (i.e., genes) not directly related to forecast precision. These deficiencies are largely due to the nature of "high dimensionality and small sample size" inherent in molecular data, and such a nature is often deemed as an obstacle to the application of deep learning, e.g., deep neural networks (DNNs), to biomedicine and cancer research. In this paper, we propose a DNN-based algorithm coupled with a new embedded feature selection technique, named Dropfeature-DNNs, to address these issues. Dropfeature-DNNs can discard some irrelevant features (i.e., genes) when training DNNs, and we formulate Dropfeature-DNNs as an iterative AUC optimization problem. As such, an "optimal" feature subset that contains meaningful genes for accurate tumor subtype and/or stage prediction can be obtained when the AUC optimization converges in the training stage. Since the feature subset and AUC optimizations are synchronous with the training phase of DNNs, model complexity and computational cost are simultaneously reduced. Rigorous feature subset convergence analysis and error bound inference provide a solid theoretical foundation for the proposed method. Extensive empirical comparisons to benchmark methods further demonstrate the efficacy of Dropfeature-DNNs in cancer subtype and/or stage prediction using HDSS gene expression data from multiple cancer types.

14 Establishing a Protocol for Activating the Massive Transfusion Protocol for Air Medical Service Trauma Patients

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Trauma is the leading cause of death world-wide in persons under the age of 40 and accounts for approximately 10% of all deaths in general. Massive hemorrhage is a major cause of early death in trauma patients in both civilian and military trauma care. In the initial management of trauma patients both interventions in hemostasis and proper preparation of blood products are crucial to prevent hemorrhagic shock, which can easily lead to early death. Massive Transfusion Protocols (MTPs) are initiated per established policies in many trauma centers, but too many centers still rely heavily on subjective clinical judgment of patient's initial vital signs. As familiarity with MTP triggers has increased, there is a growing interest and need in applying these in the civilian and military populations to initiate them earlier and to identify easy and fast ways to predict the need for MTP. From previous studies of MTP protocols and determined that many of them are very complex and require variables that are not available until trauma arrival and are thus not usable for air medical service and no single measurement of vital signs appeared to be a good predictor in determining the need for MTP activation. We focused on identifying a reliable and easy-to-calculate MTP trigger. Our goals were to (1) evaluate the reliability of air medical blood product transfusion as a trigger for MTP, (2) determine the reliability of air medical calculation of Shock Index (SI) as a trigger for MTP and (3) identify a rapid and simple scoring system for MTP based on a comparison across existing scoring systems.

15 Making Strontium-Coated Clay Nanoparticles For Bone Regeneration

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Use of Strontium (Sr) for bone tissue regeneration has gained research interest over the past few years due to its beneficial properties, in treating bone loss associated with osteoporosis, attributable to chemical similarities between Sr and calcium. Osteoporosis increases susceptibility to bone fracture by decreasing bone mass and increasing its fragility. Incorporating Sr nanoparticles in bone structure results in a strengthening of the bone and induces bone formation by osteoblasts and reduces bone reabsorption by osteoclasts. We hypothesized that by coating Sr on Halloysite nanotubes (HNT) a novel Strontium HNT (SrHNT) nanocomposite can be constructed having superior osteogenic capability with no toxic byproducts. These SrHNTs can be used as potential antimicrobial and osteogenic agent in calcium phosphate cement and other biomaterials. The aim of this project was to coat halloysite nanotubes (HNTs) with strontium in an eco-friendly, simple, and non-expensive process. The coating was confirmed by SEM (Scanning Electron Microscopy) and EDAX (Energy Dispersive X-Ray Spectroscopy). The cytotoxic effect of SrHNT was measured via Live Dead assay. We also tested the drug release via microtiter plate based antibacterial assay. The successfully coated Green SrHNTs, when doped in calcium phosphate cements (CPC), are predicted to increase the osteo-conductive and antibacterial properties of three dimensional (3D) printed bone.

16 Pharmacometabolomics and Pharmacoproteomics Analysis for Cardiovascular Disease

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Pharmaco-omics, including pharmacoproteomics and pharmacometabolomics, is a general trend of contemporary pharmacological research suggesting the use of blood biomarkers for individualized medicine strategies. Recent advances in mass spectrometry methodologies serve as powerful platforms for hypothesis generation or discovery of novel targets involved in pharmacological actions. However, outcome measurement of pharmacological treatment in humans can be challenging, due to highly complex and interconnected heterogeneous cell populations, in addition to computing and validating the large amounts of data generated. Therefore, it is required to develop bioinformatics analyses to validate raw data quality and facilitate our understanding of the interest protein sets generated by both, metabolomics and proteomics approaches.

17 Computational Docking Analysis of Human Serum Albumin Binding to the Antiviral Compound Arbidol

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Understanding the binding interactions of small molecule drugs with human serum albumin (HSA) protein is important in characterizing their systemic distribution and bioavailability. Arbidol is a drug candidate that has recently gained attention for its therapeutic potential against the novel SARS-CoV-2 virus. Arbidol is a broad-spectrum antiviral compound widely used in Russia and China, primarily for the treatment of influenza and acute respiratory diseases. Arbidol stabilizes the prefusion conformation of the hemagglutinin envelope protein of the flu virus, thus acting like a fusion inhibitor. SARS-CoV-2 spike protein is structurally similar to hemagglutinin, both are class-I fusion proteins. Furthermore, this virus also uses the spike protein to fuse to the host endosome through a similar mechanism. Currently, there are several ongoing clinical trials in various phases to evaluate the potential anti-viral efficacy of arbidol against the SARS-CoV-2 virus. Thus, arbidol holds promise as an anti-viral treatment for COVID-19. In this project we employ a multi-faceted computational approach, including molecular docking and dynamic simulations of arbidol-HSA binding, using Molecular Operating Environment (MOE) software. Our results provide a detailed assessment of the molecular binding interactions, binding energy, and the stability of the arbidol-HSA bound complex. We used two HSA site-specific ligands, warfarin (Sudlow site-I) and ibuprofen (Sudlow site-II), for a comparative analysis and to validate the docking protocols. Beyond experimental validation, our results also provide a framework to inform decision making for HSA-based drug delivery systems for use in future clinical applications.

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18 **1,3-Diarylpyrazol-5-ones as Potential Anticancer Agents for Non Small Cell Lung Cancer: Synthesis and Cytotoxic Evaluation**

Dr. Siva Murru, Huu Vo, Achyut Dahal, Mary Lo, Sitanshu S. Singh, Seetharama D. Jois
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Nitrogen heterocyclic compounds are an integral part of a huge number of natural and synthetic compounds and play important roles in the biological systems. Among those, pyrazoles and pyrazolones have shown great promise in recent years as pharmaceutical agents in medicinal chemistry. As part of our ongoing research in heterocyclic chemistry, a series of pyrazolone compounds with different substitution patterns have been synthesized using microwave reaction conditions. An evaluation of the pyrazolones in an in vitro antiproliferative activity against two NSCLC cell lines (A549 and NCIH522) showed that certain pyrazolone compounds with specific substitution patterns exhibited potent antiproliferative activities and might be promising anticancer drug candidates for further study. The details of cell cycle analysis, Western blot assay, and kinase inhibitor screening will be discussed in the presentation.

19 **Unambiguous Computational Prediction of eccDNA in Cancer Genomes**

Dr. Matthew Hayes, Angela Nguyen, Rahib Islam, Ethan Tran, Caryn Butler, Derrick Mullins, Chindo Hicks

Xavier University of Louisiana, Xavier University of Louisiana, LSU Health New Orleans

Extrachromosomal circular DNA (eccDNA) is a marker of several types of cancer, most notably in solid tumors like those from medulloblastoma. eccDNA is highly amplified and contains oncogenes, thus engendering poor prognosis in cancers derived from them. Computationally reconstructing eccDNA architectures promotes further research into studying the therapeutic impact of these oncogenic artifacts. However, reconstructing eccDNA architectures is difficult using short read sequencing in isolation because of ambiguities that exist between distinct eccDNA populations within the same tumor cell. In this study, we address the ambiguity problem by combining Hi-C sequencing data and short read whole genome shotgun sequencing data to resolve these difficult structures. Our software, called HolistIC, reconstructed eccDNA architectures at high accuracy in simulated and real cancer datasets. For addressing the eccDNA discovery problem, the study suggests that combining information from various sequencing technologies may be preferable to using short read sequencing data alone.

20 **Substance Abuse Trends in North Louisiana Young Women of Child Birth Age and Children**

Dr. Urska Cvek, Phillip C.S.R. Kilgore(1), Marjan Trutschl(1), Nadejda Korneeva(2), Steven Conrad(3), Thomas Arnold(4)

Louisiana State University Shreveport, LSU Shreveport, LSU Health Shreveport,

The Emergency Department (ED) at Louisiana State University Health Sciences Center in Shreveport (LSUHSC-S) serves a predominantly minority-based urban population with a large rural catchment area. This study focuses on the demographic variables in substance abuse trends in this region based on urine drug screen (UDS) results. Detection of substance abuse disorders among ED patients can serve as a first step in drug abuse intervention. High percentage of opiate-positive and cannabinoids-positive patients is alarming, considering the addictive nature of opiates and cannabinoids. Our results reflect a common trend nationwide and in the State of Louisiana. Between 2013 and 2017, Louisiana experienced a 36% increase in drug-related deaths, more than twice the national increase. The high percentage of children testing positive for benzodiazepines raises concerns due to the adverse effects of long-term exposure to these drugs, leading to physical dependence and withdrawal. We report on our analysis of 923,528 records of UDSs of 71,311 patients of all ages and both genders for the period of 1998-2011. We present preliminary results from our data for the period of 2012-2019. One of the goals of our study is to analyze pairwise data sets of children and their mothers and we predict that this will not only yield information concerning the substance use rates in the more recent time period, but also shed light on the parent-child relationships.

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21 Functional Annotation and Comparative Analysis of Two *Gordonia terrae* Phages - Dexdert (Cluster DE3) and Schwartz33 (Cluster DJ)

Ms. Anne Hancock, Zachary Wiggins, Zaire Bellamy, Love Moore, John Neal, Tiffany Poydras, Christopher R. Gissendanner, Ann M. Findley

University of Louisiana Monroe, University of Louisiana Monroe, Southern University, Xavier University of Louisiana

We have successfully annotated two bacteriophages that infect the *Gordonia terrae* host. *Gordonia* phage Dexdert is a member of the DE3 cluster, has a circularly permuted genome with 55,006 bp, 82 open reading frames, and a GC content of 67.5%. Schwartz33 has 59,457 bp with a 3' sticky overhang of nine bases, 82 open reading frames, and a GC content of 67.5%. Twenty-five of the open reading frames in Dexdert code for recognizable protein gene products while the Schwartz33 genome has only twenty-three functional calls. The pBLAST analyses of the remainder of the open reading frames of both phages provide no matches to any known protein product. We provide functional annotations of these phage genomes and explore their relationship to other *Gordonia* phage clusters using pBLAST and the Phamerator visualization tool. Such analyses provide insight not only into the relationship between the *Gordonia terrae* phages but can point to extended comparisons between other Actinobacter phage group isolates.

22 Reconstructing gene regulatory network for the differentiation of hematopoietic stem cells

Mrs. Duaa Alawad, Md Tamjidul Hoque

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RNA sequencing (RNA-seq) is a genomic approach for detecting and quantitative analysis of messenger RNA molecules in a biological sample; it computes biological heterogeneity across discrete cell types and continuous cell transitions. Partition-based graph abstraction (PAGA) gives an explainable graph-like map of the data manifold, based on estimating manifold partitions' connectivity. PAGA maps conserve the global topology of data, analyze data at different resolutions. Also, PAGA is used to find the abstract of the network graph, which gives us a better understanding of the network. A better understanding is essential to find the most genes that affect others to the specific clusters. We apply PAGA on hematopoietic stem cell data and infer a fundamental gene regulatory network structure. The data consists of 48 genes in 2,167 hematopoietic stem and progenitor cells (HSPCs).

23 The Influence of MED12 Knockdown on Adipogenesis

Ms. Emily Meaney, Jamie Sparkman, Emily Meaney, Joseph Straub, Sree Venigalla, Jamie Newman

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The ubiquity of obesity has increased exponentially, and the health burden of obesity-related diseases including type 2 diabetes, metabolic disorders, heart diseases, and some types of cancers is growing. Obesity is characterized by the excess accumulation of fat and adipose tissue and driven by adipogenesis, which is the process in which stem cells differentiate into adipocytes. We utilize human adipose derived stem cells (hASCs) isolated from adult fat tissue to study adipogenesis (the formation of fat tissue). This physiological potential, combined with non-invasive collection methods, make hASCs favorable in the search for new clinical stem cell treatments and for the study of cellular processes and differentiation. We are interested in understanding the function of MED12 in adipogenesis and determining its role in initiating cell type specific gene expression in hopes that this research can be used in treatments for obesity and related metabolic disorders. MED12 is a subunit of the Mediator complex kinase module that is critical in regulating cell-type specific gene expression. We have determined a decrease in MED12 leads to a decrease in adipogenesis as shown by the decrease in staining of lipid vesicles and the decrease in expression of adipogenic factors, CEPBa2, SREBP1c, and PPAR γ . This supports that MED12 does indeed play an important role in adipogenesis. We will continue to examine at what point during adipogenesis MED12 is most critical so that MED12

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may be used as a therapeutic target to control adipogenesis and treat obesity in the future.

24 An Improved Machine Learning Method to Predict the Backbone Torsion Angle Fluctuations from a Protein Sequence

Mr. Md Wasi Ul Kabir, Md Tamjidul Hoque

University of New Orleans, University of New Orleans

Protein molecules show varying degrees of flexibility throughout their three-dimensional structures. The protein backbone can be mostly defined by two torsion angles ϕ and ψ only. The backbone torsion-angle fluctuation is derived from the variation of backbone torsion angles from different NMR models. The fluctuations in the Cartesian coordinate space are used to characterize the Protein structural flexibility. The torsion-angle fluctuation is useful for protein function prediction and protein structure prediction when the torsion angles are used as restraints. This study has explored various useful features such as disorder probability, position-specific scoring matrix profiles, secondary structure probabilities, monogram, bigram, position-specific estimated energy, half-sphere exposures, and so on. Likewise, we studied Genetic Algorithm and SelectFromModel (Scikit-learn) feature selection techniques and explored some well-known machine learning methods, i.e., Extreme Gradient Boosting Regressor (XGB), Extra Tree Regressor (ETC), Light Gradient Boosting Machine Regressor (LGBM), ElasticNetCV Regressor, and Decision Tree Regressor, Convolutional Neural Network, and Long short-term memory (LSTM). We developed an ensemble-based machine learning method to effectively predict backbone torsion angle fluctuations based on sequence information only. We have found that the proposed method outperforms the state-of-the-art method.

25 Data-Driven Evaluation of New Synthetic Fisetin Analogs Identify Kinase Inhibitors with Anti-Skin Cancer Activities

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Melanoma and non-melanoma skin cancers (NMSCs), are the predominant cancers increasingly diagnosed in the United States. These aggressive conditions have been met with numerous hurdles including resistance, poor bioavailability and scar formation that impeded survival and treatment outcomes. Fisetin, a flavonoid, is a nutraceutical with anti-inflammatory and anticancer properties making it a promising hit against UV-induced and reactive oxygen species (ROS) associated skin damage. However, their clinical development is impeded by its rapid metabolic transformation. Here, a library of novel analogs of fisetin with different substituents were synthesized using microwave-assisted and characterized using spectroscopic and other analytic methods. All analogs were then assessed for their anticancer activity against human melanoma (A375) and non-melanoma skin cancer (A431) cell lines in vitro. We identify F9, and F17 as the most active compounds against A375 and A431 cell lines, with minimal effect on primary melanoma and keratinocytes. By kinase activity assay, we identified single and multi-kinase inhibitors of cancer associated targets; cyclin-dependent kinase-2 (CDK2), receptor tyrosine kinases (c-KITs), and mammalian targets of rapamycin (mTOR). Western blotting revealed a dose-dependent modulation of the skin cancer deregulated markers including CDK2 and phosphor- c-KITs, -Akt, -mTOR -p90RSK, -rS6K, -Stat3, and -ERK1/2 with the induction of expression of apoptosis-related markers caspases-3/8, Bax, Bcl-2, PARP in both cell lines. The colony formation and wound healing assay also supported the observed response. Moreover, bioinformatics analyses predicted these potent analogs F9 and F17 were superior in cell penetration properties, solubility, oral and intestinal absorption than fisetin. Our data identify novel active flavonol-analogs as promising agents for further development against skin cancers.

26 Quantification of Double Minute Chromosome Touch Patterns in Hi-C Sequencing Data

Ms. Caryn Butler, 1-Angela Nguyen, 1-Ethan Tran, 2-Matthew Hayes, 3-Chindo Hicks

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Background: Double minute chromosomes (DM) are small, circular fragments of extrachromosomal DNA. They are acentric and highly amplified. They also harbor oncogenes and genes that confer drug resistance. If DMs are reduced, this can decrease the malignancy of cancer and potentially prolong life and/or positively affect quality of life. In order to reduce DMs they must first be detected. The visualization of Hi-C sequencing data makes it possible to infer DMs based on their chromatin touch patterns. However, statistical analysis of Hi-C touch patterns can potentially reduce false positives in algorithms that predict the location of DM amplicons in Hi-C data. The purpose of this research is to statistically quantify the confidence of predicted double minute amplicons using Hi-C sequencing data.

Methods: Chromatin interactions are predicted with the GOTHiC program. The output from this program is transformed into a binary vector of 1s and 0s, with 1s being high interaction and 0s being low interaction. We use the Wald-Wolfowitz Runs Test to determine if the vector chosen to represent the double minute amplicon is in fact randomly distributed. We then compare the proportion of 1s in the chosen "DM" vector to the proportion of 1s in a "normal" vector to represent our null distribution. We then use a two proportion Z Test to determine if there are significantly more chromatin touches in the DM vector than the normal vector. **Results:** Preliminary results on a pancreatic cancer Hi-C dataset (PANC1) show that approximately 2% of bins in this dataset's DM amplicon have significant chromatin interactions throughout the genome. The normal vector, sampled from the null distribution, contained approximately 0.03% of bins with heightened interaction. This stark difference provides evidence that our method will recognize the heightened chromatin interaction for double minute amplicons. **Conclusions:** Based on preliminary data we expect to see a statistically greater number of 1s

27 Computational-Aided Drug Discovery of Anti-Viral Therapeutics for COVID-19

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The novel SARS-CoV-2 is a highly pathogenic virus and the causative agent of COVID-19 disease. Due to the lack of approved drugs for COVID-19, there is an urgent unmet medical need for new and effective therapeutics against this deadly virus. In this project we used a computational aided drug discovery (CADD) approach to rapidly identify promising drug candidates against COVID-19. Using prior knowledge of existing anti-viral drugs, we chose arbidol as a seed compound for our project. We hypothesized that arbidol and its analogs bind to the Receptor Binding Domain (RBD) of Spike protein to disrupt the viral recognition of the host ACE-2 protein and thus inhibit the first molecular event of viral entry. We used a three-pronged approach to build an arbidol-based compound library for our docking experiments. These included: I. Analogs with similar 2D/3D structures based on FP2, electrophores, spectrophores similarity metrics; II. Bioisosteric analogs informed by knowledge from prior original research; III. Bioisosteric analogs informed by knowledge from our own medicinal chemistry expertise. We chose 6M0J, the most accurate x-ray structural model of SPIKE:ACE-2, as the protein target of interest. Using virtual docking experiments of each compound with 6M0J, we prioritized compounds based on their binding interactions and affinity and selected the most promising candidates for future experimental validations.

28 Design of a Novel Antimicrobial/Antiviral Filtration System

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Louisiana Tech University, Louisiana Tech University

A novel broad-spectrum antimicrobial respiration apparatus, designed to fight bacteria, viruses, and fungi to safeguard against biological agents, is critical in halting the current pandemic's trajectory and to contain future outbreaks. We applied a simple, novel and effective electrodeposition method for coating the surfaces of halloysite nanotubes (HNTs) with metal nanoparticles (copper, silver and zinc) known to possess potent antiviral and antimicrobial properties. Metal-coated HNTs (mHNTs) were then added to polylactic acid and extruded to form a mHNT/PLA 3D printer filament. Our

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antimicrobial/antiviral mHNT/polymer composite 3D printer filament was used to fabricate a n95 style mask with an interchangeable filter with surfaces that will deactivate a virus, reduce or eliminate bacterial adhesion, preventing bacterial growth, and reducing deadly infections. The filter, made of a multilayered antimicrobial blow spun polymer and fabric, is disposable while the mask can be sanitized and reused. We will use in vitro assessment of critical clinical features and assess antibacterial growth inhibition against commonly encountered bacterial strains.

29 Notch Signaling Plays a Key Role in Regulating Adult Stem Cell Osteogenic Differentiation

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Human adipose-derived stem cells (hASCs) have significant therapeutic potential due to their ability to self-renew, differentiate down multiple lineages, and modulate the immune system. In addition to these many benefits, hASCs boast a minimally invasive harvesting procedure, making them a readily available cell source for stem cell research and tissue regeneration. Despite their broad use, very little is known about the mechanisms that control cell fate. We seek to further understand how hASCs can be used to clinically treat degenerative bone diseases by studying the mechanisms that regulate osteogenic differentiation. One way to enhance our mechanistic understanding of differentiation is through the systematic examination of the signaling pathways. The Notch signaling pathway is a highly conserved, contact dependent, cell-to-cell signaling cascade known to regulate cell state and multipotent differentiation of hASCs. This pathway consists of four unique receptors and five unique ligands. Two receptors believed to play a significant role in regulating osteogenic differentiation are Notch1 and Notch3. We are characterizing Notch1 and Notch3 expression during osteogenesis and evaluating the effect that siRNA-mediated knockdown of each receptor has on osteogenic differentiation. By studying changes in osteogenic marker expression following a reduction in Notch expression and activity, we will be able to determine how each receptor individually affects the osteogenic potential of hASCs and identify potential novel therapeutic targets to treat bone damage and loss.

30 Expression vectors for expression of Human HPRT and LDH variant in recombinant E. coli

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Southeastern Louisiana University, Southeastern Louisiana University

The goal of this project is to generate stable expression hosts for enzymes associated with malarial vectors and aerobic glycolysis in cancerous cells. The expression and isolation of these enzymes via recombinant E. coli will allow for their kinetic characterization in the presence and absence of potential small molecule inhibitors that may serve as an avenue for drug development. Vectors expressing Plasmodium HGXPRT and human IMPDH have been acquired, and the enzymes have been successfully expressed and isolated. A third vector for the expression of human HPRT has been designed, acquired, and cloned into a BL21(DE3) expression host as well. A coupled assay with H(GX)PRT and IMPDH and detecting the production of NADH at 340nm is currently being developed. It is hoped that this system can be used to test potential selective inhibitors on HGXPRT for the development of antimalarial drugs targeting the purine salvage pathway. E. coli pET-based expression vectors carrying variants of human LDH have been acquired and successfully cloned into BL21(DE3) expression hosts. This vector will allow for ready expression and purification of human LDH in order to describe the impacts of the enzyme in the development and sustainment of aerobic glycolysis in cancerous cells, also referred to as the Warburg effect. The in-house production of the variants of this enzyme will enhance the study of potential small molecule inhibitors designed to target cells undergoing aerobic glycolysis. The core of this research is the understanding of the molecular mechanisms underlying disease, and this project focuses on the integration of undergraduate student researchers at every level of project planning, experimental design, and protocol development.

31 Targeted Delivery of Doxorubicin Liposomes for Her-2+ Breast Cancer Treatment

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Dr. Anup Kundu, Chowdhury N, Chaudhry S, Hall N, Olverson G, Zhang Q, Mandal T, Dash S

Xavier University of Louisiana, Xavier University of Louisiana, Tulane University

The adverse side effects and toxicity caused by the non-targeted delivery of doxorubicin has emphasized the demand of emerging a targeted delivery system. The goal of this study is to enhance the delivery of doxorubicin by formulating an aptamer-labeled liposomal nanoparticle delivery system that will carry and deliver doxorubicin specifically into Her-2+ breast cancer cells. Twelve liposomal batches were prepared using different saturated (HSPC and DPPC) and unsaturated (POPC and DOPC) lipids by thin film hydration. The liposomes were characterized for their particle size, zeta potential, and drug encapsulation efficiency. The particles were also assessed for in vitro toxicity and DOX delivery into the breast cancer cells. The formulations, F1 through F12, had a small particle size of less than 200 nm and a high entrapment efficiency of about $88 \pm 5\%$. The best formulation, F5, had a particle size of $101 \pm 14\text{nm}$, zeta potential of $+ 5.63 \pm 0.46 \text{ mV}$, and entrapment efficiency of $\approx 93\%$. The cytotoxicity studies show that the DOX-loaded liposomal formulations are more effective in killing cancer cells than the free DOX in both MCF-7 and SKBR-3 cells. The uptake studies show a significant increase in the uptake of the aptamer-labeled liposomes (i.e., F5) by more than 60% into Her-2+ MCF-7 and SKBR-3 breast cancer cells compare to non-aptamer-labeled nanoparticles. F5 also shows ≈ 1.79 -fold increase in uptake of DOX in the Her-2+ cells compared to the Her-2- cells. This preliminary study indicates that aptamer-labeled F5 nanoparticles among several batches showed the highest uptake as well as the targeted delivery of doxorubicin into Her-2+ breast cancer cells.

32 Diesel Particulate Extract induces Cannabinoid Receptors mediated Signaling: an in silico and in vitro study

Mr. Abubakar Abdulkadir, S. Batra, S. Thota, R. Begum, N. Bidarimath

Southern University, Southern University

Diesel engine emissions are some of the most prevalent man-made pollutions in the world. Increasing use of diesel-fueled engines in the private transport sector results in high and continuous exposure of a large part of the population. Diesel particulate extract (DPE) is a complex mixture of several organic and inorganic chemical substances in solid, condensed (or liquid), and gaseous form. Exposure to diesel exhaust has been associated with multiple adverse health effects, including, but not limited to, a chronic obstructive pulmonary disorder, asthma, obesity, cardiovascular disease, and stroke. Earlier studies have demonstrated the important role of cannabinoid receptor-mediated signaling in regulating inflammatory responses. The toxins present in DPE can cause immunomodulatory effects like induction of inflammatory mediators, oxidative stress, apoptosis, and dysregulated proteostasis (also known as protein homeostasis). In this regard, we hypothesized the critical role of CB receptor-mediated signaling in DPE-induced inflammation/toxicity. A significant difficulty in the diesel particulate matter research is identifying specific components responsible for inducing inflammatory/toxic effects. Our finding using in-silico (computational modeling) showed high-binding affinities of specific DPE-components to the cannabinoid receptors. Increased transcription of cannabinoid receptors in DPE-challenged lung alveolar epithelial cells (A549) correlates well with our in-silico findings. Furthermore, we also observed DPE-induced STAT3 expression and mitogen-activated protein kinases (MAPKs), the downstream mediators of cannabinoid receptor-signaling pathways. Further studies are being planned to identify the differential responses of specific components of the particulate extract in terms of cannabinoid receptor-mediated signaling.

33 RevKnitR: An integration of Bayesian phylogenetics with the R programming environment

Dr. April Wright, Caleb Charpentier

Southeastern Louisiana University, Southeastern Louisiana University

Estimating phylogenetic trees has emerged as one of the predominant challenges in comparative biology. Phylogenetic trees provide researchers with the historical context in which traits and organisms evolved. There is abundant evidence that trying to understand trait evolution without a

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phylogenetic tree is deeply misleading. As the complexity of phylogenetic models has increased, so has the software to estimate trees. One piece of software for phylogenetics is RevBayes, which is a C++ executable. RevBayes also has an RStudio implementation. RStudio is a common way to interact with the R statistical programming language. While R is a cross-disciplinary language, it is especially common in population biology and comparative biology. In these fields the R language, upon which Rev is based, and the RStudio interface are likely to be familiar to learners. The RevKnitr interface is implemented via an R package. This package can be used stand-alone or to generate interactive reports and websites. The RevKnitr engine allows learners to run RevBayes interactively in an RStudio window. It does this by creating a cache directory and writing the Rev code to this directory. When a user runs a markdown chunk, that code is written to a script. The engine then executes the code at the command line. Each chunk is appended to the growing script. R and Rev can both be used in the RevKnitr interface. Rev can also be used to generate interactive reports and websites. The R ecosystem has extensive package infrastructure for creating websites from Markdown documents (pkgdown, blogdown), and for preparing custom books from sets of tutorials (bookdown). The RevKnitr interface is compatible with all of these tools.

34 Surface Enhanced Fluorescence of Metal Nanostructures

Dr. William Yu, Urska Cvek, Shile Huang

Louisiana State University Shreveport, Louisiana State University Shreveport

We will summarize the research efforts and outcomes in the past a few years for the synthesis and biotests of surface enhanced fluorescent metal nanoparticles for biolabeling applications.

35 In-Silico Analysis for Characterization of Biosynthetic Genes from Anticancer

Alkaloid-producing Medicinal Plants

Dr. Vonny Salim, Camaray Rouse, Zachary Ashworth, Nafay Hayat, Elahe Mahdavian, Urska Cvek

Louisiana State University Shreveport, Louisiana State University Shreveport

Camptothecin, one of the monoterpenoid indole alkaloids from medicinal plant Camptotheca acuminata has been considered as an important source of anticancer compounds. Due to low amount of alkaloid accumulation in plants, metabolic engineering has been proposed to increase their productions in recombinant systems. Functional characterization of key biosynthetic genes becomes an essential prerequisite for this engineering effort. Although large scale sequencing of various medicinal plants has accelerated the availability of genomic data, specific genes associated with the later steps of camptothecin biosynthetic pathways have not been elucidated. We aim to investigate several enzyme families, including glucosidases, cytochrome P450s, oxidases, and reductases. The functional characterization of glucosidases from our recent investigation has provided a platform to integrate the gene expression analysis, homology with biosynthetic genes in other alkaloid-producing plants and molecular modeling of substrate-enzyme binding. Further bioinformatic analysis of candidate biosynthetic genes involved in camptothecin pathways is expected to increase the efficiency of screening and detailed biochemical characterization for the ultimate goals of increased production and generating analogs of anticancer compounds.

36 Topically applied fisetin ameliorates psoriasisiform dermatitis in Balb/c mice

Dr. Jean Christopher Chamcheu, Tithi Roy¹, Samuel Boateng¹, Sergette Banang-Mbeumi¹, Roxane-Cherille Chamcheu¹, Khalid El Sayed, Anthony Walker¹, Sonika Patial², Konstantin G. Kousoulas²

University of Louisiana Monroe, University of Louisiana Monroe, Louisiana State University

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 aggressive psoriasis has remained elusive, thus the dire need to develop nutraceuticals that can inhibit target activities to benefit psoriasis treatment. We earlier reported that fisetin, a dietary polyphenolic

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ingredient, is a potent mTOR kinase inhibitor (Biochem Pharmacol.;89(3):349-60.), and recently shown it attenuates psoriasis-like features in vitro (Cells. 2019 Sep 15;8(9). pii: E1089.). Here, we examined the effect of fisetin in an imiquimod (IMQ)-induced Balb/c mouse psoriasisform dermatitis, and begun generating Myeloid-Cell Specific mTOR deficient mice for further validation of the idea. Topical application of aldara cream induced mouse psoriasisform dermatitis associated with activation of Akt/mTOR pathway components. We observed that topically applied fisetin resulted in reduction in psoriasisform features including hyperplasia, erythema, ear swelling, scaling, inflammatory mediators and phosphorylation of (Akt and mTOR) versus control mice. We are currently breeding Myeloid-Cell Specific mTOR deficient mice for used in testing fisetins' role as pathway inhibitor for psoriasis control. Validation of myeloid cell lineage mTOR deficient mice will provide useful translational data that could benefit treatment of psoriasis and other chronic skin diseases. Taken together, our data affirm suggest fisetin as a useful inhibitor of mTOR to be developed for treating psoriasis.

37 Conformationally Constrained Multicyclic Grafted Peptidomimetic as an Immunomodulator in Rheumatoid Arthritis

Mr. Achyut Dahal, Pravin Parajuli, Sitanshu S. Singh, Konstantin G Kousoulas, Seetharama Jois

University of Louisiana Monroe, University of Louisiana Monroe, Louisiana State University

Immune system mechanism can be regarded as double edge sword; one edge is for protecting our body against foreign antigens and eliminating them whereas the other edge on activation has detrimental effect leading to self-destruction of our tissues and cells. The balance towards the beneficial effect of immune system is maintained by co-stimulatory and co-inhibitory receptors expressed on T- cells and antigen presenting cell (APC).CD58 is a co-stimulatory molecule found to be over-expressed in APC in autoimmune disease like rheumatoid arthritis(RA). Inhibition of CD2-CD58 protein-protein interaction (PPI) that occurs between T-cells and APC can be a potential therapeutic intervention in treatment of such autoimmune disease. From our previous studies by alanine scanning followed by grafting on sunflower trypsin inhibitor (SFTI) we obtained a potent CD2-CD58 PPI inhibitor peptide (SFTI-AS1) with multiple conformations having an IC₅₀ of 37 nM in lymphocyte epithelial cell adhesion assay. In this study our objective is focused on conformational constraining and locking of SFTI-AS1 into a major bioactive conformer peptide. The designed peptide SFTI-DBF has been found to be conformationally locked into major single conformer evident by NMR studies. SFTI-DBF inhibited adhesion between T-cells and RA cells with an IC₅₀ of 3 nM. Binding study of SFTI-DBF with CD58 is confirmed further by molecular docking, flow cytometry and surface plasmon resonance. SFTI-DBF was able to inhibit CD2-CD58 PPI evident by Proximity Ligation Assay (PLA) and inhibits T-cell activation. SFTI-DBF was found to be stable in-vivo with half-life of 30 hours in pharmacokinetic study. In an in-vivo mice model of collagen induced arthritis, SFTI-DBF was able to significantly reduce the arthritis incidence, arthritis score and collagen antibody level. To summarize, a potent grafted peptidomimetic is designed and studied both in-vitro and in-vivo as a potential therapeutic agent for the treatment of RA.

38 Autism Spectrum Disorder in Zebrafish (*Danio rerio*) after Exposure to Four Organophosphate Pesticides

Dr. Matthew Overturf, Sarah Rogers

University of Louisiana Monroe, University of Louisiana Monroe

The objective of this study were to determine whether organophosphate pesticides altered behavior of the zebrafish (*Danio rerio*) in order to further understand the mechanism of action of autism in children when exposed to this class of pesticides. An increased association between this disease and exposure has been identified in multiple epidemiology studies. To determine if there is a correlation, 48-hour post fertilization zebrafish were exposed to chlorpyrifos, parathion, malathion, and methyl-parathion for five days at 0, 0.01, 0.1, and 1 μ M. At the end of the exposure period, animals were subjected to the following behavioral and social experiments: larvae activity, light/dark activity, startle response, and 3-

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point tracking. The two chemicals with the most significant effects on behavior and sociality were chlorpyrifos and parathion. Future studies should include alterations in the timing of exposure as well as the age at which zebrafish embryos and larvae are exposed.

39 TTR overexpression in HepG2 cells: secretion vs retention?

Dr. Paul Kim, Jacqueline Stephens

Grambling State University, Pennington Biomedical Research Center

The presence of unfolded proteins in the endoplasmic reticulum (ER stress) activates an adaptive signaling network called the unfolded protein response (UPR). Persistent UPR activation is associated with many chronic diseases. Saturated fatty acids are well known to induce ER stress and this may represent one mechanistic link between obesity and metabolic disorders. The overall goal of this project has been to better understand the mechanisms of ER stress and UPR activation. We previously demonstrated that saturated fatty acids do not alter the rates of protein synthesis or degradation in-vitro or in-vivo, suggesting that protein folding may be impaired. To explore that hypothesis, we aimed to use a probe that would sense the folding status of a target protein traveling through the ER. The probe turns on fluorescence when it binds properly folded and assembled transthyretin, a transport protein secreted by liver cells. Progress on this aim was significantly hindered by the COVID-19 pandemic, but this talk will present what work was possible.

40 Novel pH-Sensitive Liposome Formulation of Peptidomimetic-Doxorubicin Conjugate for Enhanced, Site Specific and Targeted Delivery of Anticancer Conjugate on HER2 Positive Lung and Breast Cancer

Mr. Jafrin Jobayer Sonju, Sitanshu S. Singh, Achyut Dahal, Seetharama D. Jois

University of Louisiana Monroe, University of Louisiana Monroe

Cancer treatment faces the challenge of effective and selective delivery of the cytotoxic drug to the desired site of action to minimize undesired side effects. The liposomal formulation containing targeting ligand conjugated cytotoxic drug can be an effective approach to specifically deliver chemotherapeutic drugs to cancer cells that overexpress a particular cell surface receptor. This researcher mainly focuses on the selective delivery of a peptidomimetic ligand attached doxorubicin conjugate on the HER2 positive lung and breast cancer cells carried on a pH-dependent liposomal formulation system for the enhancement of targeted anticancer treatment. The selected pH-sensitive liposome formulation showed effective pH-dependent delivery of peptidomimetic-doxorubicin conjugate in lower pH conditions mimicking tumor microenvironment (pH-6.5) compared to normal physiological conditions (pH 7.4), leading to the improvement of cell uptake. Upon selective delivery of peptidomimetic-doxorubicin conjugate to the tumor site, further specificity and treatment efficacy can be achieved to the ligand-receptor interaction of the peptidomimetic. The results suggested that the targeting ligand conjugated cytotoxic drug attached in the pH-sensitive liposomal system is a promising approach of chemotherapy and may provide a newer opportunity towards targeted anticancer therapy with the existing cytotoxic drug with enhanced efficacy as well.

41 Elevated Oxygen Consumption Rate in Response to Acute Low-Glucose Stress:

Metformin Restores Rate

Dr. Emmanuel Williams, Hazel Aberdeen

Southern University, Southern University

Advancing age is associated with gradual loss of glycemic control. Glucose levels, particularly hyperglycemia, are associated with the premature onset of many age-related diseases, including cardiovascular disease and the metabolic syndrome. A major challenge in the management of elderly patients with diabetes mellitus is preventing hypoglycemic episodes which can significantly increase morbidity and mortality. Molecular mechanisms of hypoglycemia remain unclear, but include mitochondrial dysfunction. Complex I is the most common site for mitochondrial abnormalities, representing as much as one-third of the respiratory chain deficiencies. We report an in vitro mitochondrial metabolic profile assessing short-term (up to six hours) and longer-term (12-24 hours)

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durations of low-glucose stress in C2C12 myoblasts. We observed that the anti-diabetic agent, and mitochondrial complex I inhibitor, metformin, was able to lower the elevated oxygen consumption rate during shorter-term glucose stress to levels similar to that of cells cultured in normal glucose. The "protective" effects of metformin during acute low-glucose stress also increased the cellular viability of C2C12 myoblasts. Interestingly, p49/STRAP, which is a novel SRF cofactor, was observed to increase in response to both advancing cell population doublings and in response to low-glucose stress. p49/STRAP has been shown to interact with mitochondrial complex I respiratory chain accessory subunits and to increase in expression in old age in the heart. These findings raise the possibility that metformin mediates its effect partially via p49/STRAP in C2C12 cells under conditions of low glucose stress.

42 Inhibition of FXIIIa by Sulfonated Molecules as Potential Avenue to Novel Anticoagulants

Dr. Rami Al-Horani, Srabani Kar, Madhusoodanan Mottamal
Xavier University of Louisiana, Xavier University of Louisiana

Purpose. Thrombosis remains a major public health crisis. Current treatment entails the use of anticoagulants which, despite their efficacy, are associated with significant bleeding. Thus, new approaches to safely treat thrombosis are needed. Factor XIIIa (FXIIIa) is a transglutaminase that catalyzes the last step in the coagulation process. Interestingly, venous thrombi from FXIII-deficient mice were significantly small. Studies also revealed that specific FXIIIa polymorphism protects against venous thrombosis and that heterozygous FXIII-deficient mice do not suffer from excessive bleeding. Thus, FXIIIa has been targeted to develop new anticoagulants with minimal bleeding. Few orthosteric FXIIIa inhibitors were reported, yet none was selective. We have proposed to develop allosteric inhibitors so as to achieve selectivity. Methods. A library of sulfonated molecules was screened for FXIIIa inhibition in a transglutamination assay. The effect on fibrin polymerization as well as the inhibition mechanism and selectivity were evaluated. Cellular toxicity was assessed using a proliferation assay. Molecular modeling was exploited to determine the inhibitors' putative binding site. Results. Four molecules inhibited FXIIIa with IC₅₀ of <5 μM. The inhibitors also affected fibrin polymerization. Michaelis-Menten kinetics revealed a mixed mechanism of inhibition. The best inhibitor was >200-fold selective over thrombin and factor Xa and 8-fold selective over tissue transglutaminase-2. It doubled the clotting times of human plasma but only at concentrations >700 μM. It did not affect the proliferation of three cell lines at 10 μM. Molecular modeling indicated that inhibition of FXIIIa may stem from binding to an anion-binding site involving K73, R68, K61, R56, & K54. Conclusion. The study reports two potent and potentially nonactive site inhibitors of FXIIIa belonging to two chemotypes. The inhibitors will be used in future efforts to develop effective and safer anticoagulants.

43 Understanding the Role of the Conformational Changes in the Kinesin-5 on Processivity and Inhibition

Dr. Joseph Chaney, Kingston Robinson, Jenelle DeVry, Amaya Sanders
Xavier University of Louisiana, Xavier University of Louisiana

In processive kinesins, motor domains proceed forward in a hand-over-hand stepping fashion, while performing ATP hydrolysis. Several of these biological nanomotors have been identified as very promising targets for potential cancer therapy such as kinesin-5 and kinesin-6. Their promise as clinical targets 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 dimers reveal the addition of strands to the central b-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. What has been ignored is that the docking of the NL and cover-neck to the motorhead coordinates two strand additions to the central b-sheet. During docking the NL forms two b-strands, (b9 and b10, form a beta-sheet with beta0 of the cover-neck and (beta-sheet of the central beta-sheet, respectively. These structural changes in the neck-

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linker and cover-neck of Kinesin-5 have not been reported as there is currently no dimeric structure for this protein. Thus, the importance of establishing this conformational switch in Kinesin-5 requires additional experiments for understanding and molecular validation. AIM1: Will the length of the neck-linker interfere with the coordination? To study this, we have generated inserts of three residues (DAL) into strategic positions along the neck-linker of the dimeric Kinesin-5 construct (Eg5-513). We have expressed these mutants and pursued purification in a bacterial system. Our rationale is that the introduction of (DAL) at any point of the neck-linker will initiate the start of the coil-coil. We will then test the response to inhibition to current anticancer inhibitors.

44 Comparison of Differential Gene Expression in Cultured Human Tissue exposed to Human Rhinovirus 16 and Carbamate/Organophosphate Pesticides

Ms. Taylor Austin, Waneene C. Dorsey
Grambling State University, Grambling State University

Few studies have examined transcriptomics in cytokine production caused by pesticides and viruses. Tissue injury from pesticide exposure can aggravate the innate immune system and thereby, cause the body to solicit a myriad of inflammatory responses. Similarly, a virus infection can cause the recruitment of immune regulatory mediators, invoke cytokine production, and spark other distinct inflammatory responses. In this study, we sought to compare gene expression in human cell cultures exposed to carbamate/organophosphate pesticides and the human rhinovirus, HRV16. Carbamates and organophosphates are popular insecticides used in agricultural applications and have similar mechanisms of toxicity where they inhibit the neural enzyme, acetylcholinesterase. We hypothesized that there are transcriptomic similarities mediating cytokine production caused by the human Rhinovirus and carbamate/organophosphate pesticide exposure in humans. To compare transcriptomics, we used NCBI archival data for mesenchymal stem cells treated with low doses of carbamate/organophosphate pesticides for 21 days and human trachea-bronchial cell culture treated with HRV16 for 24 hours. We employed pesticide and Rhinovirus pipeline runs to analyze our data. The Rmodel Genome GTF reference genome was used for the Homo sapiens organism and FastQ files were uploaded with pair-end reads. Data from pipeline runs demonstrated that ribosomal proteins showed more relative abundance in human tissue exposed to pesticides than to HRV16. MT genes induced by HRV16 showed more relative abundance than human tissue exposed to pesticides. We also observed that the EEF1A1 gene was the most highly activated in pesticide-treated tissue. We concluded that the HRV16 and carbamate/organophosphate pesticides activate similar genes in different tissue.

45 Simulating Double Minute Chromosomes using Java

Mr. Derrick Mullins, Matthew Hayes
Xavier University of Louisiana, Xavier University of Louisiana

Double minutes are small fragments of circular DNA. Unlike typical chromosomes, they are composed of circular fragments of DNA, up to only a few million base pairs in size and contain no centromere or telomere. They're highly amplified and formed as a byproduct of chromothripsis, or excision and circulation of genomic segments. They are known to harbor oncogenes (genes that are overexpressed) and cause cancer onset when overexpressed. This Java program simulates the evolution of double minutes using recursion, which is the repeated application calling itself. Each double minute shows start and end coordinates and the orientation of the chromosome.

46 Using Machine Learning to Discover Factors Impacting Healthcare Insurance Coverage

Ms. Devika Dua, Norman John Mapes, Brian Benson
Cedar Creek School, Cedar Creek School, Louisiana Tech University, Salubre Care LLC

This study analyzes a wide variety of factors from a health-related dataset and their correspondence with health insurance coverage. It specifically examines the central factors determining health insurance coverage discrepancy by employing machine learning algorithms that perform clustering, dimensionality reduction, decision tree models, and odds ratio computation. This study demonstrated

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that the models had a high AUC for predicting income, age, marital status, and self-rated health as the most discriminating factors and therefore can be used in minimizing discrepancy in health insurance coverage.

- 47 Design of an Arbidol-based antiviral compound library for virtual screening against SARS-CoV-2**
Ms. Jolin Rodrigues, Elahe Mahdavian
Louisiana Tech University, Louisiana State University Shreveport

In the race to identify novel therapeutics against SARS-CoV-2, we utilized highly efficient and cost-effective computer-aided drug discovery (CADD) methodology. Using prior knowledge of existing antiviral drugs, we selected Arbidol as a promising seed compound for this project. Arbidol is a non-nucleoside membrane fusion inhibitor that prevents the interaction of the influenza virus with the host cell. We hypothesized that Arbidol and its analogs bind to the Receptor Binding Domain (RBD) in spike protein-ACE2 complex, (6M0J), the crucial step in SARS-CoV-2 viral-host recognition and attachment, thus effectively blocking the viral entry mechanism. A rational drug design approach was used to build and expand the compound library based on Arbidol, thereby increasing the success rate of drug discovery. Using the Swiss Similarity tool, we screened the ChEMBL database to identify analogs that share > 85% structure similarity with Arbidol, based on fp2, electrophore, and spectrophore metrics. Using the Swiss Bioisostere tool, informed by prior original research, we identified functional group substitutions with the potential to improve Arbidol's drug response. We also designed several bioisosteric analogs, using medicinal chemistry insight to address some of Arbidol's known limitations as a drug (e.g. high rotational flexibility and poor water solubility). Furthermore, Swiss ADME and TEST tools were applied to screen for the compounds' pharmacokinetics and toxicity profiles, effectively selecting only "drug-like" compounds. In this presentation we will discuss the rational design of the compound library for our CADD project and future molecular docking experiments.

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