2021

8th Annual Louisiana Biomedical Research Network Conference on Computational Biology and Bioinformatics

Thursday, April 15
12:30 pm - 5:30 pm (CDT)

Friday, April 16
12:30 pm - 5:30 pm (CDT)

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9:00 am - 12:00 pm (CDT)

Virtual Meeting via Zoom

All Times given in Central Daylight Time Zone

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University of New Orleans
A Sequence-based Machine Learning Method to Effectively Predict DNA and RNA Binding Residues

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Louisiana Biomedical Research Network

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Session III

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The Pennsylvania State University
Herpes Simplex Viruses -- As Unique and Long-lived as their Human Hosts

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Louisiana State University School of Veterinary Medicine
ICP22 Maintains Transcriptionally Active RNA Polymerase II on the HSV-1 Genome During Lytic Infection

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Tulane University
Beyond p-Values: The Role of Statistics in Epigenetic Research

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Louisiana Biomedical Research Network

Thursday April 15, 2021 Poster Session from 4:30pm - 5:30pm CDT

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Thursday, Room #6	Derrick Mullins	Simulating Double Minute Evolution using Java	XULA
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Thursday, Room #8	Achyut Dahal	Design of Peptides as Protein-Protein Interaction Inhibitors for SARS-COV-2 and Angiotensin-Converting Enzyme2 Interaction.	ULM
Thursday, Room #9	Marjan Trutschl	Pharmacometabolomics and Pharmacoproteomics Analysis for Cardiovascular Disease	LSU-S
Thursday, Room #10	Jafrin Jobayer Sonju	pH-sensitive liposome formulation of peptidomimetic-doxorubicin conjugate for targeted delivery of anticancer conjugate on HER2 positive lung and breast cancer	ULM
Thursday, Room #11	April Wright	Discriminating among complex hierarchical models for phylogenetic inference	SELU
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Thursday, Room #13	Subhajit Chakrabarty	Seizure recognition using pattern analysis of ICA	LSU-S

Friday, April 16, 2021 Poster Session from 4:30pm - 5:30pm CDT

Session Day / Room #	Name	iPoster Title	Institution:
Friday, Room #1	Matthew Hayes	Leveraging Hi-C and Whole Genome Shotgun Sequencing for Double Minute Chromosome Discovery	XULA
Friday, Room #2	Kyle Piller	Life in the fastlane: Testing for congruence among transcriptomic signatures in model organisms	SELU
Friday, Room #3	Basanta Khakurel	Species Delimitation in Eastern Pine Snakes (Pituophis melanoleucus)	SELU
Friday, Room #4	Angela Nguyen	Cancer Genomes with eccDNA Oncogene Amplification Show Evidence of Deletion-Episome Model of Double Minute Chromosome Formation	XULA
Friday, Room #5	Aasish Rijal	A Sequence-based Machine Learning Method to effectively predict DNA and RNA Binding Residues	UNO
Friday, Room #6	Duaa Alawad	Reconstructing gene regulatory network for the differentiation of hematopoietic stem cells	UNO
Friday, Room #7	Ishita Choudhary	Compartment-specific transcriptomics of ozone-exposed murine lungs reveal sex- and cell type-associated perturbations relevant to mucoinflammatory lung diseases	LSU-BR
Friday, Room #8	Thao Vo	Vesicular and extravesicular protein signatures from the airspaces of ozone-exposed mice reflect muco-inflammatory disturbances	LSU-BR
Friday, Room #9	Chukwumaobim Nwokwu	Small RNA Sequencing and Computational Analysis Identifies Differentially Transcribed MicroRNAs that Regulate Nuclear Oxidative Damage in Human Astrocytes Exposed to Sodium Dichromate	LATECH
Friday, Room #10	Elia Brodsky	Effect of circulating PfAMA1 haplotype variants in Ghana on interaction with PfRON2 for merozoite invasion and vaccine development strategies	PineBio
Friday, Room #11	Phillip Kilgore	Augmenting Self-Organizing Maps to Depict Categorical Data	LSU-S
Friday, Room #12	Caryn Butler	Quantifying Double Minute Chromosome Touch Patterns in Hi-C Sequencing Contact Maps	XULA

OA-01 ***NIH/CIT STRIDES – Overview***
12:40 pm - 1:00 pm Dr. Todd Reilly
Thursday National Institute of Health, STRIDES Initiative

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Todd Reilly

NIH/CIT STRIDES Initiative
Chief Scientist, Percipient Consulting

NIH/CIT STRIDES - Overview

The STRIDES Initiative is a mechanism created by the NIH in an effort to support the transition to or continuation of NIH-funded, cloud-based biomedical research - this is done through access to 1) favorable pricing on cloud services, 2) an array of learning opportunities, and 3) technical consultation and direct engagement from Cloud Service Providers (CSP). In this presentation, we will discuss the STRIDES mission and the NIH- funded investigators can get involved.

OA-02 ***Transforming Biomedical Research with AWS***
1:00 pm - 1:30 pm Dr. Ankit Malhotra
Thursday Amazon Web Services

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Ankit Malhotra

Amazon Web Services (AWS)
Business development for Biomedical Research

Transforming Biomedical Research with AWS

Ankit Malhotra is the biomedical research and life sciences lead on the Amazon Web Services (AWS) Research team. At AWS, Ankit helps lower the barrier for biomedical researchers to build solutions and do their research using cloud computing. Before joining AWS, Ankit was a Staff Scientist at the Jackson Laboratory for Genomic Medicine where he led a group developing algorithms for analysis of next generation sequencing data to determine the spectrum of genetic variation in humans and how it contributes to diseases such as cancer. With a Post-Doctorate and Ph.D. in biochemistry, molecular biology, and genetics and a Master's in computer science from the University of Virginia, he has over 10 years of experience as a NIH and DoD-funded computational genomic scientist. He has authored more than 26 publications in the field with over 17000 citations.

OA-03
1:30 pm - 2:00 pm
Thursday

Powering the Open Science Flywheel
Dr. Erin Chu
Amazon Web Services

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Erin Chu

Amazon Web Services (AWS) Life Sciences Lead, Open Data

Powering the Open Science Flywheel

Herpesviruses are a widespread family of viruses. Unlike acute infections that are cleared in days or weeks, these chronic viruses are resident within an infected individual for an entire lifetime. Herpes simplex virus (HSV) lies dormant in neurons and re-appears on the skin only during intermittent periods of reactivation. This viral lifestyle makes it a particularly challenging pathogen to study in humans. This talk will highlight how the revolution of next-generation seep sequencing has revealed far more diversity and flexibility in HSV than we thought possible, and how these insights impact ongoing laboratory and clinical studies. We'll also explore how changes in human behavior are in turn re-shaping these viruses.

OA-04
2:30 pm - 3:00 pm
Thursday

Life Sciences with Google Cloud
Dr. Alexander Titus
Google Cloud

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Alexander Titus

Cloud Public Sector Strategic Business Executive

Life Sciences with Google Cloud

Alexander Titus is a strategic business executive at Google Cloud where he leads healthcare and life sciences strategy for the global public sector, as well as AI/ML applications for public sector missions. Prior to Google, Titus was the inaugural Assistant Director for Biotechnology within the Office of the Under Secretary for Defense (Research & Engineering), where he led the team developing the DoD's roadmap towards biotechnology modernization. Titus' career has woven between the private sector, public sector, and academia. Previously, he has served as an AI/ML Research Fellow on the Amazon Alexa AI team as well as in the B.Next group at the strategic investment firm In-Q-Tel, and as an Adjunct Assistant Professor of Biostatistics at Georgetown University and Biotechnology at the University of New Hampshire. Titus holds a PhD in Quantitative Biomedical Sciences from Dartmouth College, as well as a BS and BA in Biochemistry and Biology, respectively, from the University of Puget Sound.

OA-05

Multi-Cloud for Science Productivity

3:00 pm - 3:30 pm
Thursday

Dr. Ross Thomson
Google Cloud

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Ross Thomson

Google Cloud
Solutions Architect at Google

Multi-Cloud for Science Productivity

Scientific computing is an ideal candidate for cloud computing. Most institutions have some presence in the cloud. Given the variability of cloud providers (CSP) and the availability of on premise, private clouds, it is unlikely that a single CSP will meet all the needs of your institution. I present some ideas enable a multi-cloud future.

OA-06
4:00 pm - 4:20 pm
Thursday

NIH/CIT STRIDES - Training Spotlight
Mr. Matthew Gieseke
National Institute of Health, STRIDES Initiative

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Matthew Gieseke

NIH/CIT STRIDES Initiative
Cloud Instructional Development Lead at Covalent Solutions, LLC

NIH/CIT STRIDES - Training Spotlight

Matt will detail the STRIDES Training Program and the training opportunities available to NIH-funded researchers as they currently are. Matt will also provide instruction on engaging with the STRIDES Training Program.

OA-07
12:30 pm - 12:50 pm Friday

Introductory Remarks
Dr. Lakshmi Matukumalli
DRCB/NIGMS/NIH

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Lakshmi Kumar Matukumalli

NIH/NIGMS
Program director in the Networks and Development Programs Branch

Lakshmi Kumar Matukumalli, Ph.D., is a program director in the Networks and Development Programs Branch in the Division for Research Capacity Building, where

he manages grants for the IDeA Networks of Biomedical Research (INBRE), STTR Regional Technology Transfer Accelerator Hubs for IDeA States, and the Centers of Biomedical Research Excellence (COBRE) programs.

Before joining NIGMS, Matukumalli served as a program director at the National Institute of Food and Agriculture, USDA, where he managed extramural grant programs in the areas of genomics, phenomics, bioinformatics, quantitative genetics, and data sciences. Prior to that, he conducted animal genomics and bioinformatics research at the USDA Agricultural Research Service, while serving as a research faculty member at George Mason University in Virginia. Matukumalli earned M.S. degrees in biotechnology (Banaras Hindu University, Varanasi, India) and biochemical engineering (Indian Institute of Technology, New Delhi, India). He received his Ph.D. in bioinformatics and computational biology from George Mason University.

OA-08
12:50 pm - 1:50 pm
Friday

Modeling to Mitigate COVID-19 in a Large US City
Dr. Lauren Meyers
University of Texas Austin

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Lauren Ancel Meyers

University of Texas at Austin
Director, UT COVID-19 Modeling Consortium, Cooley Centennial Professor in Biology and Statistics

Modeling to Mitigate COVID-19 in a Large US City

The University of Texas COVID-19 Modeling Consortium has played a pivotal role in driving COVID-19 mitigation and public awareness in the city of Austin, Texas since March 2020. With a metropolitan population over 2.2M, Austin is the fastest growing large city in the US. Our extensive engagement with Austin's unique Executive COVID- 19 Task Force—which includes city leaders, public health officials, CEOs of all hospitals, public school superintendents and academic researchers—provides a new paradigm for action-oriented modeling. I will describe how models shaped the city's data-driven strategies for enacting and relaxing COVID measures, protecting vulnerable populations, and provisioning health care resources.

OA-09
1:50 pm - 2:25 pm
Friday

Integration of genetic and transcriptional profiles of innate cells to decipher mechanisms of TB susceptibility
Dr. Sara Suliman
Brigham and Women's Hospital

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Sara Suliman

Brigham and Women's Hospital, Division of Rheumatology, Immunity and Inflammation

Integration of genetic and transcriptional profiles of innate cells to decipher mechanisms of TB susceptibility

Most people infected with Mycobacterium tuberculosis (Mtb) never develop TB disease, suggesting host-specific risk factors for disease progression. Transcriptional profiling of samples from TB patients and Mtb-exposed controls identified innate pathways associated with progression to TB disease. However, few published studies integrate genetic variation with transcriptional profiles to decipher mechanisms of TB pathogenesis. We sought to determine how genetic polymorphisms influence expression of key innate response genes between individuals at high and low risk of progression to TB. From a prospective Peruvian cohort of household contacts of TB patients, we re-recruited fully genotyped former progressors (n=68) and non-progressors (n=67) and stored cryopreserved peripheral blood mononuclear cell samples. We generated monocyte-derived dendritic cells and macrophages by differentiating sorted monocytes in granulocyte-macrophage colony stimulating factor (GM-CSF) and interleukin 4 (IL4), or macrophage colony-stimulating factor (M-CSF), respectively. Samples were analyzed by low-input RNA-sequencing and flow cytometry. We analyzed the impact of genetic polymorphisms on expression of key target genes in an expression quantitative trait loci (eQTL) study. We identified 433 and 355 eQTL events in DCs and macrophages, respectively, 76 of which were unique to one cell type. In addition, we identified a novel interaction between a single nucleotide polymorphism rs2562754 and TB status with expression of FAH, the gene encoding for Fumaryl Acetoacetate Hydrolase, which mediates tyrosine catabolism. This eQTL analysis highlights underexplored candidate TB susceptibility pathways, which are now being functionally validated using CRISPR-based gene editing.

OA-10
2:25 pm - 2:45 pm
Friday

Leveraging Hi-C and Whole Genome Shotgun Sequencing for Double Minute Chromosome Discovery

Dr. Matthew Hayes
Xavier University of Louisiana

Double minute chromosomes are circular fragments of extrachromosomal DNA that engender cancer malignancy through oncogene amplification. Reduction of double minutes can potentially improve outcomes for cancer patients. Computational discovery of double minutes can assist in this task, but current methods for this problem rely only on whole genome sequencing data which can incorrectly determine double minute architectures due to ambiguities that arise due to shared segment intervals among distinct double minute populations. This talk presents a novel algorithm called "HolistIC" that predicts double minutes by incorporating whole genome sequencing data and Hi-C sequencing data to resolve potentially ambiguous double minute architectures. HolistIC successfully resolved ambiguous double minute architectures in simulated data. Furthermore in the sequence data of three cancer cell lines, HolistIC accurately confirmed the structure of double minutes predicted by WGS-only methods. The results demonstrate HolistIC's effectiveness in resolving potential double minute structural ambiguities which is important for developing effective therapies that target double minute chromosomes.

OA-11
3:00 pm - 3:20 pm
Friday

A Sequence-based Machine Learning Method to Effectively Predict DNA and RNA Binding Residues

Mr. Md Wasi Ul Kabir
University of New Orleans

DNA- and RNA-binding proteins play an essential role in an organism's normal life cycle. These proteins have diverse functions in various biological processes. DNA-binding proteins are crucial for DNA replication, transcription, repair, packaging, gene expression. Likewise, RNA-binding proteins are essential for post-transcriptional control of RNAs and RNA metabolism. The identification of DNA- and RNA-binding residue are essential for biological research (function annotation) and understanding many diseases' pathogenesis, yet most of the DNA- and RNA-binding proteins still need to be discovered. In this study, various properties of the protein sequences have been studied, such as amino acid composition type, Position-Specific Scoring Matrix (PSSM) values of amino acids, physicochemical properties, structural properties, torsion angles, and disorder regions. Moreover, a sliding window technique is used to extract more information from a target residue's neighbors. Finally, we proposed an optimized Light Gradient Boosting Machine (LightGBM) method to predict DNA- and RNA-binding residues. We evaluated the proposed method with independent test datasets. The results show that the method achieves Sensitivity, Mathews Correlation Coefficient (MCC), and AUC of 57.13%, 0.263, and 81.78% for the DNA-binding test set; 28.59%, 0.135, and 0.724, for the RNA-binding test set, respectively. In comparison to the state-of-the-art DRNApred method, the LightGBM method shows an improvement of 128.52%, 25.24%, 6.21%, for DNA-binding test set and 78.69%, 12.50%, and 8.19% for RNA-binding test set in terms of Sensitivity, Mathews Correlation Coefficient (MCC), and AUC metric. These results indicate that the LightGBM method outperforms the existing DRNApred method.

OA-12
3:20 pm - 4:20 pm
Friday

Systems analysis of gut microbiome influence on metabolic disease in HIV and high-risk populations

Dr. Catherine Lozupone
University of Colorado Anschutz Medical Campus

LBRN

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Catherine Lozupone

University of Colorado Denver
Associate Professor Biomedical Bioinformatics and Personalized Medicine

Systems analysis of gut microbiome influence on metabolic disease in HIV and high-risk populations

Poor metabolic health, characterized by insulin resistance and dyslipidemia, is higher in people living with HIV and has been linked with inflammation, anti-retroviral therapy (ART) drugs, and ART-associated lipodystrophy (LD). Metabolic disease is associated with gut microbiome composition outside the context of HIV but has not been deeply explored in HIV infection nor in high-risk men who have sex with men (HR-MSM), who have a highly altered gut microbiome composition. Furthermore, the contribution of increased bacterial translocation and associated systemic inflammation that has been described in HIV-positive and HR-MSM individuals has not been explored. We used a multi-omic approach to explore relationships between impaired metabolic health, defined using fasting blood markers, gut microbes, immune phenotypes and diet. Our cohort included ART- treated HIV positive MSM with and without LD, untreated HIV positive MSM, and HR-MSM. For HIV positive MSM on ART, we further explored associations with the plasma metabolome. We found that elevated plasma lipopolysaccharide binding protein (LBP) was the most important predictor of impaired metabolic health and network analysis showed that LBP formed a hub joining correlated microbial and immune predictors of metabolic disease. Taken together, our

results suggest the role of inflammatory processes linked with bacterial translocation and interaction with the gut microbiome in metabolic disease among HIV positive and negative MSM. I will also discuss informatics innovations we made while performing this analysis, including identifying and summarizing highly co-correlated features to increase power of multi'omic analysis and identifying host versus microbial origin of metabolites.

OA-13
9:10 am - 10:10 am
Saturday

Herpes simplex viruses -- as unique and long-lived as their human hosts
Dr. Moriah Szpara
Pennsylvania State Univesity

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Moriah L. Szpara

PennState University
Associate Professor of Biology and Biochemistry and Molecular Biology

Herpes simplex viruses - as unique and long-lived as their human hosts

Herpesviruses are a widespread family of viruses. Unlike acute infections that are cleared in days or weeks, these chronic viruses are resident within an infected individual for an entire lifetime. Herpes simplex virus (HSV) lies dormant in neurons, and re-appears on the skin only during intermittent periods of reactivation. This viral lifestyle makes it a particularly challenging pathogen to study in humans. This talk will highlight how the revolution of next-generation seep sequencing has revealed far more diversity and flexibility in HSV than we thought possible, and how these insights impact ongoing laboratory and clinical studies. We'll also explore how changes in human behavior are in turn re-shaping these viruses.

OA-14
10:10 am - 10:30 am
Saturday

ICP22 maintains transcriptionally active RNA Polymerase II on the HSV-1 genome during lytic infection
Dr. Claire Birkenheuer
Louisiana State University

Herpes Simplex Virus-1 (HSV-1) requires cellular RNA polymerase II (RNAPII) for transcription of its genome and efficient replication. Infected cell protein 22 (ICP22) is one of five viral proteins expressed within one hour post infection (hpi) with HSV-1. Precision Nuclear Run-on (PRO-seq) maps the location of transcribing RNAPII with strand-specific, nucleotide resolution. These features of PRO-seq overcome many limitations of ChIP like antibody target ratios, poor resolution, and lack of strand-specificity. We compared PRO-seq maps of active RNAPII in human epithelial type 2 (HeP-2) cells infected either with an ICP22 deletion HSV-1 virus (ΔICP22), or a control virus infection with a restored ICP22 orf (repair) at 3 and 6 hpi. The ΔICP22 genome had less RNAPII on the viral alpha genes 0 and 4 when compared to the repair genome at 3hpi. However, at this time RNAPII levels on the other 78 viral genes were unaffected. By 6hpi, all 80 viral genes had lost active RNAPII from the ΔICP22 genome, while d RNAPII activity had returned to the host genome. In striking contrast, the repair infection showed increased recruitment of RNAPII to the viral genome, and a further decrease in RNAPII levels on the host genome from 3 to 6 hpi. From these data we conclude ICP22 regulates transcription of the viral alpha genes 0 and 4, and over time a combined loss

of ICP22, alpha0 and alpha4 proteins inhibits RNAPII activity on the entire viral genome, while allowing it to return to host genes.

OA-15
10:45 am - 11:45 am
Saturday

Beyond p-Values: The Role of Statistics in Epigenetic Research

Dr. Michelle Lacey
Tulane University

2021 8th Annual LBRN Conference on Computational Biology and Bioinformatics

Michelle Lacey

Tulane University
Associate Professor of Mathematics

Beyond p-Values: The Role of Statistics in Epigenetic Research

A common objective in epigenetic analysis is the detection of differentially methylated regions that may be associated with variation in gene expression. For sequencing- based methods, this involves comparing two groups of samples that contain counts of methylated and unmethylated reads, and classical approaches such as logistic regression are typically employed to identify statistically significant differences. However, these algorithms largely ignore sources of both technical and biological bias and variability that violate key statistical assumptions, consequentially producing unreliable results. This talk will discuss ongoing efforts to develop improved statistical models for methylation sequencing data and will also highlight recent work with the FDA's Epigenomics Quality Control (EpiQC) Group to determine best practices for epigenetics research.

PA-01 ***Reconstructing gene regulatory network for the differentiation of hematopoietic stem cells***
Friday
Room #6

Duaa Alawad, Professor Md Tamjidul Hoque
University of New Orleans,

Single-cell RNA sequencing (scRNA-seq) is a recent technology that captures thousands of individual cells' gene expression states in a single experiment. It uncovers regulatory relationships between genes. 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. After Applying PAGA and getting the graph's abstract network, we apply GENIE3 on each node to build a small regulatory network for each cell type. The hematopoietic stem cell data is used in this research to infer a fundamental gene regulatory network structure. The data consists of 48 genes in 2,167 hematopoietic stem and progenitor cells (HSPCs)

PA-02 ***ICP22 maintains transcriptionally active RNA Polymerase II on the HSV-1 genome during lytic infection***
Thursday
Room #2

Claire Birkenheuer, Joel D. Baines
Louisiana State University, Louisiana State University

Herpes Simplex Virus-1 (HSV-1) requires cellular RNA polymerase II (RNAPII) for transcription of its genome and efficient replication. Infected cell protein 22 (ICP22) is one of five viral proteins expressed within one hour post infection (hpi) with HSV-1. Precision Nuclear Run-on (PRO-seq) maps the location of transcribing RNAPII with strand-specific, nucleotide resolution. These features of PRO-seq overcome many limitations of ChIP like antibody target ratios, poor resolution, and lack of strand-specificity. We compared PRO-seq maps of active RNAPII in human epithelial type 2 (HeP-2) cells infected either with an ICP22 deletion HSV-1 virus (ΔICP22), or a control virus infection with a restored ICP22 orf (repair) at 3 and 6 hpi. The ΔICP22 genome had less RNAPII on the viral alpha genes 0 and 4 when compared to the repair genome at 3hpi. However, at this time RNAPII levels on the other 78 viral genes were unaffected. By 6hpi, all 80 viral genes had lost active RNAPII from the ΔICP22 genome, while d RNAPII activity had returned to the host genome. In striking contrast, the repair infection showed increased recruitment of RNAPII to the viral genome, and a further decrease in RNAPII levels on the host genome from 3 to 6 hpi. From these data we conclude ICP22 regulates transcription of the viral alpha genes 0 and 4, and over time a combined loss of ICP22, alpha0 and alpha4 proteins inhibits RNAPII activity on the entire viral genome, while allowing it to return to host genes.

PA-03 ***Effect of circulating PfAMA1 haplotype variants in Ghana on interaction with PfRON2 for merozoite invasion and vaccine development strategies***
Friday
Room #10

Elia Brodsky, Benedicta A. Mensah, Elia Brodsky, Mohit Mazumder, Harpreet Kaur, Anita Ghansah
Pine BioTech, Noguchi Memorial Institute for Medical Research, University of Ghana, Pine Biotech

Apical Membrane Antigen (AMA1) - rhoptry neck protein 2 (RON2) binding is a critical interaction for Plasmodium falciparum merozoite invasion of host red blood cells. Several proposed malaria vaccine candidates designed to prevent such binding and limit merozoite entry have been studied with variable success at early in vitro and clinical trial stages. Our team analyzed PfAMA1 genomic data from Begoro and Cape Coast in Ghana collected during the peak transmission seasons over a 5-years period (2013-2017). The two towns represent parasite populations in the forest and coastal savanna ecological regions of Ghana with variable transmission rates. In our analysis we identify variable residues in positions impacting PfAMA1-PfRON2 binding. We further show that the determined haplotype variation affecting conserved regions responsible for AMA1-RON2 interaction could explain variable efficacy

observed in vaccine trials. By performing haplotype network analysis, comparing our data with MalariaGEN repository from other regions, and mapping of genomic variants onto the protein structures, we arrive at preliminary conclusions about local variation and epitope-affecting variants for consideration. The findings suggest that a combined genomic data collection with evaluation of vaccine efficacy can further enhance a comprehensive strategy for efficacious vaccine design against P. falciparum blood-stage infection in Ghana and surrounding regions. Continued genomic data collection and detailed analysis of parasite genomic data will have important consequences to inform vaccine development strategies across malaria endemic regions.

PA-04 ***Quantifying Double Minute Chromosome Touch Patterns in Hi-C Sequencing Contact Maps***
Friday
Room #12

Caryn Butler, Angela Nguyen, Ethan Tran, Matthew Hayes, Chindo Hicks
Xavier University of Louisiana, Xavier University of Louisiana, LSU Health Sciences Center New Orleans

Double minute chromosomes (DM) are small, circular fragments of highly amplified extrachromosomal DNA that harbor oncogenes (Figure 1). 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 analyses 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.

PA-05 ***Seizure recognition using pattern analysis of ICA***
Thursday
Room #13

Subhajit Chakrabarty, Marjan Trutschl, Urska Cvek
Louisiana State University Shreveport, Louisiana State University Shreveport

Introduction: Experts may identify seizures by observing spikes in electro-encephalogram (EEG) data and clinical correlation; however, that may not be data-driven entirely. Driven-driven approaches include independent component analysis (ICA) and deep learning. Objective: The objective was to examine patterns among independent components of EEG data to recognize seizures. Data sources and methods: We used publicly available data: CHB-MIT Scalp EEG Database (https://physionet.org/pn6/chbmit/). We have .edf files, signals sampled at 256 samples per second, 23 EEG signals (23x921600). Data is not denoised. Our ICA method is FastICA with various hyperparameters, such as 'symm' approach (simultaneous) and 'pow3' (kurtosis) optimization function. We empirically validate the use of a stability index, previously developed by one of the authors. Results and Significance: Though ICA is inherently inconsistent, our procedure provides consistent results. Visualization shows distinct patterns for the seizures. The 'symm' ICA approach (simultaneous) and 'pow3' (kurtosis) optimization function provides more discrimination. Conclusion: Performing ICA once is not enough! In our procedure, we do not need many iterations for convergence. We have proposed an approach that is model-free and generalizable. Future work: Our data was of epileptic seizures. We plan to perform classification of epileptic and non-epileptic seizures in future.

PA-06 ***Compartment-specific transcriptomics of ozone-exposed murine lungs reveal sex- and cell type-associated perturbations relevant to mucoinflammatory lung diseases***
Friday
Room #7

Ishita Choudhary, Ishita Choudhary, Thao Vo, Kshitiz Paudel, SonikaPatial, and Yogesh Saini
Louisiana State University, Louisiana State University

Ozone is known to cause lung injury and resident cells of the respiratory tract, i.e., epithelial cells and macrophages, respond to inhaled ozone in a variety of ways that affect their survival, morphology, and functioning. However, a complete understanding of the sex-associated and the cell type-specific gene expression changes in response to ozone exposure is still limited. Through transcriptomics, we aimed to analyze gene expression alterations and associated enrichment of biological pathways in three distinct cell type-enriched compartments of ozone-exposed

murine lungs. We sub-chronically exposed adult males and females to ozone or filtered air. RNA-Seq was performed on airway epithelium-enriched airways, parenchyma, and purified airspace macrophages. Differential gene expression and biological pathway analyses were performed and supported by cellular and immunohistochemical analyses. While a majority of differentially expressed genes (DEGs) in ozone-exposed versus air-exposed groups were common between both sexes, sex-specific DEGs were also identified in all the three tissue compartments. As compared to ozone-exposed males, ozone-exposed females had significant alterations in gene expression in three compartments. Pathways relevant to cell division and DNA repair were enriched in the ozone-exposed airways indicating ozone-induced airway injury and repair which was further supported by immunohistochemical analyses. In addition to cell division and DNA repair pathways, inflammatory pathways were also enriched within the parenchyma supporting contribution by both epithelial and immune cells. Finally, immune response and cytokine-cytokine receptor interactions were enriched in macrophages, indicating ozone-induced macrophage activation. Lastly, our analyses also revealed ozone-induced upregulation of mucoinflammation- and mucous cell metaplasia-associated pathways.

PA-07 ***Substance Abuse Trends in North Louisiana Young Women of Child Birth Age and Children***
Thursday
Room #7

Urska Cvek, Phillip C.S.R. Kilgore, Marjan Trutschl, Nadejda Korneeva, Steven A. Conrad, Thomas Arnold
Louisiana State University Shreveport, Louisiana State University Shreveport, LSU Health Sciences 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.

PA-08 ***Design of Peptides as Protein-Protein Interaction Inhibitors for SARS-COV-2 and Angiotensin-Converting Enzyme2 Interaction.***
Thursday
Room #8

Achyut Dahal, Konstantin G. Kousoulas, Ramesh Subramanian, Seetharama Jois
University of Louisiana at Monroe, Louisiana State University, University of Louisiana Monroe

Infection with the novel coronavirus, severe acute respiratory syndrome coronavirus-2(SARS-CoV-2) causes coronavirus disease (Covid-19), which is causing havoc worldwide as a global pandemic. Spike (S) glycoproteins forming the crowns on the surface of the virus have an important role in viral entry through receptor recognition and membrane fusion. S glycoprotein is present as a homotrimer in its functional form, S-protein in its monomeric unit is composed of two subunits S1 and S2. S1 subunit is involved in host recognition, whereas the S2 subunit guides fusion of the virus to the host cell membrane. S1 subunit consists of the receptor-binding domain (RBD), which is responsible for host receptor recognition and helps in the interaction of spike protein to ACE2 receptor. The ACE-2 binding interface with the RBD consists of helical and β-sheet structures forming hydrogen bonding and hydrophobic interactions. The objective of this project is to generate novel peptide molecules, which inhibit SARS-CoV-2 viral entry and virus spread. Both phenomena are mediated by the viral spike (S) glycoprotein, which is embedded in viral envelopes and expressed on infected cell surfaces, mediating entry via fusion of the viral envelope with cellular membranes and virus spread via fusion of adjacent cells and the formation of syncytia, respectively.

Based upon the crystal structure of the SARS-CoV-2 and ACE-2 complex, we designed helical and β-turn peptides targeting SARS-CoV-2 RBD, ACE2, and S2 subunit. Our preliminary docking studies on helical and β-turn peptides indicate that these peptides bind to the RBD domain of SARS-CoV-2 with docking energies of -11.91 kcal/mol and -9.7 kcal/mol and with estimated inhibition constants (Ki) of 1.9 nM and 97 nM, respectively. Thus, we believe that these peptides bind to SARS-CoV-2 with high affinity and have the potential to be developed as fusion inhibitors for Covid-19.

PA-09 Thursday Room #3 ***Comparison of Differential Gene Expression in Cultured Human Tissue Exposed to the Human Rhinovirus 16 and Carbamate/Organophosphate Pesticides***

Waneene Dorsey, Taylor Austin
Grambling State University, Grambling State University

Few studies have examined transcriptomics in cytokine production caused by pesticide and viruses. In this study, we sought to compare gene expression in human cell cultures exposed to carbamate/organophosphate pesticides and the human rhinovirus, HRV16. We hypothesized that there are transcriptomic similarities mediating cytokine production caused by the human Rhinovirus and carbamate/organophosphate pesticide exposure in humans. In our bioinformatics project, we used the NIH-National Center for Biotechnology Information 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. To compare transcriptomic similarities, we employed pesticide and Rhinovirus bioinformatics 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. Mitochondrial genes induced by HRV16 showed more relative abundance than human tissue exposed to pesticides. We concluded that the HRV16 and carbamate/ organophosphate pesticides activate similar genes but not with the same intensity.

PA-10 Thursday Room #1 ***Shotgun Metagenomic Sequencing of Vaginal Specimens Suggests Potential Involvement of Lactobacillus Phage Preceding Incident Bacterial Vaginosis***

Jacob Elnaggar, Christopher M Taylor, Evelyn Toh, Amy Dong, Kristal J Aaron, Meng Luo, Ashutosh Tamhane, Elliot J Lefkowitz,David E Nelson, Christina A Muzny
LSUHSC New Orleans, LSU Health Sciences Center New Orleans, Indiana University School of Medicine, Loyola University Chicago, University of Alabama at Birmingham

Introduction The etiology of bacterial vaginosis (BV) remains controversial. BV is the most common cause of vaginal discharge and is associated with preterm birth and increased risk sexually transmitted infections. Shotgun metagenomics, which has not been widely applied to study BV, is a next generation sequencing approach that can be used to analyze the microbiota present in a particular community. We aimed to investigate changes in vaginal microbial community composition preceding incident BV (iBV) using shotgun metagenomics. Methods African American women who have sex with women were prospectively enrolled and followed for 90 days using self-collected vaginal swabs to detect iBV. Dual-indexed sequencing libraries were constructed using the NexteraXT DNA Library preparation kit (Illumina Inc.) and sequenced on 2 lanes of an Illumina HiSeq 4000 run. Sequences were processed using Kraken2 to determine taxonomic composition. Results Vaginal specimens were sequenced from every other day collections in the 10 days leading up to iBV in 4 women. Across all women, the percentage sequencing reads classified as microbial increased substantially on the day of iBV. Reads originating from the Lactobacillus genus declined leading up to iBV while Gardnerella vaginalis, Prevotella bivia, and Atopobium vaginae increased sharply. Lactobacillus phages were also found in days leading up to iBV and steadily declined prior to iBV. This decline of Lactobacillus phages corresponded with reduction in L. crispatus, L. gasseri, and L. jensenii. Conclusion The proportion of sequencing reads classified as microbial may provide an estimate of the bacterial burden during an iBV infection. This study suggests a possible interplay between Lactobacillus phages in the development of iBV. Overall, this confirms that BV is a complex infection that may have contributions from phages, which were previously overlooked. Further investigation is required to better understand the true etiology of BV.

PA-11 ***Target genes of Hoxa1 time series sequencing; a gene regulatory network approach.***
Thursday
Room #4

Ugochi Emelogu, Yaser Banadaki, Eduardo Martinez-Ceballos
Southern University and A&M College, Southern University and A&M College

The Hoxa1 gene, a member of the homeobox family of Transcription Factors (TF), is an important regulator of embryonic development. Homeobox transcription factors control developmental processes by regulating gene expression, morphogenesis as well as behavioral and cognitive stability. In mice, Hoxa1 knockout results in developmental defects such as inner ear deficiencies, skull abnormalities, and neonatal death. In humans, HoxA1 mutations results in horizontal gaze abnormalities, central nervous system disorders, and cancer. Treatment of embryonic stem cells (ES cells) with retinoic acid (RA), which binds to the retinoic acid receptors (RARs), results in the activation of Hox genes, including Hoxa1. However, the mechanism of action of Hoxa1 is not yet known. Our strategy to understand the Hoxa1 mechanism of action is to construct the Hoxa1 gene regulatory network (GRN). For this purpose, we performed time-series analyses of mouse ES cells treated with 1μm RA for 0, 12, 24, 36, 48, and 60 hours. The RNA seq data was filtered using MATLAB. Also, information about differential gene expression was obtained from RNA sequence analysis of wild type (WT) versus knock out (KO) ES cells and control versus RA-treated. The time-series RNA seq data was then analyzed using the NARROMI algorithm implemented on MATLAB. To generate a Hoxa1-specific GRN, differential expression data from Wild Type versus Knock out cells was also input into NARROMI. For this purpose, data from TFs that were differentially expressed in ES cells were selected. The analysis by NARROMI produced a Hoxa1-related GRN with approximately 27000 nodes as it was visualized using Cytoscape. For clarity purposes, a sub-network was extracted which consists of only the 1st and 2nd Hoxa1 neighbors. NARROMI identified putative direct connections between Hoxa1 and important TFs such as Msx1, Batf3, Bbx and Hoxa5 while RNA Seq verification was done by qPCR. Our results suggest that NARROMI is a reliable algorithm to infe

PA-12 ***Leveraging Hi-C and Whole Genome Shotgun Sequencing for Double Minute Chromosome Discovery***
Friday
Room #1

Matthew Hayes, Matthew Hayes, Angela Nguyen, Rahib Islam, Caryn Butler, Ethan Tran, Derrick Mullins, Chindo Hicks
Xavier University of Louisiana, Xavier University of Louisiana, LSU Health Sciences Center New Orleans

Double minute chromosomes are acentric extrachromosomal DNA artefacts that are frequently observed in the cells of numerous cancers. They are highly amplified and contain oncogenes and drug resistance genes, making their presence a challenge for effective cancer treatment. Algorithmic discovery of double minutes (DM) can potentially improve bench-derived therapies for cancer treatment. A hindrance to this task is that DMs evolve, yielding circular chromatin that shares segments from progenitor double minutes. This creates double minutes with overlapping amplicon coordinates. Existing DM discovery algorithms use whole genome shotgun sequencing in isolation, which can potentially incorrectly classify DMs that share overlapping coordinates. In this study, we describe an algorithm called "HolistIC" that can predict double minutes in tumor genomes by integrating whole genome shotgun sequencing (WGS) and Hi-C sequencing data. The consolidation of these sources of information resolves ambiguity in double minute amplicon prediction that exists in DM prediction with WGS data used in isolation. We implemented and tested our algorithm on the tandem Hi-C and WGS datasets of three cancer datasets and a simulated dataset. Results on the cancer data sets demonstrated HolistIC's ability to predict DMs from Hi-C and WGS data in tandem. The results on the simulated data showed the HolistIC can accurately distinguish double minutes that have overlapping amplicon coordinates, an advance over methods that predict extrachromosomal amplification using WGS data in isolation.

PA-13 ***EGFR in cancer: dimers, dynamics and more.***
Thursday
Room #5

Seetharama Jois,
University of Louisiana at Monroe,

Epidermal growth factor receptors (EGFRs) are known to play a crucial role in lung cancer. Overexpression of these receptors or upon binding of ligand to these receptors leads to homo-and hetero-dimerization of these receptors. These proteins have an extracellular domain (ECD, a transmembrane helix, a cytoplasmic kinase domain, and a regulatory region. Ligand binding to EGFR or HER3 ECDs triggers a change in the conformation of the proteins, leading to their heterodimerization and, ultimately, to cell signaling. We have used modeling and molecular dynamic approach to understand the importance of domain IV of EGFR. Using NAMD, we have carried out nanosecond MD simulations of EGFR. Results indicated that domain IV of the EGFR: HER2 folded during dynamics. We have designed several peptidomimetic molecules to inhibit the EGFR heterodimerization interaction that has shown antiproliferative activity and specificity for HER2 positive cancer cell lines. Based on the design of these compounds, we have designed bicyclic peptides grafted onto a plant peptide, SFTI-1, to inhibit EGFR dimerization as a new class of grafted peptides. One particular peptidomimetic exhibited antiproliferative activity in the lower nanomolar range concentration in HER2 overexpressing lung cancer cell line. Using docking studies (AUTODOCK), we have defined the possible binding sites of these peptidomimetics on domain IV of HER2. Furthermore, SPR studies were conducted to evaluate the binding of designed peptidomimetics to EGFR. Results suggested that compounds designed to bind to HER2 protein, in particular to domain IV of HER2. Our computational and experimental studies suggest that the designed molecules inhibit HER2:HER3 interaction and can be therapeutically useful for HER2 positive breast and lung cancer. This work was supported by funding from NCI under Grant 1R15CA188225-01A1.

PA-14 ***Machine Learning-based Effective Prediction of Protein Disordered Regions***
Thursday
Room #12

Md Wasi Ul Kabir, Hoang Dai Nguyen, Md Tamjidul Hoque
University of New Orleans, University of New Orleans

Proteins without fixed or ordered three-dimensional structures are called disordered proteins. Disordered proteins can often be found in different organisms, and they play vital roles in various biological processes. Thus, accurate identification of these disordered regions has significant implications in properly annotating function and drug design for critical diseases. This research aims to use different protein features and apply a machine learning method to predict disordered regions of proteins. The structural properties of proteins, i.e., secondary structures information, backbone angles, half-sphere exposure, contact numbers, and solvent accessible surface area (ASA), provide useful information about disordered proteins. Moreover, we incorporate other features, i.e., Position-Specific Scoring Matrix (PSSM), Close Neighbor Correlation Coefficients, to enrich the feature set. A genetic algorithm is used to select the important subset of features and reduce the feature dimensionality. We explored some well-known classification algorithms, i.e., Light Gradient Boosting Machine, Logistic Regression, Extra Tree Classifier, Extreme Gradient Boosting method, to select the best machine learning method. We evaluated the proposed method with a training dataset using 10-fold cross-validations and test the model with two independent test datasets. The results show that the machine learning method attains Balanced Accuracy (BACC), F1-score, and Mathews Correlation Coefficient (MCC) of 92.0%, 0.91, and 0.84, respectively, on the training dataset. Further evaluation on independent test set reveals that it achieves BACC, F1-score, and MCC of 71.0%, 0.35, and 0.31, for CASP10 set; and 74.0%, 0.68, and 0.46 for the Disprot228 test set, respectively.

PA-15 ***Species Delimitation in Eastern Pine Snakes (Pituophis melanoleucus)***
Friday
Room #3

Basanta Khakurel, April Wright
Southeastern Louisiana University, Southeastern Louisiana University

The Eastern Pine Snake (Pituophis melanoleucus) is found throughout eastern North America with several conflicting subspecific designations. There are three different subspecific taxonomic classifications according to their geographical locations: the northern Pine snake (P. m. melanoleucus), the Florida Pine snake (P. m. mugitus), and the Black Pine snake (P. m. lodingi). There are no resolved relationships among these subspecific taxa in previous studies. We analyzed Ultra conserved elements (UCEs) to perform species tree estimation and species delimitation approaches implementing Bayesian inference methods. Species delimitation indicated that the plurality of datasets supported an ingroup of one species rather than three different subspecies. These results confirm prior findings of little divergence between the three putative subspecies, and suggesting one single species . Our study is helpful in determining the validity of UCEs in phylogenetic research of the recently evolved species like the eastern pine snake. It also contributes to the knowledge of phylogenetic patterns in the southeastern United States, removing ambiguity in the relationships and lack of geographical structuring in the traditional molecular data.

PA-16 ***Augmenting Self-Organizing Maps to Depict Categorical Data***
Friday
Room #11

Phillip Kilgore, Marjan Trutschl, Urska Cvek
Louisiana State University Shreveport, Louisiana State University Shreveport

Kohonen's self-organizing map is an unsupervised machine learning method designed to preserve the topology of its input space. Although this method has been used to efficiently summarize multidimensional data, the visualization of its constituent data has received less attention. We propose a method of addressing the visualization problem by augmenting a classical self-organizing map visualization to include an embedded histogram and evaluate its utility in depicting the self-organizing maps's constituents categorized by a discrete variable.

PA-17 ***Simulating Double Minute Evolution using Java***
Thursday
Room #6

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.

PA-18 ***Cancer Genomes with eccDNA Oncogene Amplification Show Evidence of Deletion-Episome Model of Double Minute Chromosome Formation***
Friday
Room #4

Angela Nguyen, Rahib Islam, Dr. Matthew Hayes
Xavier University of Louisiana,

Double minute chromosomes are highly amplified DNA artifacts that lead to increased oncogene expression, thus aiding the malignancy of cancer. Their mechanism of formation is poorly understood, but analysis of DNA sequencing data can potentially uncover evidence of hypothesized mechanisms of their formation. In this study, we use the whole genome sequencing data of solid and non-solid tumor genomes to study double minute chromosomes and investigate features that support the deletion-episome model of their formation. Future work will entail the development of algorithms to extract these features automatically for various hypothesized mechanisms of formation.

PA-19 ***Small RNA Sequencing and Computational Analysis Identifies Differentially Transcribed MicroRNAs that Regulate Nuclear Oxidative Damage in Human Astrocytes Exposed to Sodium Dichromate***
Friday
Room #9

Chukwumaobim Nwokwu, Adam Y. Xiao, Lynn Harrison, Gergana G. Nestorova
Louisiana Tech University, LSU Health Sciences Center,Louisiana Tech University

The exponential rise in chromium-related industrial products and activities has increased the risk of poisoning among the general population, particularly because of its ubiquity and persistence in the environment. The high lipid content of the brain, coupled with its heavy oxygen dependence and relatively weak antioxidant system, makes it highly susceptible to oxidative DNA damage by chromium free radical intermediates. This study is aimed at identifying specific miRNAs that modulate the expression and activity of the DNA repair proteins in astrocytes, which could lead to a better genotoxic assessment of exposure. Human astrocytes were treated with 10μM sodium dichromate for 16 hours followed by purification of RNA and protein. Comet assay indicated a significant increase in oxidative DNA damage. PCR and Wes® Protein assay confirmed sodium dichromate-induced reduction of the expression of the base-excision repair protein, 8-deoxyguanosine DNA glycosylase 1 (hOGG1). Small RNAseq data were generated on an Ion Torrent™ system and a list of differentially expressed miRNAs was generated using Partek® Flow® software. The biologically significant miRNAs were identified using miRNet 2.0. Our findings indicate a disproportionate decrease in miRNA expression in treated cells: 231 downregulated miRNAs and 2 upregulated miRNAs ($p < 0.05$; >2-fold). In addition to identifying multiple miRNA-mRNA pairs involved in DNA repair processes, this study uncovered a novel miRNA-mRNA pair interaction: miR-1248:OGG1. The miRNA candidates identified in this study could serve as potential biomarkers and therapeutics for sodium dichromate-induced oxidative stress in the brain that could lead to cancer and neurodegenerative disorders.

PA-20 ***Life in the fastlane: Testing for congruence among transcriptomic signatures in model organisms***
Friday
Room #2

Kyle Piller,
Southeastern Louisiana University,

Traditionally, species are developed as model organisms because they possess interesting life-history features or unique genetic attributes/physiologies that make them amenable to laboratory studies and experimentation. The Turquoise Killifish (Nothobranchiidae: Nothobranchius furzeri) is a recently developed model organism that is being used to investigate the process of aging and age-related diseases. This particular species is amendable to age-related studies because it is an annual species that can complete its entire life-cycle between 10 and 31 weeks. This is interesting because annualism is a relatively rare life-history trait among vertebrates. In addition, the genome of the Turquoise Killifish has been sequenced and annotated and several age related orthologs between the Turquoise Killifish and humans have been identified. However, it is unclear as to whether or not the same gene expression patterns of this species are unique or whether they are widespread throughout other groups of annual and non-annual species. The overall goal of this presentation is to provide a general overview of the killifish study system and a proposed research project that focuses on assessing congruence in the genetic architecture of the Turquoise Killifish to other closely related species with different life-histories traits (annual, facultative annual, and non-annual). This will be accomplished through the generation of RNA-Seq data and validation through the examination of a subset of differentially expressed genes using digital PCR methods. It is well known that replication and congruence are important in the sciences and in the case of potential model organisms, such as the Turquoise Killifish and relatives, congruence among genes and across life-cycle variants, provides stronger evidence for their importance in the aging and age related processes.

PA-21 ***A Sequence-based Machine Learning Method to effectively predict DNA and RNA Binding Residues***
Friday
Room #5

Aasish Rijal, Md Wasi Ul Kabir and Md Tamjidul Hoque
University of New Orleans, University of New Orleans

DNA- and RNA-binding proteins play an essential role in an organism's normal life cycle. These proteins have diverse functions in various biological processes. DNA-binding proteins are crucial for DNA replication, transcription, repair, packaging, gene expression. Likewise, RNA-binding proteins are essential for post-transcriptional control of RNAs and RNA metabolism. The identification of DNA- and RNA-binding residue are essential for biological research (function annotation) and understanding many diseases' pathogenesis, yet most of

the DNA- and RNA-binding proteins still need to be discovered. In this study, various properties of the protein sequences have been studied, such as amino acid composition type, Position-Specific Scoring Matrix (PSSM) values of amino acids, physicochemical properties, structural properties, torsion angles, and disorder regions. Moreover, a sliding window technique is used to extract more information from a target residue's neighbors. Finally, we proposed an optimized Light Gradient Boosting Machine (LightGBM) method to predict DNA- and RNA-binding residues. We evaluated the proposed method with two independent test datasets. The results show that the method achieves Sensitivity, Mathews Correlation Coefficient (MCC), and AUC of 57.13%, 0.263, and 81.78% for the DNA-binding test set; 28.59%, 0.135, and 0.724, for the RNA-binding test set, respectively. In comparison to the state-of-the-art DRNApred method, the LightGBM method shows an improvement of 128.52%, 25.24%, 6.21%, for DNA-binding test set and 78.69%, 12.50%, and 8.19% for RNA-binding test set in terms of Sensitivity, Mathews Correlation Coefficient (MCC), and AUC metric. These results indicate that the LightGBM method outperforms the existing DRNApred method.

PA-22 Thursday Room #10 ***pH-sensitive liposome formulation of peptidomimetic-doxorubicin conjugate for targeted delivery of anticancer conjugate on HER2 positive lung and breast cancer***

Jafrin Jobayer Sonju, Sitanshu S. Singh, Achyut Dahal, Seetharama D. Jois
University of Louisiana at Monroe, University of Louisiana at 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 research work focuses on the in vitro delivery of a peptidomimetic ligand attached doxorubicin for the HER2 positive lung and breast cancer cells transported by 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 at lower pH conditions mimicking tumor microenvironment (pH-6.5) compared to normal physiological conditions (pH 7.4), leading to the improvement of cell uptake. The results suggested that the targeting ligand conjugated cytotoxic drug with the pH-sensitive liposomal formulation is a promising approach to chemotherapy.

PA-23 Thursday Room #9 ***Pharmacometabolomics and Pharmacoproteomics Analysis for Cardiovascular Disease***

Marjan Trutschl, Marjan Trutschl, Hyung W. Nam
Louisiana State University Shreveport, Louisiana State University Shreveport, LSU Health Sciences 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.

PA-24 Friday Room #8 ***Vesicular and extravesicular protein signatures from the airspaces of ozone-exposed mice reflect muco-inflammatory disturbances***

Thao Vo, Thao Vo, Ishita Choudhary, Kshitiz Paudel, Richa Gupta, Mehmet Kesimer, Sonika Patial, Yogesh Saini
Louisiana State University, Louisiana State University, University of North Carolina at Chapel Hill

Lung epithelial lining fluid (ELF) harbors a variety of proteins that influence homeostatic and stress responses in the airspaces. Exosomes contain many proteins that vary based on the prevailing conditions. Ozone causes inflammatory responses in the airspaces of experimental animals and humans. However, in ozone-exposed lung airspaces, the protein signatures in exosomes contained within the ELF remain poorly characterized. To explore this, we hypothesized that ozone triggers the release of inflammatory proteins from various cells that reflect ozone-induced tissue pathology. Accordingly, we sub-chronically exposed adult mice to 0.8ppm ozone or air and determined exosome-bound proteomic signatures as well as the levels of soluble inflammatory mediators in the bronchoalveolar lavage fluid (BALF). Principal component analyses of the exosome-bound proteome revealed a clear distinction between air-exposed and ozone-exposed mice, as well as between ozone-exposed males and ozone-exposed females. In addition to 575 proteins that were enriched in both sexes upon ozone exposure, 243 and 326 proteins were enriched uniquely in ozone-exposed males and females, respectively. Ingenuity pathway analyses on enriched proteins between ozone- and air-exposed mice revealed enrichment of pro-inflammatory pathways. More specifically, macrophage activation-associated proteins were enriched in exosomes from ozone-exposed mice. Cytokine analyses on the BALF revealed elevated levels of G-CSF, MIP-1β, KC, IP-10, IL-6, and IL-5 in ozone-exposed mice. Finally, histopathological assessment revealed significantly enhanced intracellular localization of inflammatory proteins including MUC5B, MUC5AC, and FIZZ1 in ozone-exposed mice in cell-specific manner indicating the cellular sources of the proteins that are ferried in the exosomes upon ozone-induced lung injury. Collectively, this study identified exosomal, secretory, and cell-specific proteins and biological pathways following ozone exposure.

PA-25 ***Discriminating among complex hierarchical models for phylogenetic inference***
Thursday
Room #11

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 fossil data change over geological time. 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 molecular and morphological 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 morphological 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. This presenatation will discuss how researchers in can have confidence in their modeling approaches and can draw biological meaning from their inferences. While this presentation will focus on phylogenetics, the lessons are more broadly applicable to many mathematical systems.

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