9th Annual LA Conference on Computational Biology and Bioinformatics

Thursday, April 21
12:30 pm - 5:50 pm (CDT)

Friday, April 22
12:45 pm - 4:50 pm (CDT)

Saturday, April 23
9:00 am - 12:00 pm (CDT)

Virtual Meeting via Zoom
All Times given in Central Time Zone

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Thursday April 21, 2022 (Day 1)

12:30 – 12:38 pm ..... Day 1 Opening Remarks

12:40 - 12:58 pm ..... Lakshmi Matukumalli
NIH/NIGMS
NIGMS Update on Data Sciences and Cloud computing training

Session I

1:00 – 1:58 pm ..... Sara Sawyer
University of Colorado Boulder
Viruses at the Human-Animal Interface

2:00 – 2:18 pm ..... Christopher Taylor
Louisiana State University Health Sciences - New Orleans
Louisiana Biomedical Research Network Bioinformatics, Biostatistics, & Computational Biology Core

2:20 – 2:38 pm ..... Elia Brodsky
Pine Biotech
Analysis of Omics Data: BioMMED Bioinformatics Support Services

2:40 – 2:58 pm ..... Break

3:00 – 3:15 pm ..... Mark Bieger
Louisiana State University
The Scholarship First Agenda for Louisiana

3:17 – 3:35 pm ..... Basel Abuaita
Louisiana State University
Human neutrophils augment intestinal inflammatory responses and host defense via directing epithelial cell extrusion during Salmonella infection

3:37 – 3:55 pm ..... Michael Foster
Louisiana Tech University
Genomic Surveillance of SARS-CoV-2 in North Louisiana

3:57 – 4:15 pm ..... Lauren Cramer
University of Louisiana at Monroe
An Across Species Approach to Pharmaceutical Prioritization Using Fish Reproduction Data

4:17 – 4:27 pm ..... Day 1 Closing Remarks

4:30 – 5:50 pm ..... Poster Session

Friday April 22, 2022 (Day 2)

12:45 – 12:58 pm .....Day 2 Opening Remarks

Session II

1:00 – 1:58 pm .....Melissa Wilson
Arizona State University
Sex-biased Genome Evolution

2:00 – 2:18 pm ..... Richa Lamichhane
Louisiana State University
Sex-Specific Susceptibility of Mice to Bleomycin-Induced Pulmonary inflammation and fibrosis is Contributed by Differential Sex-Specific Transcriptomic Repertoire of Airway/Alveolar-Space Myeloid-Cells

2:20 – 2:38 pm .....Urska Cvek
Louisiana State University Shreveport
Exploring Disparities in Breast Cancer Treatment Outcomes within the State of Louisiana

2:40 – 2:58 pm .....Break

3:00 – 3:18 pm ..... Matthew Hayes
Xavier University of Louisiana
Complex Germline Structural Variant Discovery via Cluster Normalization

3:20 – 3:38 pm .....Md Wasi Ul Kabir
University of New Orleans
A Machine Learning Approach for Oyster Disease Prediction

3:40 – 4:38 pm .....April Wright
Southeastern Louisiana University
Navigating the Early Career Funding Landscape

4:40 – 4:50 pm ..... Day 2 Closing Remarks

Saturday April 23, 2022 (Day 3)

9:00 – 9:08 am .....Day 3 Opening Remarks

Session III

9:10 – 10:08 am .....Christopher Mason
Weill Cornell Medicine
Immune function, telomere length, and multi-omic adaptations to spaceflight revealed from spatial, single-cell, and environmental molecular profiling

10:10 – 10:28 am .....Ioannis Karakasiliotis
Democritus University of Thrace
Viral genome assembly and characterization hindrances from virus-host chimeric reads

10:30 – 10:43 am .....Break

10:45 – 11:43 am .....Michael Snyder
Stanford Medicine
Big Data, Health and COVID-19

11:45 - 12:00 pm..... Meeting Wrap-Up and Awards Announcement

Poster Session List

Thursday 4:30 – 5:50pm

Room	Name	iPoster Title	Institution
1	Dr. Basel Abuaita	Human neutrophils augment intestinal inflammatory responses and host defense via directing epithelial cell extrusion during Salmonella infection	LSUBR
2	Mrs. Duaa Alawad	Inferring Gene Regulatory Network using Graph Transformer Self-Attention Network	UNO
3	Mr. Eric Clifford	Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females	LSUS
4	Dr. Urska Cvek	Exploring Disparities in Breast Cancer Treatment Outcomes within the State of Louisiana	LSUS
5	Mr. Michael Foster	Genomic Surveillance of SARS-CoV-2 in North Louisiana	LATECH
6	Ms. Deriesha Gaines	RNA capture pin technology: assessment of mRNA enrichment via high throughput RNA seq	LATECH
7	Mr. Nayan Howladar	PPILC: Protein-Protein Interaction Prediction from Language of Biological Coding	UNO
8	Mr. Md Wasi Ul Kabir	Dispredict3.0: Intrinsically Disordered Protein prediction enhanced with Protein Language Model	UNO
9	Mr. Phillip Kilgore	STABILITY (Symptomatic Review during Biologic Therapy) during Inflammatory Bowel Disease Patient Infusion Therapy Visits: A Retrospective Review - 2019-22.	LSUS
10	Dr. Rahul Kumar	Generation of inducible whole-body Knockout mice using Rosa-Cre-inducible promoter	LSUBR
11	Dr. Richa Lamichhane	Sex-Specific Susceptibility of Mice to Bleomycin-Induced Pulmonary inflammation and fibrosis is Contributed by Differential Sex-Specific Transcriptomic Repertoire of Airway/Alveolar-Space Myeloid-Cells	LSUBR
12	Dr. Elahe Mahdavian	An interdisciplinary course on computer-aided drug discovery to broaden student participation in scientific research	LSUS
13	Ms. Savannah Montgomery	Inferring the Deletion-Episome Model of Double Minute Chromosome Formation Using Hi-C Sequencing Data	XULA
14	Mr. Derrick Mullins	Simulating Double Minute Chromosome and Phylogenetic Tree Evolution using Java	XULA
15	Mr. Chandra Mohan Reddy Muthumula	Identification of Constituents of Hydroethanolic Echinacea Extracts Active in Free Radical Quenching by n-Hexane and Ethyl Acetate Partitioning Aided by Chemometric Analysis	ULM
16	Mr. Luis Pena Marquez	Automatic segmentation and calculation of the Monocyte Monolayer Assay Index using deep learning	LSUS
17	Ms. Stephanie Provenzano	Bioinformatic Approaches in Elucidation of the Evolution and Functional Characterization of Natural Product Methyltransferases	LSUS
18	Mr. Aasish Rijal	A Machine Learning Approach for Oyster Disease Prediction	UNO
19	Mr. Krishna Shah	Using Language-based Features for ncRNA-protein Interaction Prediction	UNO
20	Mr. Ran Sun	Nucleosome-Receptor Structure Studies Based on Bioinformatics and Molecular Modeling	LATECH
21	Dr. Marjan Trutschl	Utilizing Self-Organizing Maps to Improve Information Delivery of Venn Diagrams	LSUS
22	Mrs. Anna Wilson	Time-Series Transcriptome Analysis of Encapsulated vs Embryo Body Mouse ES Cell Cultures Treated with Retinoic Acid	SUBR

Oral Presentation Abstracts

OA-01
Day 1: Thursday

Viruses at the Human-Animal Interface

Dr. Sara Sawyer
University of Colorado Boulder

Here, I show some of the ways that bioinformatics has contributed to our understanding of zoonosis. Zoonosis is the infection of humans with animal viruses, and was the process underpinning the SARS-1 and SARS-2 pandemics, as well as HIV-1 and most major epidemics and pandemics of the last century. I will discuss phylogeny, detection of natural selection in divergence and diversity data, and our understanding of viral evolution as viruses transmit from one host to the other. We also run a full virology lab and I will demonstrate how we can inform experimental approaches with bioinformatic findings.

OA-02
Day 1: Thursday

Human neutrophils augment intestinal inflammatory responses and host defense via directing epithelial cell extrusion during Salmonella infection

Dr. Basel Abuaita
Louisiana State University Baton Rouge

Pathological disease caused by enteric pathogens like Salmonella enterica is shaped by complex interactions between invading bacteria, intestinal cells, and immune cells. To explore the interplay between pathogen and host, we established a multi-component model comprised of human intestinal organoids (HIOs) infected with Salmonella enterica serovar Typhimurium (STM) and seeded with human polymorphonuclear leukocytes (PMNs), specifically neutrophils. Using a transcriptomics approach, we identified a dominant role for neutrophils in mounting an immune response including through increased production of pro-inflammatory cytokines, chemokines, and antimicrobial peptides. We also found that neutrophils enhanced organoid cellular stress responses to infection including activation of cell death pathways. While neutrophils migrated across the intestinal epithelial layer, they did not affect luminal colonization of Salmonella. Instead, the presence of neutrophils reduced the number of intracellular bacteria within the epithelium which was accompanied by increased epithelial cell death and extrusion. Inhibition of cell death pathways increased bacterial burden within the epithelium, consistent with a protective role for induction of cell death in the intestinal response to infection. These data support a critical function for neutrophils in promoting host defense by inducing shedding of cells from the Salmonella-infected intestinal monolayer.

OA-03
Day 1: Thursday

Genomic Surveillance of SARS-CoV-2 in North Louisiana

Mr. Michael Foster
Louisiana Tech University

SARS-CoV-2 has resulted in over 75 million cases of COVID-19 and over 950,000 deaths since its declaration on March 11, 2020. SARS-CoV-2 transmits rapidly and currently available methods of surveillance are unable to account for mutations and viral evolution. With the increased accessibility and affordability of Next Generation Sequencing (NGS), the implementation of publicly available protocols and analytical pipelines now allows for decentralized genomic surveillance, providing valuable data on emerging pathogens in real time. Our lab, in cooperation with Dr. Paul Kim at Grambling State University, performs genomic surveillance on clinical swabs obtained from local healthcare facilities. Viral RNA

is extracted and validated via RT-qPCR. Confirmed samples are amplified via multiplex PCR tiling. Samples are barcoded with sample specific oligos, combined, and purified with SPRI mag beads. The library is then sequenced on a single Oxford Nanopore MinION flow cell. Basecalling and demultiplexing is performed via ont-guppy which uses neural networks to process signal data, and fed into wf-artic, a nextflow workflow that performs alignment, variant calling, and phylogenetic analysis via the Artic field bioinformatics pipeline. The sequences are then uploaded to GISAID.org. Further visualization is done via augur/auspice. Both labs collaborate with Louisiana Tech University professor, Dr. Tom Bishop to optimize computational tools and develop efficient pipelines for analysis and data storage. Of the 213 genomes produced between our lab and GSU, 24 Delta samples were obtained in late 2021 before Omicron became the dominant variant in December. Early sequencing data from the ONT MinION was validated against Illumina data produced by LSUHSC-EVTL. Of the 213 genomes, all but two had mutations impacting diagnostic primers. Our work focused primarily on implementation and data generation but these methods could be expanded to contact tracing and outbreak determination.

OA-04
Day 1: Thursday

An Across Species Approach to Pharmaceutical Prioritization Using Fish Reproduction Data

Ms. Lauren Cramer
University of Louisiana at Monroe

The number of pharmaceuticals present in the environment has steadily increased in the past decade due to the growing human population. Moreover, there is little to no data on the effect of most pharmaceuticals in a given environment. Testing each active pharmaceutical ingredient for negative effects is difficult and not economically feasible. However, the use of Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS) can be utilized to develop a prioritization method to predict whether a particular pharmaceutical can cause fish reproductive impairment. The SeqAPASS screening tool compares the protein sequence across taxonomic groups to determine if there is a relative inherent susceptibility to chemicals. Also, it can be used to determine if there is a potential protein target or chemical/protein interaction of a certain pharmaceutical between taxonomic groups. The current study used the drug targets of 24 pharmaceuticals known to negatively impact fish reproduction to determine if there is high homology between human targets and fish. The results from this study demonstrated with each successive SeqAPASS level analysis for a drug target, homology increased, specifically between the individual amino acids within the binding sites of conserved drug targets. Pharmaceuticals that have drug targets with high homology, especially those with endocrine related pathways, could possibly lead to reproductive impairments in fish. For example, the amino acids responsible for ligand binding in each steroid receptor ranged in homology from 88.6% (progesterone) to 97.6% (estrogen receptor alpha). Furthermore, the results emphasize the shared homology between the conserved drug targets in humans and their corresponding proteins in fish.

OA-05
Day 2: Friday

Sex-biased genome evolution

Dr. Melissa Wilson
Arizona State University

I will propose how changes in industrialized society (e.g., having fewer pregnancies, and potentially even that the age at first reproduction is later) may be exacerbating sex differences in health and disease. In particular, we hypothesize that, ancestrally, sex-specific immune modulation evolved to facilitate survival of the pregnant person in the presence of an invasive placenta and an immunologically challenging pregnancy - an idea we term the 'pregnancy compensation hypothesis' (PCH). Further, we propose that sex differences in immune function are mediated, at least in part, by the evolution of gene content and dosage on the sex chromosomes, and are regulated by reproductive hormones. Finally, we propose that changes in reproductive ecology in industrialized environments exacerbate these evolved sex differences, resulting in the increasing risk of autoimmune disease observed in females, and a counteracting reduction in diseases such as cancer that can be combated by heightened immune surveillance. The PCH generates a series of expectations that can be tested empirically and that may help to identify the mechanisms underlying sex differences in modern human diseases. We then start to dig into this hypothesis by studying patterns of X-inactivation across human placentas, where we investigate regional heterogeneity in chromosome and gene-specific inactivation.

OA-06
Day 2: Friday

Sex-Specific Susceptibility of Mice to Bleomycin-Induced Pulmonary inflammation and fibrosis is Contributed by Differential Sex-Specific Transcriptomic Repertoire of Airway/Alveolar-Space Myeloid-Cells

Dr. Richa Lamichhane
Louisiana State University Baton Rouge

Idiopathic pulmonary fibrosis (IPF) is a progressive fatal interstitial lung disease that is more prevalent and have a poor prognosis in human males. Consistently, male mice are also more susceptible to experimental bleomycin-induced lung injury and fibrosis. However, the underlying mechanisms for these gender/sex-associated differences remain unknown. Here, we tested the hypothesis that the transcriptomic repertoire of airway/airspace myeloid cells determine the sex-specific susceptibility of mice to bleomycin (BLM)-induced lung injury and fibrosis. Adult C57BL/6 wild-type (WT) mice were oropharyngeally challenged with BLM (4 Units/Kg body weight) or saline. Lung injury, inflammation, and fibrosis were assessed, and airway/airspace myeloid-cells were subjected to RNA-sequencing at day-14 post-BLM challenge. As expected, male mice manifested significantly increased cellular infiltration, lung injury, and fibrosis compared to female mice at day-14. Interestingly, while BLM resulted in equivalent numbers of transcriptomic changes in both male and female myeloid cells when compared to respective saline-control groups, several pro-inflammatory genes were significantly up-regulated in male myeloid-cells when compared to female myeloid-cells in the saline-control group. Further, cross-sex bone marrow transplantation experiments revealed that male hematopoietic stem cells increased the susceptibility of female mice to BLM-induced lung inflammation. These findings suggest that there are inherent differences in gene expression between the male and female airway/airspace-myeloid cells; those male myeloid cells are inherently pro-inflammatory; and that the pro-inflammatory nature of male myeloid cells is sufficient to increase the susceptibility of female mice to BLM-induced inflammation. Our findings emphasize the importance of myeloid cells and their genetic repertoire as a contributor to gender/sex-specific differences in the susceptibility to idiopathic pulmonary fibrosis.

OA-07
Day 2: Friday

Exploring Disparities in Breast Cancer Treatment Outcomes within the State of Louisiana

Dr. Urska Cvek
Louisiana State University Shreveport

Breast cancer is the most common cancer diagnosed among US women (excluding skin cancers) and is the second leading cause of cancer death among women, after lung cancer. Breast-conserving surgery (BCS) followed by radiation therapy is now the recommended standard of care for early breast cancer with comparable survival rates (NIH, 1990 consensus statement). For appropriately selected patients, BCS provides the survival equivalent of mastectomy, a more cosmetically acceptable result with lower morbidity, and a low rate of recurrence in the treated breast. For these reasons, the national mastectomy rates fell steadily through 2006. Cancer outcomes are determined not only by innate molecular biology of the tumor, but also by potentially modifiable variables including socioeconomic factors and geographical distance from the treatment center, and also included race. The disparity in cancer treatment and outcomes due to geographic and socioeconomic variables is an increasingly recognized problem. We are interested in identifying these variations and implementing targeted strategies to improve measurable outcomes (i.e., incidence, stage at diagnosis, and survival). We followed our national-level analytics with in-depth analytics and modeling of the effect of distance between the patient's residence and the primary treatment center for more than 42,000 Louisiana breast cancer patients obtained from the Louisiana Tumor Registry database for the period of 2009-2019. In Louisiana, we found that there were significant differences in both the distance to the closest utilized facility ($p << 0.001$) and in treatment modality ($p << 0.001$) with respect to urban or rural status at the time of encounter. Greater facility distance was associated with mastectomy and rural residence respectively. Significant differences were also noted in several comorbid disease states, tumor size, race, and ethnicity for both treatment modality and urban residence (in many cases, $p << 0.001$).

OA-08
Day 2: Friday

Complex Germline Structural Variant Discovery via Cluster Normalization

Dr. Matthew Hayes
Xavier University of Louisiana

Complex genomic structural variants (CGSVs) are abnormalities that present with three or more breakpoints, making their discovery a challenge. Most existing algorithms for structural variant detection are only designed to find simple structural variants (SSVs) such as deletions and inversions; they fail to find more complex events such as deletion–inversions or deletion–duplications, for example. In this study, we present an algorithm named CleanBreak that employs a clique partitioning graph-based strategy to identify collections of SSV clusters and then subsequently identifies overlapping SSV clusters to examine the search space of possible CGSVs, choosing the one that is most concordant with local read depth. We evaluated CleanBreak's performance on whole genome simulated data and a real data set from the 1000 Genomes Project. We also compared CleanBreak with another algorithm for CGSV discovery. The results demonstrate CleanBreak's utility as an effective method to discover CGSVs.

OA-09
Day 2: Friday

A Machine Learning Approach for Oyster Disease Prediction

Mr. Md Wasi Ul Kabir
University of New Orleans

Oyster production is an essential part of the economy of the Southeastern United States. Perkinsus marinus is a parasite that is deadly to oysters, and it is one of the primary causes of oyster fatalities. This project intends to develop an accurate Machine Learning (ML) model to predict oyster disease. We used the OysterSentinel website (https://www.oystersentinel.cs.uno.edu/) to collect a large dataset of oyster disease from across the northern Gulf of Mexico.. The dataset includes decades of samples from different oyster reefs and provides oyster infection levels alongside environmental data. The dataset contains missing data, so we explored different imputation methods such as Mean/Median/Most frequent, k-nearest neighbor (k-NN), and deep learning methods to impute the missing data. We selected a subset of features with the highest importance to reduce the feature set size using the Genetic Algorithm (GA) and Incremental Feature Selection (IFS) methods. We investigated randomized parameter optimization and exhaustive grid search methods for hyperparameter tuning. Lastly, we experimented with several machine learning methods and ensemble machine learning methods to find the optimal method. The initial results show relatively low Mean Absolute Error (MAE). Additionally, we developed a Graphical User Interface (GUI) to make the process of making predictions easier. The proposed ML method, backed by an easy-to-use GUI application, will help scientists predict future oyster diseases and take the necessary steps to reduce the oyster mortality rate.

OA-10
Day 2: Friday

Navigating the Early Career Funding Landscape

Dr. April Wright
Southeastern Louisiana University

For new faculty, applying for funding is both crucial and daunting. In this talk, I will discuss how faculty can approach early career funding. In particular, applying for funding at Primarily Undergrad Institutions (PUIs) can have different dimensions than applying for funding at major research institutions. This talk will be aimed at PUI faculty looking to build a sustainable funding scheme in their lab.

OA-11
Day 3: Saturday

Immune function, telomere length, and multi-omic adaptations to spaceflight revealed from spatial, single-cell, and environmental molecular profiling

Dr. Christopher Mason
Weill Cornell Medicine

Despite the battery of human spaceflight data from NASA, ESA, and other missions, our understanding of the biology of spaceflight is still incomplete and spans only a few dozen individuals. Current data has shown that spaceflight causes changes in cell signaling, immune function, and tissue regulation, but such alterations could be better understood with more modern molecular methods. To help address this gap in knowledge, the Inspiration4 mission (deployed on the SpaceX Dragon Capsule) leveraged genome, epigenome, transcriptome, proteome, microbiome, metabolome, exosome, telomere, single-cell V(D)J immunophenotyping, and epitope profiling for the astronauts, as well as single-nucleus, multiome sequencing and multi-omic spatial mapping (human and microbial). We were able to clearly dissect the gene expression changes from spaceflight occurring at the single-cell level, particularly for concomitant chromatin (scATAC-seq) and expression (scRNA-seq) changes for macrophages, neutrophils, and CD4 T-cells, and we also mapped the first-ever in vivo human-microbial interaction maps from spaceflight (on the GeoMx spatial

imaging platform). The single-cell data showed that interleukin-6 (IL-6) was elevated in flight, and post-flight, which is a consistent response to zero gravity that has also been seen in other crew members. Also, our metagenome data showed a "blending" of the skin microbiome for of the crew within the first two days of the mission (Shannon and beta-diversity down by 0.2), particularly with rapid transfer of Caulobacter soli and other commensal species, indicating a rapid transfer of skin flora to other crew in the confines of the Dragon space capsule.

OA-12
Day 3: Saturday

Viral genome assembly and characterization hindrances from virus-host chimeric reads

Dr. Ioannis Karakasiliotis
Democritus University of Thrace

Viral metagenomics, also known as virome studies, have yielded an unprecedented number of novel sequences, essential in recognizing and characterizing the etiological agent and the origin of emerging infectious diseases. Several tools and pipelines have been developed, to date, for the identification and assembly of viral genomes. Assembly pipelines often result in viral genomes contaminated with host genetic material, some of which are currently deposited into public databases. In the current report, we present a group of deposited sequences that encompass ribosomal RNA (rRNA) contamination. We highlight the detrimental role of chimeric next generation sequencing reads, between host rRNA sequences and viral sequences, in virus genome assembly and we present the hindrances these reads may pose to current methodologies. We have further developed a refining pipeline, the Zero Waste Algorithm (ZWA) that assists in the assembly of low abundance viral genomes. ZWA performs context-depended trimming of chimeric reads, precisely removing their rRNA moiety. These, otherwise discarded, reads were fed to the assembly pipeline and assisted in the construction of larger and cleaner contigs making a substantial impact on current assembly methodologies. ZWA pipeline may significantly enhance virus genome assembly from low abundance samples and virus metagenomics approaches in which a small number of reads determine genome quality and integrity.

OA-13
Day 3: Saturday

Big Data, Health and COVID-19

Dr. Michael Snyder
Stanford University

Recent technological advances as well as longitudinal monitoring not only have the potential to improve the treatment of disease (Precision Medicine) but also empower people to stay healthy (Precision Health). We have been using advanced multiomics technologies (genomics, immunomics, transcriptomics, proteomics, metabolomics, microbiomics) as well as wearables for monitoring health in 109 individuals for up to 12 years and made numerous major health discoveries covering cardiovascular disease, oncology, metabolic health and infectious disease. We have found that individuals have distinct aging patterns that can be measured in an actionable period of time as well as seasonal patterns of health markers. We have also explored the effects of fiber using multiomics profiling. Finally, we have used wearable devices for early detection of infectious disease, including COVID-19 and built an alerting system for detecting health stressors that is scaleable to the entire planet. We believe that advanced technologies have the potential to transform healthcare.

Poster Session Abstracts

PA-01 Room 1 ***Human neutrophils augment intestinal inflammatory responses and host defense via directing epithelial cell extrusion during Salmonella infection***

Basel Abuaita, Anna-Lisa E. Lawrence, Ryan P. Berger, David R. Hill, Sha Huang, Veda K. Yadagiri, Brooke Bons, Courtney Fields, Gautam J. Sule, Jason S. Knight, Christiane E. Wobus, Jason R. Spence, Vincent B. Young, Mary X. O'Riordan

Louisiana State University Baton Rouge, University of Michigan Medical School

Pathological disease caused by enteric pathogens like Salmonella enterica is shaped by complex interactions between invading bacteria, intestinal cells, and immune cells. To explore the interplay between pathogen and host, we established a multi-component model comprised of human intestinal organoids (HIOs) infected with Salmonella enterica serovar Typhimurium (STM) and seeded with human polymorphonuclear leukocytes (PMNs), specifically neutrophils. Using a transcriptomics approach, we identified a dominant role for neutrophils in mounting an immune response including through increased production of pro-inflammatory cytokines, chemokines, and antimicrobial peptides. We also found that neutrophils enhanced organoid cellular stress responses to infection including activation of cell death pathways. While neutrophils migrated across the intestinal epithelial layer, they did not affect luminal colonization of Salmonella. Instead, the presence of neutrophils reduced the number of intracellular bacteria within the epithelium which was accompanied by increased epithelial cell death and extrusion. Inhibition of cell death pathways increased bacterial burden within the epithelium, consistent with a protective role for induction of cell death in the intestinal response to infection. These data support a critical function for neutrophils in promoting host defense by inducing shedding of cells from the Salmonella-infected intestinal monolayer.

PA-02 Room 2 ***Inferring Gene Regulatory Network using Graph Transformer Self-Attention Network***

Duaa Alawad, Ataur Katebi, Md Tamjidul Hoque

University of New Orleans, University of New Orleans, Northeastern University

Constructing gene regulatory networks (GRNs) by inferring the regulatory relationships from gene expression data has important applications in systems biology. A regulatory relationship between two genes can be inferred as a link prediction problem between two nodes in a graph. Graph neural networks allow the construction of GRNs by integrating topological neighbor propagation across the entire GRN. We propose a gene regulatory graph transformer Self-Attention Network approach to reconstruct GRNs from scratch utilizing the gene expression data. GRN inference is formulated as a graph classification problem in this work to distinguish whether a subgraph centered on two nodes contains the link between the two nodes to improve inductive generalization capability. A linked pair between a transcription factor (TF) and a target gene together with their neighbors is labeled as a positive subgraph; conversely, an unlinked pair between a TF and a target gene together with their neighbors is labeled as a negative subgraph. A graph transformer Self-Attention Network model is constructed with node features using gene expression and graph embedding. We illustrate that a noisy starting graph structure built from Pearson's correlation coefficient and mutual information can guide the GRN inference through an appropriate ensemble technique.

PA-03 Room 3 ***Drug Screen Trends in Emergency Rooms Among Childbearing-Aged Females***

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

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

LSU Health Sciences Center in Shreveport serves a largely minority-based, urban population. Prior analysis of emergency room urine drug screen results from 1998-2011 found that the African American population tested

positive for cannabinoids, opiates, and cocaine at high rates, while the Caucasian population tested positive for cannabinoids, benzodiazepines, and opiates at high rates. The focus of this study was to determine connections between visit reasons and rates of positive drug screens, tracked by race and age, among 18-35 years old females during 2012-2019. Similar to the 1998-2011 general population study, Caucasian and African-American females tested positive mostly for cannabinoids and opiates during 2012-2019. Caucasian females also tested positive for amphetamines and benzodiazepines at higher rates than African American females. African American females tested positive for cannabinoids and cocaine at higher rates than Caucasian females. From 2012-2016, Caucasian females tested positive for opiates at higher rates. Beyond 2016, African American females tested positive for opiates at higher rates. Most visits in both populations were for pain, pregnancy, or psychiatric/neurologic reasons. About 30% of pregnancy and gynecologic visits were associated with cannabinoid use, followed by opiates. Gastroenterology patients tested positive for cannabinoids in over 40% of cases and for opiates in 20%. Psychiatric/neurologic patients tested positive mostly for cannabinoids and amphetamine (36% and 15%, respectively). Sickle Cell patients (all African American) tested positive for opiates at a rate of 72%. GatewayNet analysis indicated that cannabis use likely precedes cocaine, amphetamine, benzodiazepine, and opiate use. This work is supported by the 2021 Summer Research Program of the Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P2O GM103424-19.

PA-04 ***Exploring Disparities in Breast Cancer Treatment Outcomes within the State of Louisiana***
Room 4

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

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

Breast cancer is the most common cancer diagnosed among US women (excluding skin cancers) and is the second leading cause of cancer death among women, after lung cancer. Breast-conserving surgery (BCS) followed by radiation therapy is now the recommended standard of care for early breast cancer with comparable survival rates (NIH, 1990 consensus statement). For appropriately selected patients, BCS provides the survival equivalent of mastectomy, a more cosmetically acceptable result with lower morbidity, and a low rate of recurrence in the treated breast. For these reasons, the national mastectomy rates fell steadily through 2006. Cancer outcomes are determined not only by innate molecular biology of the tumor, but also by potentially modifiable variables including socioeconomic factors and geographical distance from the treatment center, and also included race. The disparity in cancer treatment and outcomes due to geographic and socioeconomic variables is an increasingly recognized problem. We are interested in identifying these variations and implementing targeted strategies to improve measurable outcomes (i.e., incidence, stage at diagnosis, and survival). We followed our national-level analytics with in-depth analytics and modeling of the effect of distance between the patient's residence and the primary treatment center for more than 42,000 Louisiana breast cancer patients obtained from the Louisiana Tumor Registry database for the period of 2009-2019. In Louisiana, we found that there were significant differences in both the distance to the closest utilized facility ($p << 0.001$) and in treatment modality ($p << 0.001$) with respect to urban or rural status at the time of encounter. Greater facility distance was associated with mastectomy and rural residence respectively. Significant differences were also noted in several comorbid disease states, tumor size, race, and ethnicity for both treatment modality and urban residence (in many cases, $p << 0.001$).

PA-05 ***Genomic Surveillance of SARS-CoV-2 in North Louisiana***
Room 5

Michael Foster, Laura Lee, Paul Austin, Madeline Robison, Lescia Valmond, Paul Kim, Audrey Kim, Tom Bishop, Jamie Newman

Louisiana Tech University, Louisiana Tech University, Grambling State University

SARS-CoV-2 has resulted in over 75 million cases of COVID-19 and over 950,000 deaths since its declaration on March 11, 2020. SARS-CoV-2 transmits rapidly and currently available methods of surveillance are unable to account for mutations and viral evolution. With the increased accessibility and affordability of Next Generation Sequencing (NGS), the implementation of publicly available protocols and analytical pipelines now allows for decentralized genomic surveillance, providing valuable data on emerging pathogens in real time. Our lab, in cooperation with Dr. Paul Kim at Grambling State University, performs genomic surveillance on clinical swabs obtained from local healthcare facilities. Viral RNA is extracted and validated via RT-qPCR. Confirmed samples are amplified via multiplex PCR tiling. Samples are barcoded with sample specific oligos, combined, and purified with SPRI mag beads. The library is then sequenced on a single Oxford Nanopore MinION flow cell. Basecalling and demultiplexing is performed via ont-guppy which uses neural networks to process signal data, and fed into wf-artic, a nextflow workflow that performs alignment, variant calling, and phylogenetic analysis via the Artic field bioinformatics pipeline. The sequences are then uploaded to GISAID.org. Further visualization is done via augur/auspice. Both labs collaborate with Louisiana Tech University professor, Dr. Tom Bishop to optimize computational tools and develop efficient pipelines for analysis and data storage. Of the 213 genomes produced between our lab and GSU, 24 Delta samples were obtained in late 2021 before Omicron became the dominant variant in December. Early sequencing data from the ONT MinION was validated against Illumina data produced by LSUHSC-EVTL. Of the 213 genomes, all but two had mutations impacting diagnostic primers. Our work focused primarily on implementation and data generation but these methods could be expanded to contact tracing and outbreak determination.

PA-06 ***RNA capture pin technology: assessment of mRNA enrichment via high throughput RNA seq***
Room 6

Deriesha Gaines, Elia Brodsky, Harpreet Kaur, Gergana G. Nestorova
Louisiana Tech University, Pine Biotech, Louisiana Tech University

The aim to support an extended human presence in space has led to the establishment of NASA's GeneLab, which combines a database repository dedicated to ISS biological experiments and corresponding ground-based studies. The biggest constraints for real-time genetic analysis of biological specimens in space are the time that is required for the astronaut to process the sample and the reduced working area on ISS. Because of these limitations, the number of samples that are currently being analyzed in space is very low. The RNA capture pin technology can significantly reduce the time required for genetic analysis on ISS. At the core of this tool is a microscopic pin functionalized with dT(15) capture sequences for the purification of messenger RNA. The main objective of this study is to apply NextSeq 550 System for RNA sequencing to assess the selectivity of the RNA capture pin. Gold plated pins (3cmx 200µm) were functionalized with dT(15) -specific capture sequences for direct purification of RNA from the radish plant. A parallel test was included using total radish RNA purified via a commercially available plant RNA purification kit. Each experimental group included three biological replicates. The RNA sequencing analysis of the purified genetic material determined the types and relative abundance of different RNA types and the selectivity of the RNA capture pin to purify specific types of RNA. Bowtie alignment, quality control, PCA, and gene counts were performed using the T-BioInfo Platform. The mapped read counts in the total RNA and capture pin groups were 2007381 and 1180671 respectively. The principal component analysis identified that the samples clustered into two groups. The percentage of gene read counts confirmed that the total RNA sample is composed of 70% ribosomal RNA, 20% is messenger RNA, and 10% noncoding RNA. The RNA sample purified via the RNA capture pin technology contained 70% messenger RNA, 10% ribosomal RNA, and 20% noncoding RNA.

PA-07 ***PPILC: Protein-Protein Interaction Prediction from Language of Biological Coding***
Room 7

Nayan Howladar, Md Wasi Ul Kabir, Tamjidul Hoque
University of New Orleans, University of New Orleans

Protein-protein interactions in a cell are important to characterize and perform various fundamental biological processes. Due to the tedious, resource expensive, and time-consuming experimental processes, computational techniques to solve protein-protein interaction difficulties have emerged as an active research area in bioinformatics. This research aims to provide an innovative machine learning-based technique that narrows this gap by making predictions of protein-protein interaction based on carefully chosen input features and exploiting information-rich evolutionary information. We developed a Protein-Protein Interactions predictor, PPILC, that leverages the evolutionary information from the protein language model. We examined several distinct neural network architectures: Self-Attention, Linear Attention, Multi-Attention, LSTM-CONV, and found that encoder-decode architecture with linear attention performs the best. Encoder engine will take protein representation from LM and one convolution running over them to produce attention coefficients then normalize it using SoftMax and end up an attention score. Our architecture uses weighted aggregation mechanism with linear complexity where weights come from attention score. Decoder is our classification engine to predict protein interaction. We found that the PPILC outperformed other cutting-edge techniques for predicting protein-protein interactions. We believe the proposed method could serve as an important tool in protein-protein interaction prediction, further accelerating the protein drug discovery process. The model will be available as a REST API and a stand-alone application on the web.

PA-08 Room 8 ***Dispredict3.0: Intrinsically Disordered Protein prediction enhanced with Protein Language Model***

Md Wasi Ul Kabir, Md Tamjidul Hoque
University of New Orleans, University of New Orleans

Intrinsically disordered proteins (IDPs) fail to form a well-defined secondary and tertiary structure, yet they exhibit important biological functions. These disordered proteins have major implications for properly annotating protein function and drug design for diseases. The disordered protein regions are structurally and functionally distinct from ordered proteins, requiring specialized experimental and computational methods to identify and analyze them. Thus, the identification of disordered protein regions is a time-consuming task. This research aims to develop a machine learning method to predict proteins' disordered regions (IDRs) accurately. We have developed a novel disorder predictor, named Dispredict3.0, that uses the evolutionary information from a protein language model that helps to improve the performance of disorder prediction. Further, we have used the Principal Component Analysis (PCA) to reduce the dimensions of the representation and train an optimized Light Gradient Boosting Machine. The experimental results show that Dispredict3.0 outperforms the state-of-the-art method and has an improvement of 2.54%, 16.22%, 12.05%, and 17.85% in terms of AUC, F1-score, MCC, and kappa, respectively, compared to the state-of-the-art disordered method.

PA-09 Room 9 ***STABILITY (Symptomatic Review during Biologic Therapy) during Inflammatory Bowel Disease Patient Infusion Therapy Visits: A Retrospective Review - 2019-22.***

Phillip Kilgore, Prerana Ramesh, Meher Sindhoora Mavuram, Kelli Morgan, James Morris, Qiang Cai, Phillip Kilgore, Urska Cvek, Marjan Trutschl, Steven Alexander
Louisiana State University Shreveport, LSU Health Shreveport, Louisiana State University Shreveport

Several studies have documented positive correlation between improved patient outcomes with more extensive physician-patient communication in chronic diseases e.g. diabetes. Understanding how such interactions can influence and improve care is a novel opportunity in inflammatory bowel disease (IBD).

LSUHSC-S implemented brief 15-minute physician-patient interviews, so called "STABILITY" (Symptomatic Review during Biologic Therapy), during infusion therapy visits to discuss the patients' current IBD-related symptoms and assess if any changes needed to be made in the patient's treatment plan. This study aims to analyze whether outcomes for IBD patients can be improved by implementing STABILITY into their treatment regimes. A retrospective chart review was made for 177 IBD patients (36 UC, 128 CD, 13 undetermined IBD) who were seen at LSUHSC-S between 2011 and 2022. STABILITY has been mandated into all infusion therapy visits since March 2019. From the obtained survey responses, patients frequently felt that their IBD symptoms had improved (n=24, 56%), their understanding of their IBD had improved (n=36, 84%), and continued to wish see a GI physician during infusion therapy (n=40, 93%). This project will further investigate how IBD patients on STABILITY infusion therapies fare compared to LSUHSC-S patients who are solely on self-injectable biologics. Comparing patients before STABILITY (before March 2019) and after STABILITY (after March 2019), we found that fecal calprotectin was improved in female UC patients (n=9 & 47 respectively, where n refers to number of encounters; p=0.0008) and that fecal calprotectin (n=10 & 62, p=0.0003) was improved in UC patients overall. Similarly, fecal calprotectin in males with CD was also improved (n=20 & 83, p<0.0001), with fecal calprotectin in CD overall also improved (n=34 & 217, p<0.0001]). Statistical analysis was performed using Welch's unpaired t-test.

PA-10 ***Generation of inducible whole-body Knockout mice using Rosa-Cre-inducible promoter***
Room 10

Rahul Kumar, Rahul Kumar, Yun Mao, Yogesh Saini, Sonika Patial
Louisiana State University Baton Rouge, Louisiana State University

Germline deletion of certain genes causes embryonic lethality, therefore, understanding the effect of deletion of such genes on mammalian pathophysiology becomes challenging. Tamoxifen (tam)-inducible Cre recombinase (Cre-ERT2) is widely used for tissue-specific and temporal induction of gene deletion in mice. However, the employment of this approach for the generation of whole-body deletion of a gene remains untested. Activation of Cre-ERT2 is typically achieved by intraperitoneal (i.p.) or oral administration of tamoxifen. The effectiveness of tam administration via these routes, however, remains poorly characterized. R26 is a ubiquitous promoter and mice carrying the R26-Cre-ERT2 transgene assures the expression of Cre-ERT2 in all the cells. The presence of R26-mTomFl/Fl/mEGFP transgene assures the expression of fluorescent reporter proteins (mTomato or mEGFP) in all the cells. To determine the efficiency of Cre-recombination, R26-Cre-ERT2 mice were crossed with R26-mTomFl/Fl/mEGFP mice. The F1 weanlings (n=6-8/group) were subjected to different tam regimens: i.p. injections (4 injections @ 1.35mg/injection), diet (400 mg tam-citrate/kg food), or diet combined with either tam oral gavage (4 gavages @ 1.35mg/gavage) or tam i.p. injections for 2-weeks and cre recombination in different organs was determined. Tamoxifen administration resulted in loss of body weight in all the groups with relatively slow recovery in the oral gavage group. While the efficiency of Cre-recombination was variable among organs irrespective of the route of administration, major organs such as liver, heart, lungs, spleen, thymus, and kidneys showed almost complete recombination. In general, the efficiency of Cre-recombination was better with tam-injections compared to oral gavage and the tam-diet alone. Our results demonstrate that the tam-injections alone or the combination of tam-diet with injections can be employed for efficient deletion of a gene in the whole body.

PA-11 ***Sex-Specific Susceptibility of Mice to Bleomycin-Induced Pulmonary inflammation and fibrosis***
Room 11 ***is Contributed by Differential Sex-Specific Transcriptomic Repertoire of Airway/Alveolar-Space Myeloid-Cells***

Richa Lamichhane, Richa Lamichhane, Yogesh Saini, and Sonika Patial
Louisiana State University Baton Rouge, Louisiana State University

Idiopathic pulmonary fibrosis (IPF) is a progressive fatal interstitial lung disease that is more prevalent and have a poor prognosis in human males. Consistently, male mice are also more susceptible to experimental bleomycin-induced lung injury and fibrosis. However, the underlying mechanisms for these gender/sex-associated differences remain unknown. Here, we tested the hypothesis that the transcriptomic repertoire of airway/airspace myeloid cells determine the sex-specific susceptibility of mice to bleomycin (BLM)-induced lung injury and fibrosis. Adult C57BL/6 wild-type (WT) mice were oropharyngeally challenged with BLM (4 Units/Kg body weight) or saline. Lung injury, inflammation, and fibrosis were assessed, and airway/airspace myeloid-cells were subjected to RNA-sequencing at day-14 post-BLM challenge. As expected, male mice manifested significantly increased cellular infiltration, lung injury, and fibrosis compared to female mice at day-14. Interestingly, while BLM resulted in equivalent numbers of transcriptomic changes in both male and female myeloid cells when compared to respective saline-control groups, several pro-inflammatory genes were significantly up-regulated in male myeloid-cells when compared to female myeloid-cells in the saline-control group. Further, cross-sex bone marrow transplantation experiments revealed that male hematopoietic stem cells increased the susceptibility of female mice to BLM-induced lung inflammation. These findings suggest that there are inherent differences in gene expression between the male and female airway/airspace-myeloid cells; those male myeloid cells are inherently pro-inflammatory; and that the pro-inflammatory nature of male myeloid cells is sufficient to increase the susceptibility of female mice to BLM-induced inflammation. Our findings emphasize the importance of myeloid cells and their genetic repertoire as a contributor to gender/sex-specific differences in the susceptibility to idiopathic pulmonary fibrosis.

PA-12 ***An interdisciplinary course on computer-aided drug discovery to broaden student participation in scientific research***
Room 12

Elahe Mahdavian,
Louisiana State University Shreveport,

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

PA-13 ***Inferring the Deletion-Episome Model of Double Minute Chromosome Formation Using Hi-C Sequencing Data***
Room 13

Savannah Montgomery, Dr. Matthew Hayes, Angela Nguyen, Rahib Islam

Xavier University of Louisiana, Xavier University of Louisiana

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

PA-14 ***Simulating Double Minute Chromosome and Phylogenetic Tree Evolution using Java***
Room 14

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

PA-15 ***Identification of Constituents of Hydroethanolic Echinacea Extracts Active in Free Radical***
Room 15 ***Quenching by n-Hexane and Ethyl Acetate Partitioning Aided by Chemometric Analysis***

Chandra Mohan Reddy Muthumula, C. Muthumula, S. Nagumalli, O. C. McGehee, H. A. Hussin, J. D. Carstens, C. V. Landingham, K. A. El Sayed, and S. A. Meyer
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Echinacea spp. contains numerous chemical constituents known to quench free radicals, but relative potencies of these constituents in situ are unknown. To address this issue, we used partial least square (PLS) regression of spectral peaks from proton nuclear magnetic resonance (1H-NMR, 400 MHz) spectroscopy against DPPH• quenching activity. Relative areas of proton spectral regions (0.04 ppm bins; 0.00 - 10.00 ppm) of Echinacea extract were integrated for aerial parts of the three medicinal species of E. purpurea, E. pallida and E. angustifolia obtained from USDA-ARS NCRPIS, Ames, IA. We used electron paramagnetic resonance (EPR) spectroscopy to evaluate the free radical quenching activity of 75% ethanolic extracts and fractions obtained

by defatting with n-hexane and then partitioning with ethyl acetate. In addition, a commercial E. purpurea (Monterey Bay Spice Co.) extract was also evaluated. Quenching activity was measured as reduction of DPPH• signal by EPR and expressed relative to that of Trolox. Free radical quenching activity of Echinacea extract was modestly increased by defatting with n-hexane but was significantly increased by partitioning with ethyl acetate. Orthogonal PLS-regression analyses of the 1H-NMR data identified several peaks well correlated with the free radical quenching activity in the 5.10-7.70 ppm region, mostly aromatic/olefinic constituents, that partitioned with ethyl acetate. In conclusion, these results show enrichment of constituents responsible for the free radical quenching in Echinacea by removal of n hexane-soluble constituents followed by partitioning with ethyl acetate. These observations are consistent with free radical quenching activity of unfractionated Echinacea being expressed by aromatic phenolic constituents in situ.

PA-16 Room 16 ***Automatic segmentation and calculation of the Monocyte Monolayer Assay Index using deep learning***

Luis Pena Marquez, Subhajit Chakrabarty
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The classification of white cells, red blood cells and their counts have been important tasks in the clinical laboratory industry for a long time. The classification of white cells plays an important part in medical diagnosis. The counts may suggest the presence of infection, inflammation, anemia, bleeding, and other blood-associated issues. More specifically, the counting in our study is the calculation of the Monocyte Monolayer Assay Index (MMAI). The purpose of MMAI is to determine whether the patient can receive units of blood by analyzing the assay. The index is the percentage of RBCs adhered, ingested, or both (for the total) versus free monocytes. Manual methods for blood cell counting may take several hours and are highly prone to different sources of errors. Automatic methods, such as Linear Discriminant Analysis, Quadratic Discriminant Analysis, K-Nearest Neighbors, Naïve Bayes, Support Vector Machine, Convolutional Neural Network (CNN), Fast Region-based CNN, Faster Region-based CNN, Spatial Pyramidal Pooling network, Single Shot Detector and Mask Region-based CNN (Mask R-CNN), exist for classification. However, these methods currently do not perform automatic counting and calculation of MMAI. Our datasets are the Blood Cell Count Dataset (publicly available) and our own collection. For the labels in our own collection, we performed polygonal annotation using the makesense.ai tool. We trained the Mask R-CNN deep neural network model for automatic segmentation at the pixel-level, using COCO pre-trained weights. Initial results look promising, as the Mask R-CNN is able to perform automatic segmentation accurately. Future work will involve creating a custom model that will consider the MMAI in the loss function.

PA-17 Room 17 ***Bioinformatic Approaches in Elucidation of the Evolution and Functional Characterization of Natural Product Methyltransferases***

Stephanie Provenzano, Stephanie Provenzano, Ryan Miller, Phillip Kilgore, Urska Cvek, Elahe Mahdavian, Vonny Salim
Louisiana State University Shreveport, Louisiana State University Shreveport

Natural product methyltransferases (NPMTs) play crucial roles in creating a diverse array of pharmaceutically active compounds. These NPMTs are of particular importance as methylation of specialized metabolites in medicinal plants contributes to changes in the chemical properties of these compounds. Furthermore, the addition of a methyl group has been seen to stabilize compounds and decrease toxicity for human consumption. With a large number of NPMTs still to be determined, there has been recent interest in the functional characterization of these genes. However, due to a small number of biosynthetic genes that have been biochemically characterized, the NPMT classification system is ambiguous. Our goal is to delineate a more

appropriate classification system using sequence alignment via the high-throughput Basic Local Alignment Sequence Tool (BLAST), phylogenetic relationships, and conserved domains, such as the Rossman fold and protein dimer formation, using computational 3-D molecular modeling. We consider the roles of the Rossman fold binding site to AdoMet, the methyl group donor, and dimerization which dictate the architecture of the NPMTs and contributes to their unique substrate specificities. This study will provide a framework for structure-based elucidation and biochemical characterization of novel natural product biosynthetic genes.

PA-18 ***A Machine Learning Approach for Oyster Disease Prediction***

Room 18

Aasish Rijal, Md Wasi Ul Kabir, Thomas Soniat, Md Tamjidul Hoque
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Oyster production is an essential part of the economy of the Southeastern United States. Perkinsus marinus is a parasite that is deadly to oysters, and it is one of the primary causes of oyster fatalities. This project intends to develop an accurate Machine Learning (ML) model to predict oyster disease. We used the OysterSentinel website (https://www.oystersentinel.cs.uno.edu/) to collect a large dataset of oyster disease from across the northern Gulf of Mexico.. The dataset includes decades of samples from different oyster reefs and provides oyster infection levels alongside environmental data. The dataset contains missing data, so we explored different imputation methods such as Mean/Median/Most frequent, k-nearest neighbor (k-NN), and deep learning methods to impute the missing data. We selected a subset of features with the highest importance to reduce the feature set size using the Genetic Algorithm (GA) and Incremental Feature Selection (IFS) methods. We investigated randomized parameter optimization and exhaustive grid search methods for hyperparameter tuning. Lastly, we experimented with several machine learning methods and ensemble machine learning methods to find the optimal method. The initial results show relatively low Mean Absolute Error (MAE). Additionally, we developed a Graphical User Interface (GUI) to make the process of making predictions easier. The proposed ML method, backed by an easy-to-use GUI application, will help scientists predict future oyster diseases and take the necessary steps to reduce the oyster mortality rate.

PA-19 ***Using Language-based Features for ncRNA-protein Interaction Prediction***

Room 19

Krishna Shah, Duaa Alawad, Md Wasi Ul Kabir, Md Tamjidul Hoque
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Non-coding RNAs (ncRNAs) constitute about 98% of the total RNA population and are important in fundamental biological processes like post-transcriptional gene regulation. NcRNAs bind to RNA-binding proteins to elicit these functions; hence ncRNA-protein interaction (RPI) must be studied. Since the biological methods to identify RPIs are tedious and expensive, several classic and deep-learning machine learning models have been proposed as a solution. These models predict RPI probability using several features of RNA and protein, such as sequence, physicochemical properties, secondary and tertiary structure, et cetera. More importantly, with the success of the Transformer model in natural language processing (NLP), transformer models like RNABERT and Evolutionary Scaling Model (ESM) have been trained on abundantly available sequence data to create language-like representations of RNA and protein, respectively. These models encode information about several sequence features, including motifs, secondary structure, and tertiary structure, and produce embeddings that can act as a single source of input features. This study uses the embeddings from RNABERT and ESM models to train a state-of-the-art deep-learning model with CNN and BLSTM to predict the interaction probability between a protein and an RNA.

Poster Session Abstracts

PA-20 ***Nucleosome-Receptor Structure Studies Based on Bioinformatics and Molecular Modeling***
Room 20

Ran Sun, Thomas C. Bishop, Jiahao Li, John Daigre
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Next generation sequencing has enabled a wealth of biophysical data to be associated with DNA sequence, and widely available computing resources enable researchers to conduct multi-copy or ensemble based molecular dynamics studies that compare the structure and dynamics of 10's to 100's of different biomolecular complexes each containing hundreds of thousands of atoms. By combining bioinformatics and computational modeling, researchers can answer questions ranging from fundamental to clinical. Unification of these two approaches extends the capabilities of both in novel ways and enables cross validation of results from widely disparate data sets and methods. Here we demonstrate our use of a genome dashboard to leverage bioinformatics data to investigate relationships between chromatin folding and the hormone response mechanism using all-atom and coarse-grained modeling. Specifically, estrogen response elements in the human genome are identified by sequence and combined with experimentally determined nucleosome positioning data to generate models of nucleosome-receptor complexes. Molecular visualization of the 3D models is utilized to determine validity of the nucleosome-receptor complexes. All atom modeling is sufficient to identify any sterical clash and unfavorable contact of the receptor-DNA and receptor-histone. Combining the all-atom models with coarse-grain modeling based on informatics data enables us to probe the mechanism of action of this classic switching mechanism in the context of the local chromatin folding landscape. The tools and methods developed are not specific to the nucleosome-receptor complexes studied here. They can be applied to any nucleosome-protein complex for which a 3D structure or model of the protein-DNA system exits. The tools used in this project are available at https://dna.engr.latech.edu/~gdash/

PA-21 ***Utilizing Self-Organizing Maps to Improve Information Delivery of Venn Diagrams***
Room 21

Marjan Trutschl, Marjan Trutschl, Phillip Kilgore, Eric Clifford, Billy Tran, Adesewa Akande, Hyung Nam, Urska Cvek
Louisiana State University Shreveport, Louisiana State University, LSU Health Shreveport

Venn diagrams are a nearly ubiquitous tool to visualize Boolean sets; however, their method of aggregation causes information relating to the fine structure of the input data set to be lost. Although many extensions to this method have been proposed, many do not address the depiction of relationships between input records, restricting information gleaned from the visualization to generalizations about the sets in question. We developed a novel visualization technique to retain the birds-eye interpretation of Venn Diagrams while allowing for fine detail between individual records to be ascertained. We utilized Kohonen's self-organizing map (SOM) to direct placement of individual records within the Venn Diagram regions such that record similarity can be determined by their spatial similarity. Records that are collocated within a Venn Diagram region have a high degree of similarity, while those in neighboring regions have spatial similarity along their borders. We examined the utility of this new visualization through the inspection of its effects on both a synthetic dataset and an empirical proteomics data set. We found that it was able to separate data within each region within the Venn Diagram based on structure and that it could be used to highlight clustering of p-values within the empirical set.

PA-22 ***Time-Series Transcriptome Analysis of Encapsulated vs Embryo Body Mouse ES Cell Cultures***
Room 22 ***Treated with Retinoic Acid***

Anna Wilson,
Southern University and A&M College,

Poster Session Abstracts

The ability of embryonic stem cells (ESCs) to differentiate into any cell type of the body presents an opportunity to obtain neuronal progenitors capable of repairing nervous tissues. Specifically, particular studies have focused on generating GABAergic neurons from ESCs as a method to replace damaged neurons due to their ability to release the GABA inhibitory neurotransmitter. In this regard, studies have shown the potential of neural stem cell (NSC) transplantation, but a major drawback of this approach is that NSCs produced from stem cells have the ability to cause allogeneic responses, which can lead to tumor formation due to the heterogeneity of the neuronal populations being produced during culture. Thus, because teratogenesis after transplantation is possible, a better understanding on the molecular mechanism of ESC to GABAergic neuronal differentiation is required. In this regard, we previously reported that mouse ESCs encapsulated in hydrogels and treated with all-trans-retinoid acid (RA) were able to generate GABAergic neurons with high efficiency. However, the molecular mechanism associated with GABAergic differentiation through this differentiation protocol is not well known. To address this, we performed time-series transcriptome analyses on encapsulated vs standard embryoid bodies (EBs) of mouse ESCs treated with RA for two (2D-RA) or four days (4D-RA). Control cells were treated with vehicle only for two days. We found genes differentially expressed in EBs as compared to encapsulated cells. Particularly, Hap1 had decreased expression in EBs from C to 4D-RA but had constant expression in encapsulated C to 4D-RA. Hap 1 plays a role in delivery of GABAergic receptors to synapses; and therefore, Hap1 gene may be of interest in understanding the molecular mechanisms that direct ESC to synapses; and therefore, Hap1 gene may be of interest in understanding on the molecular mechanisms that direct ESC to excitatory versus inhibitory neuronal differentiation.

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