UMBC

AN HONORS UNIVERSITY IN MARYLAND

19th Annual Summer Undergraduate Research Fest

Hosted by the College of Natural and Mathematical Sciences

Wednesday, August 10, 2016

BTP	BUILD Training Program— NIH/National Institute of General Medical Sciences
HHMI Scholars	Howard Hughes Medical Institute
HPC REU	Interdisciplinary Program in High Performance Computing—A National Science Foundation's Research Experiences for Undergraduates Site
JCET	Joint Center for Earth Systems Technology
MARC U*STAR	Minority Access to Research Careers —Undergraduate Student Training in Academic Research Program—NIH/National Institute of General Medical Sciences
NSA Scholar	National Security Agency Scholar
NSF REM	National Science Foundation Research Experience and Mentoring
NSF REU	National Science Foundation Research Experience for Undergraduates Program in Chemical Sensing and Imaging at UMBC
SBTP	Summer Biomedical Training Program — CNMS and the UMBC Graduate School
SCI ART	Interface between Science and Art in the research laboratories of leading scientists, engineers and art conservators at the University of Maryland Baltimore County (UMBC), Johns Hopkins University, and the Walters Art Museum in Baltimore.
UBM	Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences—National Science Foundation

19th Annual UMBC Summer Undergraduate Research Fest

Event Schedule

Wednesday, August 10, 2016

All events will be held in the
Ballroom, University Center, 3rd Floor

8:30 am: Poster Set-up & Presenter Check-In Begins

Ballroom Lobby, University Center, 3rd Floor
Light Breakfast served

9:00 am – 10:30 am: Introductions & Oral Presentations

Ballroom, University Center, 3rd Floor

1.	Abraar Muneem and Junaid Bhatti	Independent Research
2.	Austin Gabel	MARC U*STAR
3.	Joel Tyson	MARC U*STAR
4.	Jana Hijji, Dillion Francis, and Matthew Orellana	MARC U* STAR
5.	Abigail Kramer and William Wang	HPC REU
6.	Benjamin Smith, Ethan Crasto, Sydney Kahmann and Paula Rodriguez	HPC REU, JCET

10:30 am – 12:00 noon: Poster Presentations

Ballroom, University Center, 3rd Floor

10:30 am – 11:15 am – Poster Session 1
11:15 am – 12:00 noon – Poster Session 2

12:00 noon – 12:30 pm: Mentor Recognition and Closing

Ballroom, University Center, 3rd Floor

We ask that all group photos be taken after the Closing.

Welcome

Welcome to the nineteenth annual UMBC Summer Undergraduate Research Fest. The College of Natural and Mathematical Sciences is honored to host this event. It is inspiring to see so many students participating and sharing the results of their summer research projects. Some of these projects are the result of independent agreements, but most have been made possible by grants or other funds dedicated to encouraging undergraduate research. All projects are associated with UMBC and require the support of research mentors. The mentors' passion for science and ongoing commitment to education are truly exceptional. I commend the students on their extraordinary efforts this summer, and thank each of the faculty, staff and graduate student mentors who have worked closely with them. Especially, I want to thank the staff members who are coordinating this special event - Caitlin Kowalewski, Research Coordinator; Rebecca Dongarra, Data and Events Coordinator; Kathy Sutphin, the Assistant Dean for Academic Affairs; and Justine Johnson, the Associate Director of the Meyerhoff Graduate Fellows Program. Best wishes for a very successful program.

William R. LaCourse, Ph.D.

Dean and Professor

College of Natural and Mathematical Sciences

SURF's 2016 Outstanding Mentors

At this *19th Annual Summer Undergraduate Research Fest*, we are pleased to acknowledge all of the researchers who have supported student researchers in their laboratories as "Outstanding Mentors" for 2016.

A research mentor is a trusted guide who supports and facilitates a mentee's development toward the realization of his or her short and long-term career and life goals. A research mentor also educates and encourages young scientists about the opportunities available to them as they consider careers in research. A research mentor also provides precious access to his or her research laboratory or project and gives mentees opportunities to contribute toward the 'active' scientific research activities, which may not otherwise be available to high school or undergraduate students.

On behalf of the College of Natural and Mathematical Sciences, the Program Directors and Coordinators of UMBC's summer programs, and especially the many participants in this summer's guided research experiences, we thank these mentors for their ongoing support of student research and for their willingness to invest their time and resources to contribute to UMBC's rich history of undergraduate research support.

We would also like to give special thanks to all of the post docs, graduate students and undergraduates in the mentor's research groups who have worked so diligently to support the mentoring of these SURF participants.

2016 Summer Research Mentors

Mentor Name	Presenter Name	Affiliation
Dr Kofi Adragni	Ephraim Alfa	HPC REU
	Huiyi Chen	HPC REU
	Kristen Hansen	HPC REU
	Mathew Prindle	HPC REU
Dr Songon An	Syrena Bracey	MARC U*STAR Trainee
Dr Bradley Arnold	Michael Matrona	NSF REU
Dr Sancita Balachandran	Emily Roberts	SCI ART
Dr Charles Bieberich	Shreya Agarwal	Independent Research
	Audrey Lawrence	UMBC
	Brantley Leaphart	SBTP Trainee
Dr Lee Blaney	Temitope Ibitoye	HHMI Scholar
Dr Eileen Brantley	Anna Gifty Opoku-Agyeman	MARC U*STAR Trainee

2016 Summer Research Mentors

Mentor Name	Presenter Name	Affiliation
Dr Rachel Brewster	Bryanna Canales	HHMI Scholar
	Austin Gabel	HHMI Scholar, MARCU*STAR
	Karndeep Singh	Independent Research
Dr Elizabeth Cherry	Jamshaid Shahir	MARC U*STAR, NSF REU
Dr Marie-Christine Daniel	Jashaun Bottoms	NSF REU
Dr Eduardo Davila	Tarik Hawkins	MARC U*STAR Trainee
Dr Ruben Delgado	Matthew Glover	JCET
	Shelbi Tippett	JCET
Dr Jeffrey Gardner	Da'Kuawn Johnson	MARC U*STAR Trainee
Dr Chris Geddes	Amirah Abukhdair	Independent Research
	Melissa Cyr	Independent Research
	Amanda Harvey	Independent Research
	Paula Ladd	Independent Research
	Karen Losito	Independent Research
	Verity MacDougall	Independent Research
	Daniel Pierce	Independent Research
	Melissa Roll	Independent Research
Dr Matthias Gobbert	Kallista Angeloff	HPC REU
	Carlos Barajas	HPC REU
	Sergio Garcia Tapia	HPC REU
	Rebecca Hsu	HPC REU
	Alyssa Hu	HPC REU
	Ishmail Jabbie	HPC REU
	Alexander Middleton	HPC REU
	George Owen	HPC REU
	Darren Stevens II	HPC REU
	Benjamin Whiteley	HPC REU
	Uchenna Osia	HPC REU
Dr Erin Green	Jeremiah Quijote	UBM
Dr Lisa Kelly	Elisa Castillo	NSF REU
Dr Minjoung Kyoung	Blake Ford	NSF REU
	Anthony Huynh	Independent Research
Dr William Lacourse	Quincy Richburg	SBTP Trainee
	Kayla Sims	SBTP Trainee
Dr Erin Lavik	Catherine Barron	NSF REU
Dr Jeff Leips	Tonya Burge	HHMI Scholar
	Kerria Burns	UMBC
Dr Wen Li	Taylor Patrick	MARC U*STAR Trainee
Dr Weihong Lin	Olubukola Abiona	MARC U*STAR Trainee
Dr Susan Lindquist	Austin Maduka	MARC U*STAR Trainee

2016 Summer Research Mentors

Mentor Name	Presenter Name	Affiliation
Dr Daniel Lobo	Junaid Bhatti	Independent Research
	Mark Ebeid	UBM
	Samantha Herath	UBM
	Caroline Larkin	Independent Research
	Abraar Muneem	Independent Research
	Mikhail Plungis	Independent Research
Dr Beth McGinty	Sarah Pollock	MARC U*STAR Trainee
Dr Patricia McGuiggan	Emily Roberts	SCI ART
	Laurence Spekterman	SCI ART
Dr Stephen Miller	Tsegaye Arficho	NSF REM
	Lian Jackson	NSF REM
	Ayana Mitchell	NSF REM
Dr Nagaraj Neerchal	Ethan Crasto	HPC REU
	Ross Flieger-Allison	HPC REU
	Sydney Kahmann	HPC REU
	Lois Miller	HPC REU
	Paula Rodriguez	HPC REU
	Benjamin Smith	HPC REU
	Danielle Sykes	HPC REU
	Pablo Valle	HPC REU
Dr Kevin Omland	Michael Rowley	UBM
Dr Bradford Peercy	Mary Aronne	HPC REU
	Samantha Clapp	HPC REU
	Soohwan Jung	HPC REU
	Abigail Kramer	HPC REU
	William Wang	HPC REU
Dr Matthew Pelton	Kyle Belluomo	NSF REU
Dr Marcin Ptaszek	Marcus Jordan	MARC U*STAR Trainee
	Kalen Sullivan	NSF REU
Dr Ryan Robucci	Meshach Hopkins	NSA Scholar
Dr Zeev Rosenzweig	Marie Desrochers	SC IART
	Sam Maina	SCI ART
	Hyo Park	NSF REU
	Rebecca Pontius	NSF REU
	Alex Taylor	SCI ART
Dr Katherine Seley-Radtke	Yafet Arefeayne	HHMI Scholar
Dr Gymama Slaughter	Lillie Cimmerer	SCI ART
	Khalid Elawad	SCI ART
	Janaya Slaughter	SCI ART
	Arowa Suliman	SCI ART
	Joel Tyson	MARC U*STAR Trainee

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2016 Summer Research Mentors

Mentor Name	Presenter Name	Affiliation
Dr Michelle Starz-Gaiano	Victoria Davenport	Independent Research
	Sylvia Edoigiawerie	UBM
	Nathan Shenkute	Independent Research
	Amelia Smith	Independent Research
Dr Maureen Stone	Ange Lydie Tchouaga	MARC U*STAR Trainee
Dr Michael Summers	Sophia Abbott	Independent Research
	Olufemi Ajayi	Independent Research
	Tawa Alabi	HHMI Scholar
	Sapna Basappa	Independent Research
	Natalia Batchenkova	Independent Research
	Paige Canova	Independent Research
	Hannah Carter	Independent Research
	Arthur Chinery	SBTP Trainee
	Bryce Edwards	Independent Research
	Dillon Francis	MARC U*STAR Trainee
	Heather Frank	Independent Research
	Julia Harmon	SBTP Trainee
	Jana Hijji	HHMI Scholar
	Aishwarya Iyer	HHMI Scholar
	Talayah Johnson	SBTP Trainee
	Nansen Kuo	Independent Research
	Ugonna Mbaekwe	HHMI Scholar
	Daniel Morris	Independent Research
	Ubiomo Oboh	Independent Research
	Colin O'Hern	Independent Research
	Matthew Orellana	HHMI Scholar
	Colin Poodry	SBTP Trainee
	Christina Quasney	Independent Research
	Amalia Rivera Oven	Independent Research
	Bailey Roberts	SBTP Trainee
	Carly Sciandra	Independent Research
	Phoebe Somani	HHMI Scholar
	Emre Tkacik	HHMI Scholar
	Stanley Wang	Independent Research
	Alexis Waller	BTP Trainee
	Jaeuk Yang	Independent Research
	Ae Lim Yang	Independent Research
Dr Susumu Tonegawa	Eudorah Vital	HHMI Scholar, MARC U*STAR
Dr Ryan White	Mai Lam	NSF REU

Alphabetical Listing of Poster Presenters

First Name	Last Name	POSTER #	POSTER SESSION
Sophia	Abbott	**64***	**Session 1**
Olubukola	Abiona	**20**	**Session 1**
Amirah	Abukhdair	**3***	**Session 2**
Shreya	Agarwal	**2**	**Session 1**
Olufemi	Ajayi	**55***	**Session 2**
Tawa	Alabi	**22***	**Session 2**
Ephraim	Alfa	**50***	**Session 1**
Kallista	Angeloff	**46***	**Session 1**
Yafet	Arefeayne	**72**	**Session 2**
Tsegaye	Arficho	**8**	**Session 2**
Mary	Aronne	**47***	**Session 1**
Carlos	Barajas	**46***	**Session 1**
Catherine	Barron	**35**	**Session 1**
Sapna	Basappa	**60***	**Session 2**
Natalia	Batchenkova	**7***	**Session 2**
Kyle	Belluomo	**36**	**Session 1**
Junaid	Bhatti	**17***	**Session 1**
Jashaun	Bottoms	**37**	**Session 1**
Syrena	Bracey	**59**	**Session 2**
Tonya	Burge	**76**	**Session 1**
Kerria	Burns	**14**	**Session 2**
Bryanna	Canales	**78**	**Session 1**
Paige	Canova	**80**	**Session 2**
Hannah	Carter	**68***	**Session 1**
Elisa	Castillo	**38**	**Session 2**
Huiyi	Chen	**50***	**Session 1**
Arthur	Chinery	**27***	**Session 2**
Lillie	Cimmerer	**28*, 29***	**Session 1, 2**
Samantha	Clapp	**47***	**Session 1**
Ethan	Crasto	**49***	**Session 1**
Melissa	Cyr	**15***	**Session 1**
Victoria	Davenport	**11***	**Session 2**
Marie	Desrochers	**32***	**Session 1**
Marie	Desrochers	**33***	**Session 2**
Mark	Ebeid	**70***	**Session 1**
Sylvia	Edoigiawerie	**57**	**Session 2**
Bryce	Edwards	**73**	**Session 2**

** Indicates research that is co-presented, half of the group is assigned to present during session 1 and the other half is assigned to present during session 2.*

Alphabetical Listing of Poster Presenters (continued)

First Name	Last Name	POSTER #	POSTER SESSION
Khalid	Elawad	**28*, 29**	**Session 1, 2**
Ross	Flieger-Allison	**48***	**Session 1**
Blake	Ford	**39**	**Session 2**
Dillon	Francis	**58**	**Session 1**
Heather	Frank	**19***	**Session 1**
Austin	Gabel	**16**	**Session 2**
Sergio	Garcia Tapia	**44***	**Session 1**
Matthew	Glover	**1***	**Session 2**
Kristen	Hansen	**50***	**Session 2**
Julia	Harmon	**23***	**Session 2**
Amanda	Harvey	**15***	**Session 1**
Tarik	Hawkins	**69**	**Session 1**
Samantha	Herath	**70***	**Session 2**
Jana	Hijji	**62**	**Session 1**
Meshach	Hopkins	**6**	**Session 2**
Rebecca	Hsu	**44***	**Session 1**
Alyssa	Hu	**44***	**Session 2**
Anthony	Huynh	**9**	**Session 1**
Temitope	Ibitoye	**12**	**Session 2**
Aishwarya	Iyer	**62**	**Session 2**
Ishmail	Jabbie	**45***	**Session 1**
Lian	Jackson	**54**	**Session 1**
Da'Kuawn	Johnson	**71**	**Session 2**
Talayah	Johnson	**64***	**Session 2**
Marcus	Jordan	**75**	**Session 1**
Soohwan	Jung	**47***	**Session 2**
Sydney	Kahmann	**49***	**Session 1**
Abigail	Kramer	**47***	**Session 2**

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Alphabetical Listing of Poster Presenters (continued)

First Name	Last Name	POSTER #	POSTER SESSION
Nansen	Kuo	**19***	**Session 1**
Paula	Ladd	**3*, 15***	**Session 1,2**
Mai	Lam	**34**	**Session 1**
Caroline	Larkin	**18**	**Session 2**
Audrey	Lawrence	**25***	**Session 2**
Brantley	Leaphart	**25***	**Session 1**
Karen	Losito	**21***	**Session 1**
Verity	MacDougall	**63**	**Session 2**
Austin	Maduka	**4**	**Session 1**
Sam	Maina	**32*, 33***	**Session 1, 2**
Michael	Matrona	**40**	**Session 2**
Ugonna	Mbaekwe	**60**	**Session 1**
Alexander	Middleton	**46***	**Session 2**
Lois	Miller	**48***	**Session 1**
Ayana	Mitchell	**61**	**Session 2**
Daniel	Morris	**7***	**Session 1**
Abraar	Muneem	**17***	**Session 2**
Ubiomo	Oboh	**68***	**Session 2**
Colin	O'Hern	**65**	**Session 1**
Anna Gifty	Opoku-Agyeman	**77**	**Session 1**
Matthew	Orellana	**58**	**Session 2**
Uchenna	Osia	**46***	**Session 2**
George	Owen	**45***	**Session 2**
Hyo	Park	**41**	**Session 1**
Taylor	Patrick	**83**	**Session 1**
Daniel	Pierce	**26**	**Session 1**
Mikhail	Plungis	**24**	**Session 2**
Sarah	Pollock	**79**	**Session 1**
Rebecca	Pontius	**42**	**Session 2**
Colin	Poodry	**66***	**Session 1**
Mathew	Prindle	**50***	**Session 2**
Christina	Quasney	**19***	**Session 2**
Jeremiah	Quijote	**74**	**Session 1**
Quincy	Richburg	**51**	**Session 2**
Amalia	Rivera Oven	**82**	**Session 1**

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Alphabetical Listing of Poster Presenters (continued)

First Name	Last Name	POSTER #	POSTER SESSION
Bailey	Roberts	**23***	**Session 1**
Emily	Roberts	**30*,31***	**Session 1, 2**
Paula	Rodriguez	**49***	**Session 2**
Melissa	Roll	**21***	**Session 2**
Michael	Rowley	**5**	**Session 1**
Carly	Sciandra	**27***	**Session 1**
Jamshaid	Shahir	**10**	**Session 2**
Nathan	Shenkute	**52**	**Session 1**
Kayla	Sims	**56**	**Session 2**
Karndeep	Singh	**67**	**Session 1**
Janaya	Slaughter	**29*, 28***	**Session 1, 2**
Benjamin	Smith	**49***	**Session 2**
Amelia	Smith	**11***	**Session 1**
Phoebe	Somani	**22***	**Session 1**
Laurence	Spekterman	**31*, 30***	**Session 1, 2**
Darren	Stevens II	**44***	**Session 2**
Arowa	Suliman	**29*, 28***	**Session 1, 2**
Kalen	Sullivan	**43**	**Session 1**
Danielle	Sykes	**48***	**Session 2**
Alex	Taylor	**33*, 32***	**Session 1, 2**
Ange Lydie	Tchouaga	**84**	**Session 2**
Shelbi	Tippett	**1***	**Session 1**
Emre	Tkacik	**53***	**Session 2**
Joel	Tyson	**-**	**ORAL**
Pablo	Valle	**48***	**Session 2**
Eudorah	Vital	**13**	**Session 2**
Alexis	Waller	**19***	**Session 2**
William	Wang	**47***	**Session 2**
Stanley	Wang	**66***	**Session 2**
Benjamin	Whiteley	**45***	**Session 2**
Jaeuk	Yang	**55***	**Session 1**
Ae Lim	Yang	**53***	**Session 1**

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Oral Presentations

1	Abraar Muneem and Junaid Bhatti	Independent Research
2	Austin Gabel	HHMI, MARC U*STAR
3	Joel Tyson	MARC U*STAR
4	Jana Hijji, Dillion Francis, and Matthew Orellana	MARC U*STAR
5	Abigail Kramer and William Wang	HPC REU
6	Benjamin Smith, Ethan Crasto, Sydney Kahmann and Paula Rodriguez	HPC REU, JCET

Program Acronyms

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UBM	Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences—National Science Foundation
UMBC	University of Maryland, Baltimore County

PAVING THE WAY FOR REGENERATIVE MEDICINE: CURATING PLANARIAN EXPERIMENTS IN A CENTRALIZED MATHEMATICAL DATABASE

Junaid Bhatti[1], Abraar Muneem[1], and Daniel Lobo[1]
[1]Department of Biological Sciences, University of Maryland Baltimore County, 1000 Hilltop Circle, Baltimore, MD 21250

For more than a century, scientists have been captivated by the regenerative capabilities of the planarian flatworm, which can regenerate a full body from almost any type of amputation. To understand the mechanisms controlling this extraordinary ability, research approaches based on surgical, pharmacological, and genetic manipulations have been used extensively to produce a huge dataset of experimental results disseminated through the literature. The rise of sophisticated machine learning algorithms and computational power has brought upon a novel way of studying these fascinating creatures. The Lobo Lab has developed a mathematical ontology for encoding regenerative experiments, together with an artificial intelligence method to automatically infer mechanistic models of regeneration. In this project, we have curated hundreds of additional experiments into a formal database, called Planform, which stores, in a mathematical language, thousands of planarian experiments and results performed in the past decade. The data includes the details of the experimental interventions, such as drug additions, genetic interference, and surgical manipulations, and their effects on the resultant morphologies. This curated dataset not only deal with the growth and shape of the worm, but also show how the presence, or the lack, of key genes, results in different patterns and morphologies in the worm. Planform is a freely-available, centralized collection of information that helps the scientific community search efficiently for experiments and morphologies published in the literature. More importantly, this resource is essential for the application of artificial intelligence methods to automatically reverse-engineer models that explain the regulatory mechanisms controlling the regeneration in these worms. The new dataset is already published and freely available in the dedicated website (http://lobolab.umbc.edu/planform), helping human scientists and the automated computational approach to find better models of planarian regeneration. All these efforts will pave the way for the next-generation applications in human regenerative medicine.

We thank the members of the Lobo lab and the planarian regeneration community for helpful discussions. This work is partially supported by the National Science Foundation (NSF) under award #1566077.

Oral Presentation 1 – Joint Presentation

UNDERSTANDING INDUCTION OF SUSPENDED ANIMATION IN ZEBRAFISH

Austin Gabel[1], Young-Sam Lee[2], Rachel Brewster[1]
[1]Department of Biological Sciences, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250
[2]Department of Biochemistry, Johns Hopkins University, 3400 N. Charles St.

Deprivation of oxygen, or ischemia, is observed in stroke, heart attack and cancer, and leads to severe depletion of intracellular energy. Depletion of adenosine triphosphate (ATP), the major cellular energy source, is believed to be irreversibly damaging to living tissues. Some organisms have adaptive mechanisms that prevent them from completely expending ATP under low or zero oxygen conditions. These processes are not well understood, but a prevailing idea is that arrest of activity or "suspended animation" prevents complete depletion of ATP. Zebrafish embryos arrest under anoxia within thirty minutes, suggesting arrest is triggered possibly involving a key change in metabolites. A favored model for oxygen sensing supports that the decrease ATP and corresponding increase in adenosine monophosphate (AMP) serve as the proximal signal to trigger arrest. Working in collaboration with Dr. Young-Sam Lee at Johns Hopkins University, we are utilizing metabolic profiling, an unbiased approach, to identify rapidly changing metabolites after exposure to anoxia in Zebrafish. Interestingly, the levels of lactate, a byproduct of anaerobic respiration, change dramatically and may precede the previously reported changes in AMP:ATP ratio. Current experiments are attempting to elucidate a possible role of lactate in signaling developmental arrest, as well as identifying other key metabolites.

This investigation was supported by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences.

Oral Presentation 2

A NOVEL, HIGH-DENSITY, POLYIMIDE NEURAL PROBE AND ITS BIOCOMPATIBILITY

Joel Tyson[1], Minhquan Tran[2], Gymama Slaughter[2]
[1]Department of Chemical, Biochemical and Environmental Engineering, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250
[2]Department of Computer Science and Electrical Engineering, UMBC, 1000 Hilltop Circle, Baltimore, MD 21250

Since the birth of neuroscience, neuroscientists have successfully used probes implanted in brain tissue to gather chemical, electrical and ligand-mediated signals in different parts of the brain over the short term. However, long term, chronic implantation of neural probes has eluded the field due to damage caused by general incompatibility with surrounding tissue. Surrounding brain tissue damage can be a result of the probe's size, inflexibility, and cytotoxicity. Development of a probe suitable for chronic implantation holds the promise of giving neuroscience a high-resolution picture of neurodegenerative diseases and long-term brain disorders.

We are addressing this need by fabricating multichannel, flexible neural probes using standard CMOS techniques. The probes are designed to enable simultaneous recording of neurophysiological activities at multiple sites in the brain using an array of four shanks with 16 gold pyramidal recording electrodes per shank measuring approximately 250 μm^2. The electrodes are connected to bonding pads by interconnect wires and are sandwiched between two non-absorbent, polyimide dielectric layers with windows in the first layer to expose the electrode and bonding pad sites.

The probe electrodes were tested using impedance spectroscopy and found to have an effective resistance of 158 kΩ on average at an AC frequency of 1kHz. Current experiments include the attachment of multi-walled, carbon nanotubes to the electrodes using DC potential amperometry. Preliminary data shows a reduction of impedance at 1kHz to as little as 9.87 kΩ after treatment.

Biocompatibility was tested using PC-12 Adh cell culture incubated on the probe, polyolefin, and extracellular matrix proteins, laminin and collagen. Cell viability and proliferation were measured using trypan blue- based hemocytometry. The results suggest that the polyimide neural probe exhibits desirable characteristics fSSor chronic implantation- high viability (>80%) and low proliferation (<40%), suggesting a low level of cytotoxicity.

This work was supported in part by the National Science Foundation (Award ECCS- # 1342912) and by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences.

Oral Presentation 3

5′ START SITE HETEROGENEITY OF THE HIV-1 RNA AND ITS EFFECT ON STRUCTURE AND FUNCTION

Dillon Francis[2], Matthew Orellana[1], Jana Hijji[3], Joshua Brown[1], Dr. Michael Summers[1]
[1]Department of Chemistry and Biochemistry, Howard Hughes Medical Institute, University of Maryland, Baltimore County, 1000 Hilltop Circle, Baltimore, MD 21250
[2]Department of Chemistry, University of West Florida, 11000 University Pkwy, Pensacola, FL 32514
[3]University of Maryland-College Park, College Park, MD 20742

The 5′ Leader (5′-L) of the human immunodeficiency virus-1 (HIV-1) RNA genome is highly conserved and constantly in an equilibrium between the monomer and dimer conformations. In the monomer conformation, the RNA is preferentially translated into proteins necessary for reproduction, while in the dimer conformation, the RNA is packaged as the genome for a new virion. The exact start site of the RNA has not been listed consistently in the literature in the past years. It was found that *in vivo*, there exists a mixed population of capped viral RNA with start sites that begin with one, two, or three guanosines (Cap1G, Cap2G, and Cap3G, respectively). This discrepancy had a profound effect on the folding patterns of the RNA, as it was observed using native gel electrophoresis Cap1G 5′-L favored the dimer conformation, whereas the Cap2G and Cap3G preferred the monomer conformation. This difference in start sites therefore influences the structure and function of the RNA. We use nuclear magnetic resonance spectroscopy to determine the exact structural mechanism by which start site differences direct this change. Using specific nucleotide- and site- specific labeling schemes, we were able identify a sensitive signal that is unique to the Cap2G construct only. Assigning signals in the full 5′-L is difficult due to the numerous signal overlap. To overcome this problem and assign the residue that the sensitive signal belongs to, we constructed smaller oligo controls of the full 5′-L. Our future works include making oligo control constructs of the TAR hairpin with different start sites to compare the signals.

This research was funded by NIH/NIGMS grant *1P50GM103297*, and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. Matthew Orellana was supported, in part, by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program, UMBC, and the Meyerhoff Scholars Program. We would like to thank our principal investigator Michael Summers for allowing us this opportunity to work in the lab, our graduate student Joshua Brown for his mentorship and guidance, and our lab members for their support.

Oral Presentation 4 – Joint Presentation

THE INTERACTION OF CALCIUM AND METABOLIC OSCILLATIONS IN PANCREATIC β-CELLS

REU Site: Interdisciplinary Program in High Performance Computing
Mary Aronne[1], Samantha Clapp[2], Soohwan Jung[3], Abigail Kramer[4], William Wang[5],
Graduate assistant: Janita Patwardhan[1], Faculty mentor: Bradford E. Peercy[1],
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Diabetes is a disease characterized by an excessive level of glucose in the bloodstream, which may be a result of improper insulin secretion. Insulin is secreted in a bursting behavior of pancreatic β-cells in the islets of Langerhans, which is affected by oscillations of cytosolic calcium concentration. We used the Dual Oscillator model to explore the role of calcium in calcium oscillation independent (CaI) versus calcium oscillation dependent (CaD) modes as well as the synchronization of metabolic oscillations in electrically coupled cells. We observed that voltage and calcium coupling result in increased synchronization and are more effective in CaD modes. Also increasing voltage coupling results in greater synchronization. Furthermore, we studied heterogeneous cellular bursting arrangements in the islets and their effects on synchronization. Calcium coupling has a larger impact on synchronization than voltage coupling, in the heterogeneous bursting scenarios. To better represent an entire islet, we altered previous code by further optimizing run-time and memory usage to allow for a greater number of cells.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Mary Aronne was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Janita Patwardhan was supported by UMBC.

Oral Presentation 5 – Joint Presentation

ENHANCED DATA EXPLORATION AND VISUALIZATION TOOL FOR LARGE SPATIO-TEMPORAL CLIMATE DATA

REU Site: Interdisciplinary Program in High Performance Computing
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This project builds on the research from past REU projects by enhancing a Graphical User Interface (GUI) for data exploration and visualization of spatio-temporal climate data from the Missouri River Basin (MRB) region. Teams from 2014 and 2015 REUs have built GUIs using the R software to facilitate the statistical downscaling process for precipitation and maximum/minimum temperatures using historical simulated data from the Global Climates Models (GCM) MIROC5 and HadCM3. Modeling attempts for temperature were largely accurate while precipitation proved more difficult to predict due to the semi-continuous distribution of rainfall. Therefore, our project seeks to complement predictive efforts by using visualizations to reveal spatio-temporal patterns such as underlying correlations and other trends in the data.

In this project several aspects of the GUI are enhanced by using the R package, Shiny, which allows greater control of the GUI design and thus will enable us to give more data visualization and exploration options. Specifically, the enhanced GUI enables an easy inter-comparison of MIROC5, HadCM3, and NCAR-CCSM4 in terms of prediction accuracy using bias, root mean-squared error (RMSE), and other metrics of interest for daily precipitation. Temporal trends and autocorrelation are determined through the use of time series plots, principal oscillation patterns (POPs), and sample autocorrelation function plots. Spatial correlation and patterns can be explored using contour plots, surface plots, and semivariograms. We will also provide calculation and visualization of cross-correlation matrices, empirical orthogonal functions (EOFs), and canonical correlation analysis (CCA).

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Oral Presentation 6 – Joint Presentation

Poster Session 1

First Name	Last Name	POSTER #	Program Affiliation
Sophia	Abbott	**64***	Independent Research
Olubukola	Abiona	**20**	MARC U*STAR Trainee
Shreya	Agarwal	**2**	Independent Research
Ephraim	Alfa	**50***	HPC REU
Kallista	Angeloff	**46***	HPC REU
Mary	Aronne	**47***	HPC REU
Carlos	Barajas	**46***	HPC REU
Catherine	Barron	**35**	NSF REU
Kyle	Belluomo	**36**	NSF REU
Junaid	Bhatti	**17***	Independent Research
Jashaun	Bottoms	**37**	NSF REU
Tonya	Burge	**76**	HHMI Scholar
Bryanna	Canales	**78**	HHMI Scholar
Hannah	Carter	**68***	HHMI
Huiyi	Chen	**50***	HPC REU
Samantha	Clapp	**47***	HPC REU
Lillie	Cimmerer	**28***	SCI ART
Ethan	Crasto	**49***	HPC REU, JCET
Melissa	Cyr	**15***	Independent Research
Marie	Desrochers	**32***	SCIART
Mark	Ebeid	**70***	UBM
Khalid	Elawad	**28***	SCIART
Ross	Flieger-Allison	**48***	HPC REU
Dillon	Francis	**58**	MARC U*STAR Trainee
Heather	Frank	**19***	Independent Research
Sergio	Garcia Tapia	**44***	HPC REU
Amanda	Harvey	**15***	Independent Research
Tarik	Hawkins	**69**	MARC U*STAR Trainee
Jana	Hijji	**62**	UMBC
Rebecca	Hsu	**44***	HPC REU
Anthony	Huynh	**9**	Independent Research
Ishmail	Jabbie	**45***	HPC REU
Lian	Jackson	**54**	NSF REM
Marcus	Jordan	**75**	MARC U*STAR Trainee
Sydney	Kahmann	**49***	HPC REU, JCET

Poster Session 1 (Continued)

First Name	Last Name	POSTER #	Program Affiliation
Nansen	Kuo	**19***	Independent Research
Paula	Ladd	**3***	Independent Research
Mai	Lam	**34**	NSF REU
Brantley	Leaphart	**25***	SBTP Trainee
Karen	Losito	**21***	Independent Research
Austin	Maduka	**4**	MARC U*STAR Trainee
Sam	Maina	**32***	SCIART
Ugonna	Mbaekwe	**60**	HHMI Scholar
Lois	Miller	**48***	HPC REU
Daniel	Morris	**7***	Independent Research
Colin	O'Hern	**65**	Independent Research
Anna Gifty	Opoku-Agyeman	**77**	MARC U*STAR Trainee
Hyo	Park	**41**	NSF REU
Taylor	Patrick	**83**	MARC U*STAR Trainee
Daniel	Pierce	**26**	Independent Research
Sarah	Pollock	**79**	MARC U*STAR Trainee
Colin	Poodry	**66***	SBTP Trainee
Jeremiah	Quijote	**74**	UBM
Amalia	Rivera Oven	**82**	Independent Research
Bailey	Roberts	**23***	SBTP Trainee
Emily	Roberts	**30***	SCIART
Michael	Rowley	**5**	UBM, Independent Research
Carly	Sciandra	**27***	Independent Research
Nathan	Shenkute	**52**	Independent Research
Karndeep	Singh	**67**	Independent Research
Janaya	Slaughter	**29***	SCIART
Amelia	Smith	**11***	Independent Research
Phoebe	Somani	**22***	HHMI
Laurence	Spekterman	**31***	SCIART
Arowa	Suliman	**29***	SCIART
Kalen	Sullivan	**43**	NSF REU
Alex	Taylor	**33***	SCIART
Shelbi	Tippett	**1***	JCET
Jaeuk	Yang	**55***	Independent Research
Ae Lim	Yang	**53***	Independent Research

REMOTE SENSING MONITORING OF CANADIAN WILDFIRE SMOKE AND ITS IMPACT ON BALTIMORE AIR QUALITY

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High spatial and temporal resolution Elastic *li*ght *d*etection *a*nd *r*anging (lidar) measurements allows to monitor long-range transport of particulates, such as dust and smoke, that impact local and regional air quality. These lidar measurements enhance current knowledge and understanding on how vertical layering and long range transport of natural and anthropogenic particle pollution may alter the relationship between column aerosol optical depth and surface particle pollution concentrations. We analyze the impact and frequency of the transportation of Canadian wildfire smoke to the Mid-Atlantic. We will present a statistical analysis of data from ground based air quality monitors and remote sensing instrumentation (lidar, satellite, and sun photometer) which yield the chemical, physical, and optical properties of particle pollution during these events.

This research is supported by NOAA-CREST/CCNY Foundation CREST Grant-NA11SEC481004.3, the Joint Center for Earth Systems Technology, and NOAA Office of Education Educational Partnership Program.

Poster 1

HABITAT USAGE AND NESTING BEHAVIOR OF THE CRITICALLY ENDANGERED BAHAMA ORIOLE

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The Bahama Oriole (*Icterus northropi*) is currently listed as a critically endangered species restricted to one island in the Bahamas. It was only recently classified as its own species in 2010, and very little research has been conducted regarding its behavior and population dynamics. In 2011, it was estimated that only 141-254 individuals still survived in the wild, and due to its recent extirpation from Abaco in the 1990's, it is only found on the island of Andros.

In May 2016, a team of UMBC undergraduate researchers led by Dr. Kevin Omland traveled to Andros to conduct preliminary research on the Bahama Oriole. We conducted point count surveys to census their population densities across five distinct habitat classifications: pine forest, hardwood forest, mixed pine/hardwood, agriculture/secondary growth, and developed land. Previous to this study, it was believed that the Bahama Oriole nested mostly in the coconut palm (*Cocos nucifera*) in developed habitats. However, we documented the orioles using all five habitat types. Furthermore, we documented nesting in different tree species, including pine trees (*Pinus caribaea* var. *bahamensis*) and species of understory palm deep in the pine forest. We will return to Andros in January to continue censusing during the non-breeding season.

This work was funded by The Explorer's Club, the NSF Interdisciplinary Training for Undergraduates in Biological and Mathematical Sciences (UBM), and the MBZ Species Conservation Fund.

Poster 5

STRUCTURAL DETERMINATION OF THE HIV-1 RRE-REV COMPLEX BY NMR

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Human immunodeficiency virus (HIV) needs to traffic its RNA genome toward the plasma membrane for packaging into new virions. Initially, unspliced and singly spliced viral RNAs are retained within the host cell nucleus. These RNAs contain a noncoding region of the HIV genome known as the Rev response element (RRE). HIV translates the accessory protein Rev that binds to RNAs containing the RRE. This RNA-Rev complex uses the CRM1 nuclear export system to transport the complex into the cytoplasm for translation or packaging.

We plan to characterize the structure of the RRE-Rev complex by Nuclear Magnetic Resonance (NMR). First, the RRE and Rev will be analyzed individually in their unbound, monomeric form. We worked toward identifying structural elements by comparing spectra of the full length RRE to those of an array of smaller fragments based on computational secondary structure predictions. Larger molecules such as the full length RRE produce NMR spectra that can be difficult to analyze due to broad, overlapping peaks. To simplify the spectra, the RRE was transcribed using various labeling schemes in which certain protons were replaced with deuterium. Signals replaced with deuterium are not present in ^{1}H-^{1}H NOESY spectra making proton assignment more manageable. To further simplify the spectra, we used segmentation, a technique in which two strands are designed such that the annealed product resembles full length RRE. These strands are differentially deuterated where specific signals are visualized while others are silenced. Once the RRE structure is understood, high-purity Rev is needed to study the complex. Currently, metal affinity chromatography of Rev is being optimized.

We hope to utilize these techniques to characterize the RRE, Rev, and RRE-Rev complex. By understanding the three-dimensional structure further directions can be made toward inhibiting viral genome export.

This research was funded by NIH/NIGMS grant #*1P50 GM103297*, and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. Special thanks are given to Michael Summers and Jan Marchant for their incredible support and guidance.

Poster 7

DEVELOPING TRANSIENT TERTIARY COMPLEXES WITH VARIOUS BINDING AFFINITIES

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Transient protein-protein interactions (PPI) occur in various processes throughout the cell and many types of diseases result from the alterations of these transient interactions. This is mainly due to the fact that we lack proper tools that can quantitatively characterize critical transient PPIs in real time.

We designed a set of protein-protein interactions as a function of binding stability to utilize them to evaluate our new tool, nano-reaction chamber to characterize transient PPIs. Mammalian target of rapamycin (mTOR) is a well-studied protein kinase that forms complexes that can regulate cell growth. Rapamycin inhibits the mTOR complex 1 (mTORC1) by binding on FK506 binding protein (FKBP) and FKBP-rapamycin binding (FRB) domain of mTOR with binding affinities of Kd = 26 μM ± 0.8 μM and Kd = 0.2 nM, respectively.[1] Mutations to these proteins will decrease binding affinity, which will lead to short-lived, transient interactions. Tyrosine 82 hydroxyl on FKBP was shown to interact with C8 carbonyl on rapamycin, so we next, use site-directed mutagenesis to modify that amino acid as well as other amino acids located nearby in the rapamycin binding pocket.[3] Finally, we will produce various transient tertiary complexes of the rapamycin, FKBP and the mTOR and use them to evaluate the new tool. This work enables us to demonstrate the feasibility of the new nano-reaction chamber and will contribute to quantitatively tackling critical and druggable short-lived PPIs in signaling and metabolic pathways.

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2 Tsang, C. K., Qi, H., Liu, L. F., & Zheng, X. F. S. (2007). Targeting mammalian target of rapamycin (mTOR) for health and diseases. Drug Discovery Today, 12(3–4), 112-124. doi:http://dx.doi.org/10.1016/j.drudis.2006.12.008

3 Van Duyne, G. D., Standaert, R. F., Schreiber, S. L., & Clardy, J. (1991). Atomic structure of the rapamycin human immunophilin FKBP-12 complex. Journal of the American Chemical Society, 113(19), 7433-7434. doi:10.1021/ja00019a057

Poster 9

CHARACTERIZING A ROLE OF THE *FAS3* GENE IN CELL MIGRATION

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Cell migration is an important area of scientific investigation as it is required for proper embryonic development, healing of injuries, and fighting against infection in organisms. While cell migration has these positive roles, it is also the mechanism responsible for cancer metastasis. In an attempt to obtain a full understanding of this process, we use the model organism *Drosophila melanogaster* because the genes regulating cell migration in flies are largely conserved in humans. The ovaries in the female fruit fly contain egg chambers that require a set of cells, called the border cells, to migrate for proper egg development. Within this cluster, there are polar cells which secrete migration signals to other cells in the group. Previous work has shown that manipulation of the *Fas3* gene, which encodes a homophilic adhesion protein, alters cell migration. We used a *D. melanogaster* mutant that has the *green fluorescent protein* gene fused to *Fas3* to visualize the location of Fas3 protein in the developing eggs. We found that the protein is located between the polar cells in the border cell cluster, promoting adhesion between the polar cells. To observe effects of Fas3 loss, we created homozygous mutants using two different alleles. We also used mutants that have insertions which result in knockdown of the gene's function. Since the polar cells need to adhere together to secrete migration signals, we expect to find that *Fas3* does have a role in border cell migration. Future research may reveal the exact means by which *Fas3* regulates cell migration in Drosophila, leading researchers to explore possible implications for similar adhesion proteins in human cell migration.

This research was funded in part by a National Science Foundation Career Award to Dr. Michelle Starz-Gaiano.

Poster 11

PAVING THE WAY FOR REGENERATIVE MEDICINE: CURATING PLANARIAN EXPERIMENTS IN A CENTRALIZED MATHEMATICAL DATABASE

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For more than a century, scientists have been captivated by the regenerative capabilities of the planarian flatworm, which can regenerate a full body from almost any type of amputation. To understand the mechanisms controlling this extraordinary ability, research approaches based on surgical, pharmacological, and genetic manipulations have been used extensively to produce a huge dataset of experimental results disseminated through the literature. The rise of sophisticated machine learning algorithms and computational power has brought upon a novel way of studying these fascinating creatures. The Lobo Lab has developed a mathematical ontology for encoding regenerative experiments, together with an artificial intelligence method to automatically infer mechanistic models of regeneration. In this project, we have curated hundreds of additional experiments into a formal database, called Planform, which stores, in a mathematical language, thousands of planarian experiments and results performed in the past decade. The data includes the details of the experimental interventions, such as drug additions, genetic interference, and surgical manipulations, and their effects on the resultant morphologies. This curated dataset not only deal with the growth and shape of the worm, but also show how the presence, or the lack, of key genes, results in different patterns and morphologies in the worm. Planform is a freely-available, centralized collection of information that helps the scientific community search efficiently for experiments and morphologies published in the literature. More importantly, this resource is essential for the application of artificial intelligence methods to automatically reverse-engineer models that explain the regulatory mechanisms controlling the regeneration in these worms. The new dataset is already published and freely available in the dedicated website (http://lobolab.umbc.edu/planform), helping human scientists and the automated computational approach to find better models of planarian regeneration. All these efforts will pave the way for the next-generation applications in human regenerative medicine.

We thank the members of the Lobo lab and the planarian regeneration community for helpful discussions. This work is partially supported by the National Science Foundation (NSF) under award #1566077.

Poster 17

PROTEIN: RNA INTERACTIONS THAT NUCLEATE HIV-1 VIRAL ASSEMBLY

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36 million people are currently infected with human immunodeficiency virus (HIV), a retrovirus responsible for the onset of the acquired immunodeficiency syndrome (AIDS). Upon transmission, the virus invades $CD4^+$ T cells and integrates its proviral genome into the host genome leading to a life-long infection. During the viral life cycle, interactions between the unspliced viral RNA and its translated product, the Gag polyprotein, initiate the packaging of two copies of the HIV genome. Gag contains three structured domains: Matrix (MA), Capsid (CA), and Nucleocapsid (NC). The NC domain of Gag binds to regions of the 5'-leader (5'-L) within the dimeric HIV-1 genome to initiate genome packaging and viral assembly.

We seek to characterize the Gag-RNA interactions essential to genome packaging using a truncated 5'-L derivative and a hexameric NC protein. The basic unit of the immature viral shell is a hexamer of Gag; mutations at the hexameric interface significantly reduce Gag's selectivity towards dimeric viral RNA. We hypothesize that the hexameric structure of the CA domain contributes to the dimeric RNA genome selection. However, hexamer-hexamer interactions in the C-terminal Domain (CTD) of CA lead to protein aggregation and precipitation in the presence of RNA. To circumvent these problems, we have fused the NC domain of Gag to a hexameric protein scaffold, which mimics hexameric Gag but forms isolated hexamers and does not aggregate in solution. The truncated 5'-L contains only the necessary regions needed for NC binding and packaging. With these RNA and protein constructs, we aim to deduce the qualitative conditions, thermodynamic parameters, and structural information of these Gag-RNA interactions using electrophoretic mobility shift assays, isothermal titration calorimetry, X-ray crystallography, and cryo-electron microscopy. These studies will further our understanding of the mechanism of HIV genome selection, a step of the life cycle that can be targeted with therapeutics.

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Poster 19

MATRIX BINDING TO $tRNA^{LYS3}$ IN HIV-1 INFECTED CELLS IS pH DEPENDENT

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When entering a host cell, the HIV-1 RNA genome is reverse transcribed into double stranded DNA by reverse transcriptase using human $tRNA^{Lys3}$ as a primer. Packaging of virions starts with the recognition of unspliced viral RNA by Gag and GagPol proteins, which form a complex that is targeted to the plasma membrane (PM) by the matrix domain (MA) on Gag. This binding is mediated through the Highly Basic Region (HBR) and N-terminal myristoyl group on MA and phosphatidylinositol 4,5-bisphosphate [$PI(4,5)P_2$] on the PM. In addition to $PI(4,5)P_2$, MA binds specific tRNAs including $tRNA^{Lys3}$. MA mutant studies suggest that $tRNA^{Lys3}$ binds to the HBR, which may regulate MA binding to $PI(4,5)P_2$ in the PM. However, it is unclear whether the N-terminal myristoyl group, which exists in an equilibrium between sequestered and exposed conformations, impacts MA-$tRNA^{Lys3}$ interactions. Isothermal titration calorimetry (ITC) was used to titrate $tRNA^{Lys3}$into myristoylated (myrMA), unmyristoylated (unmyrMA), and exposure-deficient L8I matrix proteins.

NMR data shows that matrix is predominately in the sequestered form at pH 7, but decreasing the pH will shift the equilibrium toward the exposed conformation. MA's ability to bind $tRNA^{Lys3}$ is pH dependent, as ITC results showed that at pH 5.5, myrMA and L8I binds less strongly to $tRNA^{Lys3}$ than at pH 7. Additionally at pH 7, myrMA behaves like unmyrMA and L8I. This suggests that the myristoyl group is responsible for changes seen at different pHs. The difference seen at pH 5.5 suggests that $tRNA^{Lys3}$ cannot bind exposed myrMA or that myrMA multimerizes in solution and prevents $tRNA^{Lys3}$ binding. These proposed mechanisms can be verified by solving the structure of myrMA-$tRNA^{Lys3}$ complex in solution.

Funding for this research was provided by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program, the Meyerhoff Scholars Program, the HHMI Exceptional Research Opportunities (EXROP) Fellowship, and the Summer Biomedical Training Program (SBTP) at UMBC.

Poster 22

GENE CLONING OF THE HIV-2 MATRIX PROTEIN

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In 1983, the human immunodeficiency virus (HIV) was discovered to be the leading cause of acquired immune deficiency syndrome (AIDS). HIV infects a type of T-lymphocyte cell critical to the immune system, and uses it as a means to spread and infect other cells, resulting in compromised immune function. There are two main subtypes of HIV: type 1 and 2 (HIV-1 and HIV-2, respectively). Although HIV-1 is responsible for the majority of AIDS infections, HIV-2 represents a significant number of cases in West Africa and is becoming increasingly prevalent in other areas. No cure for HIV exists, so research to better characterize HIV replication is necessary in order to identify novel drug targets. Assembly of the Gag polyprotein (Gag) to the plasma membrane is a plausible drug target. Gag assembles to the cellular membrane by the matrix protein (MA). HIV-2 MA requires the myristate, a fourteen carbon fatty acid, for its function. This myristate is linked to HIV-2 MA by the enzyme N-myristyltransferase (NMT). Previously, yeast NMT (yNMT) was used to prepare myristylated HIV-2 MA, but yNMT did not fully myristylate HIV-2 MA, resulting in the requirement for additional protein purification. This project aims to use human NMT (hNMT) to myristylate HIV-2 MA with the objective of preparing fully myristylated protein by performing gene cloning. In doing these analyses, ultimately myristylated HIV-2 MA may be prepared without the requirement for additional purification processes.

This project is supported by NIH/NIAID 5R37AI030917 and the Howard Hughes Medical Institute.

Poster 23

A NEW MOUSE MODEL OF HUMAN PROSTATE CANCER DRIVEN BY MYC OVEREXPRESSION AND PTEN LOSS

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Most forms of prostate cancer depend on the presence of androgen, a class of male hormones, which binds to androgen receptors located on the surface of the prostate cells and support growth. Androgen independent prostate cancer occurs after the disease has progressed to a state where it no longer relies on the presence of androgen, thereby making traditional treatments, including hormone deprivation therapy, ineffective. The goal of this project was to determine the *in vivo* growth characteristics of two newly-derived androgen independent mouse prostate cancer cell lines developed from a genetically engineered mouse model. Clonal cell lines from liver and lymph node metastatic sites in the BMPC mouse prostate cancer model (FVB/N background) were injected subcutaneously into athymic nude mice (Balb/c background) and FVB/N mice. Growth curves of xenograft tumors located in the immunocompromised athymic nude mice and FVB/N mice were determined by daily measurements of tumor size. The study showed that the cell line derived from the liver metastasis produced xenograft tumors in the athymic nude mice, as well as allograft tumors in the FVB mice. The results from the cell line grown from the lymph nodes will be presented. These data suggest that allografts of metastatic BMPC cell lines grown in immunocompetent FVB mice are a viable option for future pre-clinical trials of potential treatments for androgen independent prostate cancer. With the advent of new immunomodulatory biologics, this system provides a much needed platform to test the efficacy of these promising agents.

This work was supported by a grant from the Prostate Cancer Foundation.

Poster 25

STRUCTURE AND MECHANISM OF AN RNA THERMOSENSOR

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RNA thermosensors (RNATs) are non-coding RNA molecules found in the 5′-untranslated region (5′-UTR) of mRNAs and regulate the expression of the downstream gene as a function of temperature. RNATs are proposed to adopt a structure that occludes the ribosome-binding site (RBS) at low temperature, thus preventing translation. At elevated temperatures, the RBS is exposed, promoting translation. We are interested in the RNAT found in the 5′-UTR of prfA, a transcriptional activator that regulates the expression of a number of virulence genes in *Listeria monocytogenes*, which is an important human pathogen. Unlike well-characterized RNATs (4U, ROSE, and CSS), which gradually melt as a function of increasing temperature, the prfA RNAT utilizes a different mechanism, where there is a large functional change either permitting or inhibiting translation over a very narrow temperature range. Between 30 °C and 37 °C, there is no expression of PrfA, but at 38 °C there is significant amounts of PrfA expression. Using NMR spectroscopy we will probe the structure and mechanism of the prfA RNAT at different temperatures. Using a selective deuteration approach, we have obtained high-quality 1D proton and 2D proton-proton NOESY spectra of the 110-nt prfA RNAT at various temperatures. These preliminary spectra indicate that there is a large structural change over a narrow temperature window (3 °C). A detailed understanding of the structure and mechanism of the prfA RNAT will allow for the targeted design of a novel RNAT that functions at either higher or lower temperatures. Additionally, since PrfA controls a number of virulence genes in *Listeria monocytogenes*, it is a promising target for therapeutic development. The three-dimensional structure of the prfA RNAT will facilitate the design of small molecules that can bind to and "turn off" the prfA RNAT, even at elevated temperatures, which would normally promote translation.

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Poster 27

MUSIC AND MUSEUMS: AN INVESTIGATION INTO THE EFFECTS OF ACOUSTIC NOISE ON MUSEUM DISPLAYS AND ARTWORK

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Acoustic noise from social events that incorporate music can cause detrimental effects to museum objects by inducing vibration in these precious objects and the magnitude of the induced-vibration experienced by these objects is related to the intensity and frequency of the music along with the display environment. In this project we hypothesized that there is a correlation between the intensity of the acoustic noises at certain frequencies and the induced-vibration of museum display elements. Here, several glass object placed on a display were subjected to tones at controlled frequencies and intensities under numerous display conditions. The induced-vibrations were detected through the use of a wireless tri-axial accelerometer. The threat that these vibrations pose to museum objects can be modeled under multiphysics conditions to show that they are at risk of increased structural damage and stress.

Initial findings suggest that at intensities below 80 dB there is no significant evidence of a relationship between the vibration experienced and the display elements. Conversely, early trials suggest that at intensities exceeding 90 dB, changes in the vibration experienced inside the display case relate to the frequency of the tone being played, the presence of the Plexiglas cover and whether or not the display is freestanding.

We can infer that museum display elements do affect the vibration observed by the art objects and museums should account for the type of tones the art is exposed to when determining display environments. Future work will include a more extensive characterization of the effect of various intensities and frequencies of acoustic noise on the structures that support the artwork.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 28

ACOUSTIC INDUCED VIBRATION ANALYSIS OF GLASS ART OBJECT

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Museums display and preserve priceless pieces of cultural heritage however, music played during museum events could be endangering the very objects they are tasked with protecting. This project aims to characterize how art objects vibrate when subjected to acoustic stimulation at their resonant frequencies. This research investigates the effect of acoustic vibrations on glass objects using a tri-axial accelerometer. Vibration effects were modeled via the use of COMSOL Multiphysics and SolidWorks software.

The acceleration of the accelerometers was obtained to determine the vibration of the objects, the signal was then analyzed using the Fast Fourier Transform (FFT) to take the signal to the frequency domain. The data was also filtered and reconstructed in Matlab. This project aims to characterize how art objects vibrate when subjected to acoustic stimulation at their resonant frequencies.

Initial findings suggest a wine glass has three vibration mode shapes occurring at three distinct frequencies. At the first mode shape, the wine glass exhibited a bending behavior from side to side about the stem at 263.11 Hz, whereas at 660.12 Hz the top half of the wine glass expanded vertically illustrating the second mode shape. Lastly, the third mode shape exhibited an oscillating compression behavior at the lip of the glass. This third deformation appears to occur at the dominant resonant frequency 1212.9 Hz. Vibrations occurring at any of these three frequencies for extended periods of time can result in structural failure of the wine glass. In the future, the effect of the object's material, geometry, and defects on its vibration should be investigated.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 29

QUANTITATIVE ODDY TESTS OF MATERIALS USED FOR BOOK CONSERVATION, RESTORATION, DISPLAY, AND STORAGE

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A variety of materials are used to conserve, restore, store, and display books and paper including fabrics, adhesives, paper, and cleaning materials. These materials can off-gas harmful chemicals that can deteriorate the books and paper. The Oddy test, or the Accelerated Corrosion test, is used to determine if these materials might harm the books and paper they are supposed to protect. In this test, the materials are placed in a sealed container with copper, silver, and lead coupons. If corrosion of the metals is observed, it is assumed that the materials will also damage the books and paper and should not be used. Using the Walters Art Museum's Oddy Test Protocol, tests were run at Johns Hopkins University's Heritage Science for Conservation Laboratory on materials commonly used by the JHU conservators. Some modifications were made to the protocol including integrating Whatman #1 filter paper to test whether paper deterioration can be measured, comparing different polishing techniques on the copper and silver coupons, and integrating analytical techniques to detect corrosion. Before the test began, physical and chemical tests were performed on the sample materials and metal coupons to determine a baseline. These tests include mass, thickness, optical microscopy, Atomic Force Microscopy (AFM), colorimetry, and Infrared Spectroscopy. Corrosion is then measured 28 days after the start of the test, and these tests are still running. Once the testing is finished, we will repeat the baseline measurements and note any changes. In the future, we would like to integrate techniques such as Gas Chromatography (GC), High Performance Liquid Chromatography (HPLC), and Mass Spectrometry (MS) into the testing to measure and identify gas emission.

This project is supported by the Baltimore SCIART research experience for undergraduate students, a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore funded by the Andrew Mellon Foundation.

Poster 30

THE SECRET LIFE OF AN ANCIENT EGYPTIAN WEAVER: ADVANCEMENTS TO IDENTIFY DYES AND FIBERS ON AN ANCIENT EGYPTIAN BASKET

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A small, oval, coiled basket of the Ancient Egyptian New Kingdom Era (1550-1292 BCE) is on loan to the Johns Hopkins Archaeological Museum from the Eton College. The fibers and dyestuffs of the basket need to be identified to narrow its provenance and help link it to similar baskets identified during that era. This research aims to build a database of proposed dyes from Eton College including their historical background and their spectral, chemical, compositional, and anatomical properties as a step towards identification of the dyes. Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR) was performed on sample dyes to analyze their functional groups to be used for identification. X-Ray Photoelectron Spectroscopy (XPS) was used to identify metal elements found in the pigments representative of the dyes of interest. Scanning Electron Microscopy (SEM) was used to identify anatomical feature of fibers from the basket, thereby allowing us to identify the plant fiber used. Future research needs to create a replicated dye-fiber environment of the basket to compare to samples from the basket. They will both be analyzed using ATR-FTIR and XPS and then compared to each other for identification. Following this, conclusions can be drawn regarding what dyes are present, as well as a narrowing of its provenance.

This project is supported by the Baltimore SCIART research experience for undergraduate students, a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore funded by the Andrew Mellon Foundation.

Poster 31

GO FOR THE GOLD: AN INVESTIGATION INTO THE USE OF COSMETIC SPONGES FOR TARNISH REMOVAL FROM GILDED SILVER OBJECTS

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Since ancient times, cultures worldwide have been gilding objects to give them a metallic gold surface. Today art conservators are tasked with preserving these objects' integrity. Recent work at the Walters Art Museum revealed a problem for cleaning tarnished gilded silver objects. While cosmetic sponges have been used for the mechanical removal of silver tarnish, recent practice demonstrated that sponges remove thin gold layers just below tarnish on gilded silver objects, causing them to lose historic and aesthetic features. The goal of this study was to understand the effects of these mechanical conservation methods for tarnish removal, specifically by characterizing the sponge compositions, both on molecular and microscopic levels. Another aspect of this study was to understand whether or not extracts from the sponges were remaining on the object's surface after cleaning. We hypothesized that sponges with rougher texture would remove more gold and tarnish than those with smoother textures, and that solvents used to moisten sponges dissolved some sponge components, depositing them on the object surface. A variety of analytical techniques including Gas Chromatography (GC) and Inductively Coupled Plasma Mass Spectrometry (ICP:MS) as well as Scanning Electron Microscopy (SEM) with Energy-Dispersive X-ray Spectroscopy (EDS) and Fourier Transform-Infrared (FTIR) spectroscopy were used to study these problems. Our main finding so far is that sponges with greater roughness in their microscopic surface texture do remove more tarnish and gold from gilded silver object surfaces. Ongoing and future work will measure the abrasiveness of swabs as well as test the success of variations on the described cleaning techniques.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 32

SETTLING FOR SILVER: UNDERSTANDING THE INTERACTION OF ACIDIFIED THIOUREA SOLUTIONS AND THE SURFACES OF TARNISHED GILDED SILVER OBJECTS

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Tarnish is a challenge for silver preservation in applications from industrial electronics to jewelry. Aesthetically prized for its shine and color, silver's appearance is altered by tarnish layers, making its surface become dull and darker in color. For art conservators, traditional chemical cleaning methods for silver objects use an acidified thiourea solution. Despite best efforts to rinse this reactive solvent from the object's surface post-cleaning, museum staff have noticed that objects cleaned with thiourea re-tarnish at an accelerated rate. The goal of this study was to understand how thiourea solutions react with the surface of gilded silver objects and to characterize the complexes formed by this interaction. Our hypothesis is that thiourea is forming complexes with silver sulfides in the tarnish layer, and these may react more readily with the atmospheric environment. To study the potentially damaging effects of thiourea solutions on a valuable museum object, our laboratory recreated the object's surface by gold-plating silver coupons with electroless deposition. A variety of analytical techniques including Inductively Coupled Plasma Mass Spectrometry (ICP:MS) as well as Scanning Electron Microscopy (SEM) with Energy-Dispersive X-ray Spectroscopy (EDS) were used to study these problems. Our main finding so far is that in cleaning the coupons with multiple thiourea solutions separately prepared with three acids, different levels of pressure and mechanical effort are required for full tarnish removal. Ongoing and future work will analyze the coupon surfaces post-cleaning, as well as characterize the thiourea complexes formed on the surfaces of the coupons.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 33

DETERMINING THE ANALYTICAL PERFORMANCE OF VARIOUS MUTANT RNA AND DNA APTAMER-BASED BIOSENSORS FOR THE DETECTION OF THE AMINOGLYCOSIDE ANTIBIOTIC, GENTAMYCIN SULFATE

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There is a need for reliable and effective biosensors that can enable, for example, studies of biological systems to answer important biochemical questions and to provide therapeutic monitoring of patients for improved patient care. Electrochemical biosensors that utilize the conformation-switching ability of various aptamers are selective for specific analytes, sensitive to changes in analyte concentration, and can be easily altered for the detection of other analytes of interest. In this project, electrochemical aptamer-based sensors were modified with various mutated RNA and DNA aminoglycoside aptamers to determine the quantitative effects on sensor performance. These sensors were then used for the detection of the aminoglycoside antibiotic, gentamycin sulfate, in buffer and fetal bovine serum using square wave voltammetry (SWV) in order to determine the specificity, selectivity and sensitivity of each of these aminoglycoside aptamers. It was determined that these various aminoglycoside aptamers can detect gentamycin sulfate in both buffer and fetal bovine serum, but with a greater electrochemical signal change and binding affinity for gentamycin sulfate in fetal bovine serum. In order to further characterize the specificity, selectivity and sensitivity of these aminoglycoside aptamers for gentamycin sulfate, repeated trials should be conducted. In order to better predict the behavior of these aminoglycoside aptamers as reliable and effective biosensors in human beings, experiments should be conducted in increasingly complex biological media, such as blood.

This project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 34

DEVELOPING A 3D RETINAL TISSUE SCAFFOLD USING PEG-BASED HYDROGELS

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There is a need for an *ex vivo* model of the retina in order to further our understanding of retinal diseases. The objective of this project was to develop a method to create a 3D tissue scaffold of the retina with poly (ethylene glycol) (PEG)-based hydrogels. PEG-based hydrogels make excellent candidates for tissue scaffolds, because they are biodegradable, can be fine-tuned to mimic the extracellular matrix (ECM) of the target tissue, have a highly porous architecture, and can be rendered bioactive. The previous methods of forming hydrogels involve carbonyldiimidazole (CDI) activation and photopolymerization. These methods are not ideal as they are either too slow or require UV light, which is damaging to retinal tissue. As a solution, we synthesized a hydrogel via a Michael-type addition of PEG-diester-dithiol (PEG-SH) onto four-arm PEG vinyl sulfone (PEG-VS). In this reaction, the hydrogel crosslinks in under 30 seconds and without UV light. The PEG hydrogel itself is inert, so poly (L-lysine) was incorporated into the PEG-VS hydrogel precursor in order to make it cell-adhesive. In addition, we developed a casting technique to produce the hydrogel in virtually any desired shape with approximately 13 µm thickness. This technique will allow us in the future to produce the hydrogel into the multiple layers of the retina. In addition, we will characterize the mechanical properties of the new hydrogel, such as its storage modulus, swelling ratio, and mesh size. We propose that a well-characterized retinal 3D tissue scaffold will provide further insight for engineering retinal tissue for cell-replacement therapies following injuries and many other applications.

The project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 35

ELECTROMAGNETIC SIMULATION OF METAL NANOPARTICLES AND METAL NANOPARTICLE ASSEMBLIES

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The goal of this project is to perform rigorous electromagnetic simulations of two gold nanoparticles coupled to a quantum dot. It has been shown before that coupling two silver nanoparticles to a quantum dot produces a different scattering and absorption spectrum that a single silver nanoparticle exhibits. We are interested in seeing how light will respond to an identical system, but with gold nanoparticles instead of silver. A graduate student working in the same lab will attempt to experimentally measure the scattering and absorption of light on the exact system that I intend to model, whereby after we will be able to compare the calculations I performed to the experimental results.

To accurately model this system, a solid quantitative understanding of the coupled electric and magnetic fields inside the gold particle is necessary. To achieve this, I will use a numerical approach such as the Finite-Difference Time-Domain method. This numerical method calculates the electric and magnetic fields by solving Maxwell's Equations directly, making it a very intuitive and flexible method for determining the fields of interest. Once we know the fields, we can then relate these fields to the energy flux over the surface of the metal nanoparticle to yield a clear picture of the absorption and scattering due to the metal nanoparticle. To ensure that our simulations are giving us accurate results, we will first model a single uncoupled silver nanoparticle, as the absorption and scattering spectrum of this system is analytically solvable, letting us tell quantitatively whether our calculations are correct. From there, we will model the two silver nanoparticles coupled to a quantum dot and compare these with previously published results. Once we are confident our simulations are giving us accurate results, we will transition into modeling the desired gold nanoparticle quantum dot system.

THE DEVELOPMENT OF GOLD NANOPARTICLE-CORED DENDRIMERS AS A MULTIFUNCTIONAL DRUG DELIVERY SYSTEM FOR CHEMOTHERAPY

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Chemotherapy is administered in a manner that is not tumor-specific, and the drugs are generally distributed throughout the body. When the drugs become active in parts of the body other than the tumor, they are highly toxic, causing severe side effects. Gold nanoparticles have the potential to improve the transport and effectiveness of chemotherapeutic agents because their size aids in targeting tumors through the enhanced permeability and retention effect. The nanoparticles can also be designed for multiple functions by decorating them with tree-like molecules called dendrons and terminating the dendrons with different chemotherapeutic drugs, imaging dyes, and targeting agents. The dendrons can then combined around a central gold nanoparticle to form a multifunctional dendrimer.

In this project, second-generation poly(propyleneimine) dendrons were synthesized and attached to a tetraethylene glycol spacer terminated with thioctic acid. The thioctic acid molecule contains a cyclic disulfide group that will infer strong attachment onto the gold core. Once the spacers and dendrons were coupled, the dendron was grown to third-generation (8 branches) and its termini were modified so that the cisplatin drug molecules could be attached through a cleavable bond (acyl hydrazone) to allow for specific release into cancer cells. All intermediates were characterized using ^{1}H NMR spectroscopy (for the dendron) or mass spectrometry (for the cisplatin derivatives). The final product was characterized by NMR, thermogravimetric analysis and ICP-MS. Future studies will include attaching the cisplatin-terminated dendrons to gold nanoparticles.

The project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 37

QUANTUM DOTS CHEMICAL STABILITY AND THEIR INTERACTIONS WITH ZEBRAFISH EMBRYOS

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Quantum dots (QD) are being incorporated into many consumer products including: television screens, cell phone screens, computers and more. Their unique optical properties enable the expansion of modern technologies; however, they are made with heavy metals that are known to be toxic. The most commonly used QD is composed of cadmium, a known toxin. There is concern that the wide scale manufacturing and use of luminescent QD will have adverse impacts on the environment. However, not all quantum dots have the same chemical composition. By altering the core, shell and surface chemistry of a QD, it can increase colloidal stability and decrease the toxicity. In this account, we have systematically evaluated the toxicity of two QD formulations on embryonic zebrafish. We evaluated the biodistribution and abundance of apoptosis in 48-hour post fertilization zebrafish embryos exposed to QD composed of ZnSe or CdSe cores. Both QD compositions have a ZnS shell and a surface ligand of Di-hydrolipoic acid- 750MW Polyethylene glycol-methoxy. Colloidal stability of CdSe/ZnS/DHLA(750MW)PEG-OCH_3 was analyzed through absorbance, steady-state fluorescence and lifetime fluorescence measurements over the course of a week. According to steady-state fluorescence intensity, QD capped with the DHLA-(750MW)PEG -OCH_3 ligand were stable in water, E3 media, 10mM of phosphate buffer, and Phosphate Buffer Saline (PBS) solution containing 10mM phosphate 135mM of sodium chloride, while the QD in minimal media showed signs of degradation. This is in contrast to QD that are capped with mono-thiolated ligands like mercaptoundecanoic acid, which has been frequently used in biological experiments. The improvement in chemical stability will enable chronic exposure experiments of living organisms to QD, which were not accessible to the community until the development of the DHLA-PEG ligand capping ligand technology. Future stability studies should include DHLA-PEG ligands with various charges, as well as looking for alternatives to Cadmium based cores.

The project is supported by the Research Experience for Undergraduates and Undergraduate Veterans (REU/REV) Program of the National Science Foundation Center for Chemical Innovation on Sustainable Nanotechnology (CSN). CSN is funded by NSF Award No. CHE-1503048.

Poster 41

SYNTHESIS OF NOVEL HYDROPORPHYRIN ORGANOPLATINUM PHOTONICS MATERIALS AS ACTIVATABLE SINGLET OXYGEN PHOTOSENSITIZERS

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Photonic materials that can function as activatable singlet oxygen photosensitizers are of great interest because of their potential applications including *in vivo* imaging and cancer therapy. However, photonic materials based on tetrapyrrolic macrocycles that can selectively be activatable have yet to be reported. The aim of this research is the synthesis of novel hydroporphyrin organoplatinum photonics materials, and investigate the structure-photophysics relationship of such materials. This research would allow us to establish guidelines for the design of selectively activatable singlet oxygen photosensitizers.

Numerous syntheses were completed and analytical methods such as matrix assisted desorption/ionization-time of flight (MALDI-TOF) mass spectrometry, UV-Vis spectrophotometry, ^{1}H NMR, and singlet-oxygen ($^1O_2$) production were used to characterize products. Further experimentation with syntheses and photophysical properties are currently under investigation.

Future plans include the optimization and additional synthesis of other organoplatinum photonics materials while determining their structure – photophysical properties with pertinence to singlet oxygen production.

The project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 43

TENSOR PROPERTIES AND DECOMPOSITIONS IN DATA ANALYSIS

REU Site: Interdisciplinary Program in High Performance Computing
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A continuing effort to determine efficient ways to deal with large and high-dimensional data sets has led many to the area of multilinear algebra. With today's increasing computing power, it is now a more attractive option to make use of tensors to represent and analyze these data sets. Whereas matrices are two-way arrays with each element specified by two indices, tensors are N-way arrays with its elements specified by N indices. In this sense, tensors are higher-dimensional generalizations of matrices, and they can be sparse in many cases of data analysis.

We explore the properties of tensors as they are used to represent data, and take advantage of the ability to matricize them to apply readily known linear algebra techniques that apply to conventional matrices. We compare computations with tensors such as the Tucker decomposition to established techniques such as the singular value decomposition of matrices or principal component analysis. The Tucker decomposition attempts to express a tensor as a product of a potentially compressed tensor (known as the core tensor) and three factor matrices which are orthonormal. Many algorithms try to fit an Alternating Least Squares model to compute a plausible approximation. The objective is then to analyze the core tensor in hopes of obtaining a summary of the original data, and to find ways to compress it without losing meaningful information to obtain a simpler representation. Several areas and applications that have benefited from using tensors are psychometrics, chemical analysis, signal processing, and data mining. Data sets from different types of applications are used in our comparisons.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Darren Stevens II was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Jonathan Graf was supported by UMBC.

Poster 44

PERFORMANCE COMPARISON OF A TWO-DIMENSIONAL ELLIPTIC TEST PROBLEM ON INTEL XEON PHIS

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The Intel Xeon Phi is a processor with a theoretical peak performance of approximately 1 TFLOP/s in double precision. This project compares the performance of code on the Intel Xeon Phi. Specifically, we benchmark a reference code on two generations of the Intel Xeon Phi, code-named Knights Corner (KNC) and Knights Landing (KNL), and contrast to performance on one compute node with two CPUs. The second generation of Intel Xeon Phi, Knights Landing, just became available in Spring 2016. KNL uses MCDRAM memory, which is nearly 50% faster than the GDDR5 in the KNC version. KNL can have up to 72 cores interconnected by a 2D mesh network, whereas KNC only has on the order of 60 cores connected by a bi-directional ring bus. The KNL can be run as a processor or coprocessor, and can support a full stand-alone Linux OS. KNC can only be a coprocessor and can only support a Linux micro-OS.

The benchmark code solves a classical elliptic test problem, the two-dimensional Poisson equation with homogenous Dirichlet boundary conditions on a unit square domain. The partial differential equation is discretized by the finite difference method and the resulting system of linear equations with a symmetric positive definite system matrix solved by the conjugate gradient method. The same C implementation of the benchmark code with hybrid MPI+OpenMP parallelization is used on all hardware platforms.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Ishmail Jabbie was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Jonathan Graf was supported by UMBC. The authors would like to thank the Performance Research Laboratory, University of Oregon for providing access to the KNL hardware.

Poster 45

ELECTRICAL EXCITATION, CALCIUM SIGNALING, AND PSEUDO-MECHANICAL CONTRACTION IN CARDIOMYOCYTES: EXTENDING A PARTIAL DIFFERENTIAL EQUATIONS MODEL

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Calcium dysregulation is a significant cause of fatal cardiac arrythmias, but it is an incompletely understood phenomenon and difficult to predict. Heartbeat rhythm is governed by periodic membrane depolarizations causing the release of calcium ions into the cytosol of individual cardiomyocytes; the reaction of this calcium with contractile proteins triggers the overall contraction of the heart. These calcium wave patterns can be modelled as a system of coupled partial differential equations linking the excitation, signaling, and contraction of individual cardiomyocytes.

The starting point of this research is a model that includes the electrical system of the cell and establishes a one-way link from the electrical system to the chemical system. We extend the model to connect the chemical system to the electrical system and to incorporate a pseudo-mechanical component of calcium dynamics in cardiomyocytes. We extend the model further to include the impact of the efflux of calcium onto the electrical system.

A parallel implementation of a special-purpose numerical code using MPI is necessary to enable the long-time solutions of this large-scale system of partial differential equations. Numerical simulations examine the behavior of the system that arises from the feedback loops between the calcium system, the electrical system, and the pseudo-mechanical system.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Uchenna Osia was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Jonathan Graf was supported by UMBC.

Poster 46

THE INTERACTION OF CALCIUM AND METABOLIC OSCILLATIONS IN PANCREATIC β-CELLS

REU Site: Interdisciplinary Program in High Performance Computing
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Diabetes is a disease characterized by an excessive level of glucose in the bloodstream, which may be a result of improper insulin secretion. Insulin is secreted in a bursting behavior of pancreatic β-cells in the islets of Langerhans, which is affected by oscillations of cytosolic calcium concentration. We used the Dual Oscillator model to explore the role of calcium in calcium oscillation independent (CaI) versus calcium oscillation dependent (CaD) modes as well as the synchronization of metabolic oscillations in electrically coupled cells. We observed that voltage and calcium coupling result in increased synchronization and are more effective in CaD modes. Also increasing voltage coupling results in greater synchronization. Furthermore, we studied heterogeneous cellular bursting arrangements in the islets and their effects on synchronization. Calcium coupling has a larger impact on synchronization than voltage coupling, in the heterogeneous bursting scenarios. To better represent an entire islet, we altered previous code by further optimizing run-time and memory usage to allow for a greater number of cells.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Mary Aronne was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Janita Patwardhan was supported by UMBC.

Poster 47

DIMENSIONALITY REDUCTION USING SLICED INVERSE REGRESSION IN MODELING LARGE CLIMATE DATA

REU Site: Interdisciplinary Program in High Performance Computing
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This project aims at using a data-analytic tool called Sliced Inverse Regression (SIR) to reduce the dimension in the regression of monthly precipitation on historical data of several climate variables provided by Global Climate Models (GCM). The SIR approach enables us to identify a small number of linear combinations from a large list of predictor variables while still maintaining the prediction accuracy. Following SIR, we implement a simple non-parametric prediction method, the Nadaraya-Watson Estimator (NWE). NWE is adapted for a Tobit model in order to account for the semi continuous nature of the precipitation data to improve prediction accuracy.

We apply the SIR method on the data from the Missouri River Basin (MRB). We implement the methodology to data from the GCMs: MIROC5, HadCM3, and NCAR-CCSM4 with a temporal coverage of 1949-2010 at over 30,000 locations. The cluster Maya is used to parallelize the estimation by dividing the region into sub regions, each of which is assigned one node of the cluster. Some of the predictor variables that are included are precipitation, maximum/minimum temperature, sea-level pressure, relative humidity, and surface wind speed. Additional predictor variables are added to account for the spatial properties of the reduced dimensions. The results of the prediction carried out using SIR and NWE are compared to an alternate regression model to observe the accuracy of the results.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Danielle Sykes was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Poster 48

ENHANCED DATA EXPLORATION AND VISUALIZATION TOOL FOR LARGE SPATIO-TEMPORAL CLIMATE DATA

REU Site: Interdisciplinary Program in High Performance Computing
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This project builds on the research from past REU projects by enhancing a Graphical User Interface (GUI) for data exploration and visualization of spatio-temporal climate data from the Missouri River Basin (MRB) region. Teams from 2014 and 2015 REUs have built GUIs using the R software to facilitate the statistical downscaling process for precipitation and maximum/minimum temperatures using historical simulated data from the Global Climates Models (GCM) MIROC5 and HadCM3. Modeling attempts for temperature were largely accurate while precipitation proved more difficult to predict due to the semi-continuous distribution of rainfall. Therefore, our project seeks to complement predictive efforts by using visualizations to reveal spatio-temporal patterns such as underlying correlations and other trends in the data.

In this project several aspects of the GUI are enhanced by using the R package, Shiny, which allows greater control of the GUI design and thus will enable us to give more data visualization and exploration options. Specifically, the enhanced GUI enables an easy inter-comparison of MIROC5, HadCM3, and NCAR-CCSM4 in terms of prediction accuracy using bias, root mean-squared error (RMSE), and other metrics of interest for daily precipitation. Temporal trends and autocorrelation are determined through the use of time series plots, principal oscillation patterns (POPs), and sample autocorrelation function plots. Spatial correlation and patterns can be explored using contour plots, surface plots, and semivariograms. We will also provide calculation and visualization of cross-correlation matrices, empirical orthogonal functions (EOFs), and canonical correlation analysis (CCA).

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Poster 49

USING HISTORICAL DATA FOR RETROSPECTIVE PREDICTION OF RAINFALL IN THE MIDWEST

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The Missouri River Basin (MRB) is an important food-producing region in the United Stated and Canada. Climate variability and water availability affect crops production in this region. Past climate data have been recorded at various locations in the basin over a period of ten years. We use the data for a retrospective prediction of rainfall.

As the dimension of the data is relatively large, a sufficient dimension reduction approach is used to reduce the dimensionality of the data while preserving the regression information pertinent to rainfall. We use the nascent dimension reduction methodology called Minimum Average Deviance Estimation or MADE to reduce the dimensionality of the climate data. Since MADE is still a tool in development, we explored two of its intrinsic prediction methods and compared them to the Nadaraya-Watson prediction approach by a cross-validation method.

A parallel implementation of MADE and its prediction methods were carried out. A performance study was performed along with the application of the best prediction method to the MRB climate data.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Ephraim Alfa was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Poster 50

IMMUNE FUNCTION AND EFFECTS ON BLOOD CELLS IN RESPONSE TO THE FEEDBACK INHIBITION OF JAK/STAT SIGNALING BY APONTIC

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The immune system is the primary line of defense against infections in all multicellular organisms. This complex interconnected system is regulated by several pathways and proteins. Our lab mainly focuses on the JAK/STAT pathway that plays a critical role in regulating immune function. We hypothesize that this signaling pathway activates several downstream target genes that are involved in the process of phagocytosis. We used *Drosophila melanogaster* as our model organism to study the effect of altering the expression of a gene that we know regulates the JAK/STAT pathway called apontic (apt). A primary immune response is the engulfment and destruction of a pathogen in a process called phagocytosis, which is carried out by blood cells (hemocytes). In the study we are evaluating how the phagocytic ability in Drosophila changes in accordance to overexpressing as well as knocking down apontic in blood cells by using the Gal4/UAS system. In addition, we are also assessing the change in hemocyte count near the dorsal vessel to determine if this plays a role in the immune response. Knowing that the JAK/STAT pathway is involved in providing immune response to infections in humans, results from this study will likely provide an understanding about some of the key target genes that regulate the immune function in mammals.

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Poster 52

MATRIX BINDS SPECIFICALLY TO $tRNA^{Lys3}$

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Human immunodeficiency virus-1's (HIV-1) matrix domain (MA) of the Gag polyprotein targets Gag to the cell membrane through interactions between MA's highly basic region and phosphatidylinositol 4,5-bisphosphate [$PI(4,5)P_2$] on the cell membrane. Targeting to the plasma membrane is critical for the assembly of the virus. In addition to interacting with the plasma membrane, CLIP studies by the Bieniasz lab showed that MA specifically binds to certain tRNAs, including $tRNA^{Lys3}$, *in vivo*. Host $tRNA^{Lys3}$ acts as a primer for reverse transcription and also is packaged into budding virions. We confirmed that $tRNA^{Lys3}$ and MA form a complex *in vitro* using gel electrophoresis, and determined the thermodynamic properties of the interaction using isothermal titration calorimetry (ITC) to better understand how the interaction takes place. $tRNA^{IleGAT,}$ which was proven not to bind to MA through CLIP studies, was compared to $tRNA^{Lys3}$ using ITC. $tRNA^{Lys3}$ forms a one to one ratio with MA, while $tRNA^{IleGAT}$ forms a 0.5:1 ratio with matrix. Studying the interaction of HIV-1 MA and tRNAs will better our understanding of how these specific tRNAs regulate interactions with the plasma membrane. In the future we seek to determine the tRNA-MA complex structure, which could provide a target for future antiretroviral drugs for AIDS and HIV patients.

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Poster 53

THE OVEREXPRESSION OF CALVIN CYCLE ENZYME FRUCTOSE-BISPHOSPHATE ALDOLASE TO INCREASE GROWTH RATE IN ALGAE

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Algae are plant-like organisms that can be used for sustainable production of biofuels and other commercially valuable products. *Chlamydomonas reinhardtii,* a single celled green alga, has been used as a model organism to research algal biofuel production, due to its sequenced genome, ability to be genetically manipulated and its fast growth rate. Carbon dioxide (CO_2) is limiting for algal growth, so it is believed that certain enzymes that function in the Calvin cycle, which converts CO_2 into carbohydrates, may be key targets for improving photosynthesis and growth. Fructose-bisphosphate aldolase (FBA) functions in the regeneration phase of the Calvin cycle, and overexpression of this enzyme in higher plants improves growth significantly. We are testing the idea that overexpressing FBA will also increase flux through the Calvin cycle in algae. Using recombinant DNA techniques, we have generated *C. reinhardtii* transformants that contain the coding region for *C. reinhardtii* FBA under the control of *psbD* and *psbA* 5' and 3' regulatory sequences, respectively, integrated into the chloroplast genome. We are currently using western blot analysis to determine expression levels of FBA in theses transformants. Next we will use an algal multicultivator to compare the growth rate of the best expressing transformants to that for the recipient (wild type) strain. If overexpression of FBA improves *C. reinhardtii* growth, we will apply these methods to other algae, such as the biotechnology production organism *Chlorella.*

These results were obtained as part of the Research Experience and Mentoring (REM) program in the Department of Biological Sciences at the University of Maryland Baltimore County. This program is funded by a grant (REM supplement to NSF-EFRI-1332344) from the National Foundation (NSF) Directorate for Engineering (ENG) Office of Emerging Frontiers in Research and Innovation (EFRI).

Poster 54

MYRISTIC ACID'S EFFECT ON MYRISTOYLATION OF THE MATRIX PROTEIN

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Human immunodeficiency virus (HIV) is a serious global health problem that has resulted in 35 million deaths since the beginning of the epidemic. In the US alone it affects approximately 1.2 million Americans. In Maryland 1 out of 49 are at a risk for HIV in the population, meaning about 27.7 out of every 100,000 people. HIV has a matrix (MA) protein, which guides the Gag-genome complex to the plasma membrane of the cell to bind for assembly of new virions. We explored the necessity of supplemental myristic acid for myristoylation of HIV-1 MA protein. Ordinarily myristic acid is added during MA synthesis in *E. coli*, but this lowers the pH level, producing a small yield of protein. We hypothesized that if the *E. coli* cells in the media have sufficient native myristic acid, then the addition of myristic acid to the cells will not decrease the myristoylation rate in MA. If the myristic acid is not necessary, the yield will significantly rise, due to a more favorable environment for cells. To test this myrMA was expressed in *E. coli* cells with and without the addition of myristic acid, and purified through PEI precipitation, ammonium precipitation, cation exchange FPLC and size exclusion FPLC. Once the preparations were done, the myristoylation rate and protein yield was measured using hydrophobicity FPLC. Protein yield was confirmed with a Nanodrop spectrophotometer. Hydrophobicity FPLC showed that all matrix proteins were myristoylated. Without myristic acid the yield is 0.44 μmol and with myristic acid the yield was 0.27 μmol. In conclusion, we found that the addition of myristic acid produces a higher yield, but is not necessary for efficient myristoylation. Future protocols will include the addition of myristic acid.

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Poster 55

5′ START SITE HETEROGENEITY OF THE HIV-1 RNA AND ITS EFFECT ON STRUCTURE AND FUNCTION

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The 5′ Leader (5′-L) of the human immunodeficiency virus-1 (HIV-1) RNA genome is highly conserved and constantly in an equilibrium between the monomer and dimer conformations. In the monomer conformation, the RNA is preferentially translated into proteins necessary for reproduction, while in the dimer conformation, the RNA is packaged as the genome for a new virion. The exact start site of the RNA has not been listed consistently in the literature in the past years. It was found that *in vivo*, there exists a mixed population of capped viral RNA with start sites that begin with one, two, or three guanosines (Cap1G, Cap2G, and Cap3G, respectively). This discrepancy had a profound effect on the folding patterns of the RNA, as it was observed using native gel electrophoresis Cap1G 5′-L favored the dimer conformation, whereas the Cap2G and Cap3G preferred the monomer conformation. This difference in start sites therefore influences the structure and function of the RNA. We use nuclear magnetic resonance spectroscopy to determine the exact structural mechanism by which start site differences direct this change. Using specific nucleotide- and site- specific labeling schemes, we were able identify a sensitive signal that is unique to the Cap2G construct only. Assigning signals in the full 5′-L is difficult due to the numerous signal overlap. To overcome this problem and assign the residue that the sensitive signal belongs to, we constructed smaller oligo controls of the full 5′-L. Our future works include making oligo control constructs of the TAR hairpin with different start sites to compare the signals.

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Poster 58

SCREENING SMALL MOLECULE LIGANDS WITH THE CORE ENCAPSIDATION SIGNAL OF HIV-1 RNA AS A POTENTIAL DRUG TARGET

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Over 1.2 million people in the United States are infected with the human immunodeficiency virus type 1 (HIV-1). Current treatments target proteins that play important roles in various stages of the HIV-1 life cycle, but due to the high mutation rate of the virus, these drugs can only work for so long. One alternative is to develop therapeutics that target functional RNA elements within the highly-conserved 5′-untranslated region (UTR).

The core encapsidation signal (CES) was identified as a region within the 5'-UTR that is capable of directing packaging of the virus's dimeric genome. In the absence of this RNA element, HIV-1 virions cannot efficiently package their genomes, and therefore cannot produce infectious virions. The important role the CES plays makes it a potential drug target, and therefore the three-dimensional structure of this RNA was recently determined. Our research focuses on understanding how ligands bind to and modulate the CES structure. We use techniques such as nuclear magnetic resonance (NMR) spectroscopy and isothermal titration calorimetry (ITC) to characterize the sites of ligand binding and affinity. SOFAST HMQCs were performed on free and ligand bound CES and the resulting spectra were compared. Ligands that resulted in changes in the HMQC spectrum relative to that of free CES were identified as hits and further screened by ITC.

Out of 82 molecules, we identified 24 molecules as hits. We are currently using ITC to identify the binding affinity of these 24 small molecules. While these ligands bind to CES, it is not known whether they function as inhibitors of the genome packaging step of the HIV-1 replication cycle. Based on our experimental data, in vivo studies will be performed to further examine these effects. Our findings will aid in the development of a new drug that specifically targets the RNA genome.

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Poster 60

ASSIGNING THE SECONDARY STRUCTURE OF THE HIV-1 MONOMER-DIMER CONFORMATIONS

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The human immunodeficiency virus-1 (HIV-1) is a pandemic that affects thirty-seven million people worldwide, resulting in over 1.2 million AIDS-related deaths yearly. In order to attack this retrovirus and reduce the amount of deaths associated with HIV, we must first look at the HIV-1 replication cycle. During the late phase of the retroviral replication cycle, the 5′ Leader (5′-L) can remain as a monomer or base pair with another 5′-L molecule to form a dimeric complex. There is currently no drug therapy that targets this highly conserved portion of the viral RNA. In this monomer-dimer equilibrium, the monomer allows the RNA genome to be translated into Gag-pol, while the dimer is responsible for assembling an RNA-protein complex to be packaged into new virions. To further understand its function, we plan to characterize the secondary structure of the two conformations using nuclear magnetic resonance (NMR) spectroscopy. However, studying large RNAs by NMR is difficult because only four residues are present, thus resulting in limited chemical shift dispersion. We overcame this obstacle by using fragmentation techniques. Fragmentation uses smaller, synthesized hairpins that resemble portions of the longer stem loop. The NMR data of these fragments can be overlaid with the data from the full length 5′-L to assign and confirm the existence of structural elements. This method allowed us to confirm several structural elements in both the monomer and the dimer conformation. Our future work includes assigning the bottom of the TAR hairpin and the polyA stem loop in the dimer as well as confirm the U5: DIS interaction and the U5: AUG interaction in a native monomer and dimer construct, respectively.

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Poster 62

STRUCTURAL COMPARISON OF TRUNCATED AND FULL-LENGTH FELINE IMMUNODEFICIENCY VIRUS MATRIX PROTEIN BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

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The human immunodeficiency virus (HIV) remains a global health issue and warrants further research to address resistance to current treatment. To combat this issue, an animal model is necessary for understanding the processes that facilitate successful replication. Cats offer potential because the feline immunodeficiency virus (FIV) shares similar features to HIV. One of these features includes the trafficking of the Gag polyprotein to the plasma membrane, a process that is dependent on the N-terminal matrix (MA) domain. MA is comprised of a specific, six amino acid myristylation sequence that serves as a site for recognition and binding of a myristate moiety. Previous research has revealed that most mammals share a common myristylation signal, however FIV MA diverges from this pattern. Our research investigates the purpose of this unique myristylation signal by better characterizing the structure and function of the native FIV MA using nuclear magnetic resonance (NMR) spectroscopy. FIV MA features an unstructured, non-functional C-terminus, and truncation of this region has provided better stability, solubility, and higher yields compared to the full length (FL) FIV MA, ultimately resulting in better NMR spectra. FIV MA FL is most stable at pH 7, whereas solubility of truncated FIV MA was optimized at pH 8. In order to ensure that this change in pH did not significantly change the structure of FIV MA, NMR data was collected on FIV MA FL at pH 8 for comparison to spectra at pH 7. By making these comparisons between the truncated and full-length samples, this work can provide insight on methods that facilitate collection of long-term NMR experiments using a more soluble, stable, and highly concentrated FIV MA.

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Poster 64

CHARACTERIZATION OF THE UNIQUE MYRISTYLATION SIGNAL OF THE FELINE IMMUNODEFICIENCY VIRUS MATRIX PROTEIN

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The feline immunodeficiency virus (FIV) is a retrovirus, similar to the human immunodeficiency virus (HIV) in humans that suppresses and inhibits activity of the immune system in cats. Given that humans and cats have similar immune responses to these viruses, cats may serve as an animal model to develop HIV treatment. Both retroviruses feature the Gag polyprotein (Gag) with a matrix (MA) domain that targets and binds Gag to the plasma membrane during retroviral replication. The myristate moiety, a saturated fatty acid, is necessary for MA function. The myristate is covalently linked to MA co-translationally via N-myristyltransferase (NMT), an enzyme that recognizes a six amino acid myristylation signal. The myristylation signal of FIV MA is unique in comparison to the common mammalian myristylation signal whereas feline proteins follow the common sequence. This research aims to understand why FIV MA features a non-consensus myristylation signal. To answer this question, mutations were introduced to the native FIV MA myristylation signal to incorporate the common feline protein myristylation signal (FIV MA NOS). Preliminary studies indicated that, while native FIV MA was myristylated, FIV MA NOS was not myristylated. This work describes the characterization of the influence of specific residues in the FIV MA NOS mutant on myristylation efficiency. Mutations were introduced by mutagenesis and myristylation efficiencies of these mutants were judged by mass spectrometry results. Ultimately, these studies will help to understand why the myristylation signal of FIV MA is evolutionarily unique.

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Poster 65

STRUCTURAL ELUCIDATION OF THE REV-RRE COMPLEX IN HIV-1

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HIV-1 is a virus that leads to acquired immune deficiency syndrome, also known as AIDS. It is highly pathogenic, with approximately 2 million new cases every year, and up to 40 million people currently infected. The RRE and its binding partner the Rev protein are important for viral replication, as they are needed to help transfer viral RNA out of the nucleus.

The main goal of our research is to discover the structure of the RRE. Using a computer program known as Mfold, we have created several secondary structure predictions. Using NMR we have evaluated the full length RRE as well as specific fragments of that sequence. Comparing the NMR spectra from those fragments to the spectrum from the full length RRE, we are able to validate certain portions of our predicted RRE structure.

Another current objective in our research is to purify the Rev protein, which we overexpressed in *E.coli*. We are optimizing the purification process and will eventually analyze the protein using a range of methods, so that we can investigate and analyze the protein's structure as well as its interaction with the RRE.

Knowledge of the structures of the RRE and Rev protein, and how they interact, may allow therapeutics to be developed to target this stage of viral replication.

This work was supported by the Howard Hughes Medical Institute and National Institutes of Health Grant # 1P50 GM103297.

Poster 66

VAN-GOGH-LIKE 2, FRIZZLED, AND KNYPEK CONTROL DISTINCT ASPECTS OF POLARIZED CELLULAR MIGRATION DURING NEURAL CONVERGENCE

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The planar cell polarity (PCP) pathway plays a significant role in facilitating neural convergence (NC) – the narrowing of the neural plate before the formation of the neural tube. NC in zebrafish requires elongation and midline-directed polarized migration of neural plate cells. Failure of NC or the later stages of neural tube morphogenesis can result in severe neural tube defects (NTDs) which have been observed in all vertebrates studied. Although perturbation of the PCP pathway is associated with NTDs in model organisms and humans, the underlying neural cell behaviors remain elusive.

In order to investigate the cellular effects of the PCP pathway, we use *Knypek (Kny^{fr6}), Van gogh-like* 2 *(Vangl^{vu67}),* and *Frizzled 7a^{+}/7b^{-} (Fzd7a^{e3-}; Fzd7b^{hu3495})*, three zebrafish lines carrying null mutations. We confirmed the published result that mutations in the PCP pathway result in delayed NC. Our comparative cellular analysis revealed how cell elongation, membrane dynamics, and trajectory are affected in homozygotes. We show that wild type (WT) neural plate cells elongate and medially restrict membrane protrusions, thus narrowing the neural plate.

Preliminary data show that cells in all mutants initially failed to elongate, specifically *Vangl* and *Fzd* mutant cells extend randomized protrusions while *Kny* mutant cells show temporally restricted protrusive activity. In the PCP pathway, *Kny* is a *Fzd* co-receptor thought to present *Fzd* with various Wnt ligands, suggesting that the differences between these mutants are a ligand-independent aspect of PCP signaling during NC. While current literature understands how PCP genes regulate cell polarity and migration, the effect of these genes is poorly understood in neural tissue as the genes contribute to NTDs. By studying cell behavior in neural tissue, we may reveal how the PCP pathway promotes NC and identify additional genes affecting NTDs.

Thank you to Dr. Brewster, my mentor Sharlene Brown, and the current and past lab members for your guidance, contributions, and continuous support. This work was supported by funding from a Meyerhoff Graduate Fellowship, a U.S. Department of Education GAANN Fellowship, NIH R01GM085290, NIH R033HD076615, and Confocal Imaging: NSF MRI Grant DBI-0722569.

Poster 67

PROBING INTRAMOLECULAR INTERACTIONS IN THE HIV-1 5′-LEADER DIMERIC CONFORMATION

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The human immunodeficiency virus (HIV-1) is the causative agent of acquired immunodeficiency syndrome (AIDS), which was associated with 1.1 million deaths in 2015. The late phase of HIV-1 replication cycle is characterized by the equilibrium between the monomer and dimer conformations of the 5′ Leader (5′-L) in the RNA genome. Our model predicts that in both conformations, a hallmark interaction occurs with the Unique 5 region (U5) which characterizes the respective conformations; in the monomer, the U5 region is bound to the Dimer Initiation Site (DIS), and in the dimer, the AUG hairpin. The dimer is essential for virus reproduction, it binds to nucleocapsid and acts as the genome for a new virion during packaging. We synthesized a construct with modification that locked it into the dimeric conformation but prevented intermolecular dimerization. We called this construct locked dimer (LD). Using nuclear magnetic resonance (NMR) spectroscopy is particularly challenging for large RNA such as the 5′-L or LD. We overcame that obstacle by probing a small oligo control which mimics the chemical environment for the U5:AUG interaction. We then compared the spectrum from this oligo to the LD construct and found that the signals overlapped, confirming the existence of the U5:DIS interaction in LD. We next plan to compare these spectra with the native 5′-L. If the spectra overlap, that will be the first evidence of the U5:AUG interaction in the native dimeric 5′-L.

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Poster 68

A MATHEMATICAL AND COMPUTATIONAL FRAMEWORK FOR DISCOVERING MODELS OF SHAPE AND FORM REGENERATION

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Regenerative medicine aims to repair, rebuild, and restructure new tissue in an injured or amputated organism to fully restore functionality. Remarkably, planarian worms have the ability to regenerate a complete body, including new organs such as the brain, eyes, pharynx with the correct size and position, from almost any amputated piece. Understanding the mechanisms by which planarian flatworms regenerate can revolutionize medical techniques and treatment. Current models of planarian regeneration explain the emergence of appropriate body region patterning during regeneration, but no model or appropriate modeling technique exists to explain the restoration and allometric re-scaling of form and shape that occurs and are essential for planarian regeneration. In this work, we have combined a mathematical and computational approach for the discovery of mechanistic models of large-scale tissue regeneration and growth. We have developed a novel mathematical formalism based on partial differential equations to model full-body tissue regeneration. Importantly, this modeling framework includes cell density and growth and is able to describe mechanistic genetic networks controlling the restoration of shape and forms. In addition, we have integrated this new formalism into an artificial intelligence methodology for the automated reverse-engineering of quantitative models directly from experimental data. As a proof of concept, we have applied our novel framework to infer the mechanisms responsible for the allometric restoration of body shape in amputated trunk-pieces of planarian worms. Using a dataset of planarian experiments and their resultant morphologies, we have discovered a suitable, dynamic genetic model that accurately recapitulates the regeneration of shape and form in planarian worms after surgical amputations. This work paves the way for the understanding of how shape and form is restored through a regenerative process, an essential step towards the much sought-after tissue regeneration applications in human medicine.

We thank Santiago Schnell, the members of the Lobo Lab, and the planarian regeneration community for helpful discussions. We would also like to thank Jeffrey Leips and Nagaraj Neerchal for their support through the UBM program (NSF award #1031420). This work is also partially funded by the National Science Foundation (NSF) under award #1566077.

Poster 70

GENE EXPRESSION NETWORKS OF HISTONE METHYLTRANSFERASES IN *S. CEREVISIAE*

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Histone methyltransferases play a key role in the modification of chromatin to regulate gene expression. In 2014, Martin et al. discovered new functional consequences of deleting either one or both histone methyltransferases Set1 and Set5 in budding yeast, revealing that both are important for repressing lowly expressed genes near telomeres and retrotransposons. In the same year, Kemmeren et al. published microarray data for 706 strains of yeast lacking well-know chromatin regulators. Our study revisits the Martin et al. *set1*Δ, *set5*Δ, and *set1*Δ *set5*Δ mutant data and the Kemmeren et al. *set4*Δ data to investigate the functions of histone methyltransferases. After determining significant differentially expressed genes compared to a wild type (WT) strain, we performed Spearman's rho based correlation analysis between the *set1*Δ, *set5*Δ, *set1*Δ *set5*Δ, and *set4*Δ mutants and the microarray data containing the additional 706 strains. The correlation analysis and gene ontology (GO) analysis indicates that *SET4* has overlapping roles with gene *GPB2* which is involved in pseudohyphal and invasive growth, and that *SET1* and *SET5* have overlapping roles with genes that are involved with telomeres. Overall, this analysis expands our understanding of the functions and pathway relationships in gene expression regulation for three conserved histone methyltransferases Set1, Set5, and Set4.

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Poster 74

SYNTHESIS OF WATER-SOLUBLE BODIPY DERIVATIVES VIA "CLICK" REACTION

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The goal of this project was to synthesize BODIPY that was soluble in aqueous media through the addition of PEG-chains. BODIPY possesses spectroscopic properties that make it very useful for biomedical applications; however, these kinds of molecules are normally insoluble in aqueous media, such as human blood. In order to remedy this issue, we present PEG-ylated BODIPY compounds that are synthesized through the use of microwave-assisted "click chemistry". More specifically, azide derived PEG chains were reacted with BODIPY that contained a 2, 4, 6-tripropargyloxyphenyl substituent in order to yield a water soluble compound that does not aggregate in aqueous media. So far, this has only been observed for BODIPY, as it retains its optical properties while being water-soluble. Work is currently being done to observe similar trends in chlorins and porphyrins.

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Poster 75

VERIFYING THE GENES THAT PLAY A ROLE IN *DROSOPHILA MELANOGASTER* SURVIVAL OF *E. FAECALIS* BACTERIA

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Like many physiological traits, the ability of individuals to fight infection varies among individuals in natural populations. This variation has a strong genetic component. A previous genome wide association study (GWAS) identified single nucleotide polymorphisms (SNPs) involved in age-related immune dysfunction of *Drosophila melanogaster*. Using flies derived from a natural population at one and six-weeks of age, the study identified SNPs associated with survival and clearance of bacterial infection. The objective of this work is to use these GWAS findings to validate candidate genes involved in the immune response of *Drosophila melanogaster* at one week of age. We hypothesized that the reduced expression of a gene would produce negative effects on the immune system that would reduce the capacity to survive and clear infection of *Enterococcus faecalis*, a pathogenic bacterium. To test this hypothesis, we will manipulate the expression of genes (previously identified in a genetic mapping experiment) to test their effects on immune function. The expression of *dally*, a previously identified candidate gene, will be ubiquitously knocked down using RNA interference combined with the GAL4-UAS system, and the offspring will then be injected with the pathogenic bacteria, *E. faecalis.* Twenty-four hours post-infection, the flies will be checked for survivorship and assessed for their ability to clear infection. The findings from this experiment will be used to understand the genetic basis of variation in the immune system and contribute to the formation of treatments designed to restore immune function.

Tonya Burge was supported, in part, by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program, UMBC, and the Meyerhoff Scholar's Program.

Poster 76

STEMNESS GENE ALPHA6 INTEGRIN MEDIATES TAMOXIFEN RESISTANCE IN ESTROGEN RECEPTOR POSITIVE BREAST CANCER

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De novo and acquired resistance to the tamoxifen (TAM), an agent that's commonly used to treat estrogen receptor positive (ER+) breast cancer, have significantly diminished its clinical efficacy. Hence, a need exists to target molecules within breast cancer cells that promote tamoxifen resistance. Emerging evidence suggests breast tumor initiating cells (TICs) contribute to anti-cancer drug resistance, owing to their ability to evade treatment and self-renew. α6 integrin promotes TIC capability and survival via pathways associated with TAM resistance. Furthermore, previous studies indicate an association between α6vB (α6 integrin variant B) cytoplasmic expression and TIC potential. TAM increases TIC properties in mammary tumors, promotes mammosphere formation (an in vitro model enriched for TICs) and increases α6 integrin expression. In contrast, anti-tumor aryl hydrocarbon receptor (AhR) agonist aminoflavone (AF) disrupts mammosphere formation and thwarts α6 integrin expression. Consequently, we hypothesized that α6 integrin overexpression confers TAM resistance and suppressing α6 integrin expression counteracts TAM resistance. Quantitative reverse transcriptase PCR (qRT-PCR) showed elevated basal α6 integrin expression in both luminal A (with acquired TAM resistance) and luminal B (with de novo TAM resistance) ER+ cell lines. The Alamar Blue assay revealed that TamR cells exhibited sensitivity to AF. Semi-quantitative RT-PCR indicated α6B overexpression in TamR cells and the ability of AF to reduce both α6 integrin variant A and α6vB expression in TamR and parental cells. Anti-α6 integrin blocking antibody NKI-GoH3 sensitized TamR cells to the active TAM metabolite 4-hydroxy-tamoxifen and enhanced AF efficacy in these cells. These findings suggest α6 integrin behaves as a novel mediator of TAM resistance and highlight the therapeutic potential of anticancer AhR agonists such as AF to effectively counteract such resistance. This is significant since combating TAM resistance is expected to decrease breast cancer related mortality and improve clinical outcomes.

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Poster 77

UNDERSTANDING THE ROLE OF ELECTRON TRANSPORT CHAIN BLOCKAGE IN THE DEVELOPEMENTAL ARREST OF ZEBRAFISH

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Ischemia, a state of oxygen deprivation, is apparent in conditions such as heart attack, stroke, and cancer. Under anoxia (complete absence of oxygen), zebrafish embryos respond by halting their development, which reduces their oxygen dependence and prevents ATP depletion. Oxygen serves as the final electron acceptor in oxidative phosphorylation, the metabolic pathway that oxidizes nutrients and generates ATP via the Electron Transport Chain (ETC). Previous research has correlated developmental arrest with ETC blockage and reduced ATP production. Indeed, exposure of embryos to potassium cyanide (KCN), an ETC blocker, triggers developmental arrest under normal oxygen. It is therefore likely that KCN mimics the effect of an endogenous ETC blocker that is produced in response to anoxia. However, the signaling mechanisms connecting anoxia, ETC blockage, and developmental arrest, remain controversial. The goal of my research project is to compare the arrest response induced by anoxia and KCN. If ETC blockage is the signal downstream of anoxia that causes arrest, then the arrest response in anoxia and KCN should be very similar. I will evaluate the temporal profile of arrest under both conditions using cell proliferation as a quantitative assay. In addition, I will examine the organization of the microtubule cytoskeleton in anoxia and KCN-arrested embryos, since microtubules play a key role in epiboly progression. I expect that both anoxia and KCN will trigger a rapid arrest of proliferation, although KCN may induce a faster response since it directly targets the ETC. Furthermore, I anticipate that anoxia and KCN will both disrupt microtubule organization, resulting in epiboly arrest. These studies will increase our understanding of the adaptive response to anoxia and the underlying signaling mechanism. Future work will focus on the identification of the endogenously-produced ETC blocker.

Poster 78

IMPLEMENTERS' ATTITUDES TOWARD HEALTH HOMES FOR PEOPLE WITH SERIOUS MENTAL ILLNESS IIN THE PSYCHIATRIC REHABILITATION SETTING

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The passage of the Affordable Care Act allowed states to create Medicaid health homes, focused on improving somatic care for high-cost, high-need populations like consumers with serious mental illness (SMI). Health homes are designed to improve health outcomes for persons with SMI by coordinating the delivery of behavioral and somatic healthcare services. Maryland is the only state in the nation implementing the health home model in psychiatric rehabilitation programs (PRPs), a community-setting serving a high-need segment of persons with SMI. The objective of this project is to assess implementers' perceptions of facilitators and barriers to health home implementation in the PRP setting. We administered a 24-item, paper-and-pencil survey to 175 staff at PRP health homes in Maryland. The survey measured staff perceptions of the role of PRPs in improving physical health. The results show that 92% of the staff agreed that PRPs should incorporate improving physical health into their missions. 86% of the staff agreed that PRPs should monitor and manage health conditions like diabetes, and 91% agreed that PRPs should address all the health and social needs of their clients. These results suggest strong implanter buy-in to the health home program, which is an important factor in improving consumers' health outcomes.

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THE ROLE OF SPECIFIC tRNAs IN REGULATING MATRIX AND PLASMA MEMBRANE BINDING FOR INITIATION OF HIV-1 VIRION ASSEMBLY

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Currently 37 million people around the world are living with human immunodeficiency virus (HIV). The HIV-1 RNA genome is reverse transcribed into DNA using $tRNA^{Lys3}$ as a primer. Virion packaging is initiated when Gag and GagPol proteins are targeted to phosphatidylinositol 4,5-bisphosphate (PIP_2) on the plasma membrane (PM) via the highly basic region (HBR) of the matrix (MA) domain on the Gag protein. Mutations on the HBR can relocalize Gag to multivesicular bodies, disrupting the replication cycle. This is supported by liposome studies, which show that K18, K30, and K32 mutations in the HBR decrease MA binding to membranes containing PIP_2. The K26/27T mutation in the HBR decreases MA's specificity for PIP_2-containing membranes. Other studies show that RNA binding to MA maintains specificity of MA-PM interactions, as addition of enzymes to degrade RNA result in increased non-specific membrane binding. CLIP studies suggest that MA binds to specific host cell tRNAs, including $tRNA^{Lys3}$. We hypothesize that tRNA binding to MA acts as a regulatory mechanism in maintaining specificity to PIP_2 containing membranes, where PIP_2 out competes tRNA for MA binding, initiating virion assembly. To investigate this regulatory mechanism, we created and purified MA mutants that disrupt membrane binding, and using isothermal titration calorimetry we tested the effect such mutations have on tRNA-MA interactions. Compared to wildtype MA, the K18T mutant bound similarly to tRNA, while K30T and K32T mutants showed a decrease in tRNA binding. The K26/27T double mutant abolished MA's ability to bind tRNA, but single K26T and K27T mutants weakened the interaction. This suggests that the HBR, important for PM targeting, plays a role in binding to specific tRNAs and may regulate MA's interaction with membranes. Understanding such regulation may provide a target for future HIV therapeutics.

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Poster 82

CONTROL OF FREELY BEHAVING OPTOGENETIC RODENTS USING A BI-DIRECTIONAL NEURAL INTERFACE

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About 285 million people are vision impaired worldwide. The motivation of this project is to contribute to research in prosthetic vision, by using neural interfaces to provide light stimulation to optogenetic nerve cells in the visual cortex of the rodents. These devices may serve as a prototype or base technology that will eventually lead to the development of prosthetic vision. Our research focus was to validate whether a bi-directional neural interface can be used to produce prosthetic vision in freely behaving optogenetic rodents. The focus of this project is on the development and evaluation of a valid animal behavioral model to test the viability of the neural interface. In this study animals were trained to perform a reward based activity inside a training cage, which involved pressing a lever upon comprehending the given visual stimulus and receiving a food reward. Experiments were conducted that focused on the evaluation of the behavioral model using the reward based activity, which involved N=5 Long Evans female rodents, over 8 days of trial, with each trial taking place 30 minutes each occurring once a day for all experimental and training activities. Time delay data, the time interval between the presentation of the visual stimulus and the lever being pressed by the animal, was acquired from pre-surgical rodents using Intan RHD 2000 interface software and Open Ephys data acquisition system. It was found that the average time interval of receiving stimulus and pressing the lever associated with completing an experimental trial was 3-5 secs. Future investigation regarding the results received from the pre-surgical time delay data include how often the rodents are successful in pressing the lever, before the visual stimulus is removed. Future works will include the successful implantation of the neural interface, subsequent post-surgical experimentation and time delay data collection and analysis.

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Poster 83

Poster Session 2

First Name	Last Name	POSTER #	Program Affiliation
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Olufemi	Ajayi	**55***	Independent Research
Tawa	Alabi	**22***	HHMI
Yafet	Arefeayne	**72**	HHMI Scholar
Tsegaye	Arficho	**8**	NSF REM
Sapna	Basappa	**60***	Independent Research
Natalia	Batchenkova	**7***	Independent Research
Syrena	Bracey	**59**	MARC U*STAR Trainee
Kerria	Burns	**14**	UMBC
Paige	Canova	**80**	Independent Research
Elisa	Castillo	**38**	NSF REU
Arthur	Chinery	**27***	SBTP Trainee
Lillie	Cimmerer	**29***	SCI ART
Victoria	Davenport	**11***	Independent Research
Marie	Desrochers	**33***	SCIART
Sylvia	Edoigiawerie	**57**	UBM
Bryce	Edwards	**73**	Independent Research
Khalid	Elawad	**29***	SCIART
Blake	Ford	**39**	NSF REU
Austin	Gabel	**16**	HHMI Scholar, MARC U*STAR Trainee
Matthew	Glover	**1***	JCET
Kristen	Hansen	**50***	HPC REU
Julia	Harmon	**23***	SBTP Trainee
Samantha	Herath	**70***	UBM
Meshach	Hopkins	**6**	UMBC
Alyssa	Hu	**44***	HPC REU
Temitope	Ibitoye	**12**	HHMI Scholar
Aishwarya	Iyer	**62**	UMBC
Talayah	Johnson	**64***	SBTP Trainee
Da'Kuawn	Johnson	**71**	MARC U*STAR Trainee
Soohwan	Jung	**47***	HPC REU
Abigail	Kramer	**47***	HPC REU
Paula	Ladd	**15***	Independent Research
Caroline	Larkin	**18**	Independent Research
Audrey	Lawrence	**25***	UMBC
Verity	MacDougall	**63**	Independent Research

Poster Session 2 *(Continued)*

First Name	Last Name	POSTER #	Program Affiliation
Sam	Maina	**33***	SCIART
Michael	Matrona	**40**	NSF REU
Alexander	Middleton	**46***	HPC REU
Ayana	Mitchell	**61**	NSF REM
Abraar	Muneem	**17***	Independent Research
Ubiomo	Oboh	**68***	Independent Research
Matthew	Orellana	**58**	HHMI Scholar
Uchenna	Osia	**46***	HPC REU
George	Owen	**45***	HPC REU
Mikhail	Plungis	**24**	Independent Research
Rebecca	Pontius	**42**	NSF REU
Mathew	Prindle	**50***	HPC REU
Christina	Quasney	**19***	Independent Research
Quincy	Richburg	**51**	SBTP Trainee
Emily	Roberts	**31***	SCIART
Paula	Rodriguez	**49***	HPC REU, JCET
Melissa	Roll	**21***	Independent Research
Jamshaid	Shahir	**10**	MARC U*STAR Trainee, NSF REU
Kayla	Sims	**56**	SBTP Trainee
Janaya	Slaughter	**28***	SCIART
Benjamin	Smith	**49***	HPC REU, JCET
Laurence	Spekterman	**30***	SCIART
Darren	Stevens II	**44***	HPC REU
Arowa	Suliman	**28***	SCI ART
Danielle	Sykes	**48***	HPC REU
Alex	Taylor	**32***	SCIART
Ange Lydie	Tchouaga	**84**	MARC U*STAR Trainee
Emre	Tkacik	**53***	HHMI Scholar
Pablo	Valle	**48***	HPC REU
Eudorah	Vital	**13**	HHMI Scholar MARC U*STAR Trainee
Alexis	Waller	**19***	BTP Trainee
William	Wang	**47***	HPC REU
Stanley	Wang	**66***	Independently working with my mentor
Benjamin	Whiteley	**45***	HPC REU

REMOTE SENSING MONITORING OF CANADIAN WILDFIRE SMOKE AND ITS IMPACT ON BALTIMORE AIR QUALITY

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High spatial and temporal resolution Elastic *li*ght *d*etection *a*nd *r*anging (lidar) measurements allows to monitor long-range transport of particulates, such as dust and smoke, that impact local and regional air quality. These lidar measurements enhance current knowledge and understanding on how vertical layering and long range transport of natural and anthropogenic particle pollution may alter the relationship between column aerosol optical depth and surface particle pollution concentrations. We analyze the impact and frequency of the transportation of Canadian wildfire smoke to the Mid-Atlantic. We will present a statistical analysis of data from ground based air quality monitors and remote sensing instrumentation (lidar, satellite, and sun photometer) which yield the chemical, physical, and optical properties of particle pollution during these events.

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Poster 1

STRUCTURAL DETERMINATION OF THE HIV-1 RRE-REV COMPLEX BY NMR

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Human immunodeficiency virus (HIV) needs to traffic its RNA genome toward the plasma membrane for packaging into new virions. Initially, unspliced and singly spliced viral RNAs are retained within the host cell nucleus. These RNAs contain a noncoding region of the HIV genome known as the Rev response element (RRE). HIV translates the accessory protein Rev that binds to RNAs containing the RRE. This RNA-Rev complex uses the CRM1 nuclear export system to transport the complex into the cytoplasm for translation or packaging.

We plan to characterize the structure of the RRE-Rev complex by Nuclear Magnetic Resonance (NMR). First, the RRE and Rev will be analyzed individually in their unbound, monomeric form. We worked toward identifying structural elements by comparing spectra of the full length RRE to those of an array of smaller fragments based on computational secondary structure predictions. Larger molecules such as the full length RRE produce NMR spectra that can be difficult to analyze due to broad, overlapping peaks. To simplify the spectra, the RRE was transcribed using various labeling schemes in which certain protons were replaced with deuterium. Signals replaced with deuterium are not present in ^{1}H-^{1}H NOESY spectra making proton assignment more manageable. To further simplify the spectra, we used segmentation, a technique in which two strands are designed such that the annealed product resembles full length RRE. These strands are differentially deuterated where specific signals are visualized while others are silenced. Once the RRE structure is understood, high-purity Rev is needed to study the complex. Currently, metal affinity chromatography of Rev is being optimized.

We hope to utilize these techniques to characterize the RRE, Rev, and RRE-Rev complex. By understanding the three-dimensional structure further directions can be made toward inhibiting viral genome export.

This research was funded by NIH/NIGMS grant #*1P50 GM103297*, and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. Special thanks are given to Michael Summers and Jan Marchant for their incredible support and guidance.

Poster 7

IMPROVING ALGAL BIOFUEL PRODUCTION BY EXPRESSION OF CARBON CONCENTRATING MECHANISM ENZYMES

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Growing concerns over climate change are driving interest in development of renewable bioenergy to replace fossil fuels. Genetic manipulation of algae can make biofuel production more efficient. The photosynthetic green alga *Chlamydomonas reinhardtii* is a well-studied model organism that is easy to grow and manipulate at the molecular genetic level. This project focusses on a set of genes believed to be important for a carbon-concentrating mechanism (CCM) that acclimates algae to normal, CO_2-limiting conditions. Carbonic anhydrases are components of the CCM that catalyze the interconversion of carbon dioxide and bicarbonate, and thereby make inorganic carbon more accessible to the cell. The purpose of this project is to increase the intracellular concentrations of CO_2 in *C. reinhardtii* by overexpressing periplasmic and thylakoid membrane carbonic anhydrases, CAH1 and CAH3, respectively. *C. reinhardtii CAH1* and *CAH3* coding regions were synthesized with *C. reinhardtii* codon bias and epitope tags and the gene fragments were subcloned into expression vector pARG which contains the *ARG7* gene required for arginine biosynthesis. We transformed the *CAH1and CAH3* vectors into an *arg7* mutant strain and selected several ARG survivors for western blot analysis to determine the expression of protein. We will select the best expressing lines for growth curve and dry weight analyses to determine whether the transformants overexpressing *CAH1 or CAH3* are able to grow faster than the wild-type *C. reinhardtii* strain. In future both genes could be expressed together. The next step will be to manipulate these methods for microalgae that naturally produce higher lipid levels than *C. reinhardtii*, such as *Chlorella vulgaris*.

These results were obtained as part of the Research Experience and Mentoring (REM) program in the Department of Biological Sciences at the University of Maryland Baltimore County. This program is funded by a grant (REM supplement to NSF-EFRI-1332344) from the National Foundation (NSF) Directorate for Engineering (ENG) Office of Emerging Frontiers in Research and Innovation (EFRI).

Poster 8

USING DELAY DIFFERENTIAL EQUATIONS TO STUDY CALCIUM ALTERNANS IN A MODEL OF INTRACELLULAR CALCIUM CYCLING

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Cardiac arrhythmias are irregular beatings of the heart caused by disruptions in the electrical activity that triggers contraction. Electrical alternans, a period-2 behavior characterized by long and short action potential durations, is a mild arrhythmia that often degenerates into more life-threatening cardiac arrhythmias such as ventricular fibrillation. Of particular interest is calcium alternans, which is characterized by alternating large and small intracellular calcium concentrations in response to periodic stimuli and can lead to alternans at the cellular and tissue levels. Experimental findings have shown that this calcium cycling can exhibit alternans even when there is no alternans in the electrical dynamics, behavior that can be reproduced with the Shiferaw et al. model (2003) we use here. Despite the need to understand mechanisms for calcium-driven cardiac alternans, however, many ordinary differential equation models of intracellular calcium cycling do not produce alternans, thus restricting the scope of such models for studying alternans behavior. Delay differential equations (DDEs), which in many contexts produce complex dynamics, may be a promising tool for promoting alternans in cardiac models and have been shown previously to enhance alternans in the Shiferaw et al. model in a limited context. We extend this prior work by applying DDEs more broadly to the same model; specifically, we introduce DDEs in the equations for the calcium current gating variables, currents, and the release function. After suppressing alternans in the original model, we show that alternans can be induced by DDEs in certain compartments of the cell. We analyze the changes in the calcium concentrations, currents, and gating variables in response to these DDEs and discuss the mathematical and physiological implications of our findings. Our results provide further insight to understanding the role intracellular calcium cycling plays in the development of alternans.

This investigation was supported, in part, by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) from the National Institutes of Health, National Institute for General Medical Sciences. Our work was also supported by in part by the National Science Foundation through Grant DMS-1358583. We also thank Alfonso Bueno-Orovio, Rodrigo W. dos Santos, Johnny M. Gomes, and Yohannes Shiferaw for useful discussions.

Poster 10

CHARACTERIZING A ROLE OF THE *FAS3* GENE IN CELL MIGRATION

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Cell migration is an important area of scientific investigation as it is required for proper embryonic development, healing of injuries, and fighting against infection in organisms. While cell migration has these positive roles, it is also the mechanism responsible for cancer metastasis. In an attempt to obtain a full understanding of this process, we use the model organism *Drosophila melanogaster* because the genes regulating cell migration in flies are largely conserved in humans. The ovaries in the female fruit fly contain egg chambers that require a set of cells, called the border cells, to migrate for proper egg development. Within this cluster, there are polar cells which secrete migration signals to other cells in the group. Previous work has shown that manipulation of the *Fas3* gene, which encodes a homophilic adhesion protein, alters cell migration. We used a *D. melanogaster* mutant that has the *green fluorescent protein* gene fused to *Fas3* to visualize the location of Fas3 protein in the developing eggs. We found that the protein is located between the polar cells in the border cell cluster, promoting adhesion between the polar cells. To observe effects of Fas3 loss, we created homozygous mutants using two different alleles. We also used mutants that have insertions which result in knockdown of the gene's function. Since the polar cells need to adhere together to secrete migration signals, we expect to find that *Fas3* does have a role in border cell migration. Future research may reveal the exact means by which *Fas3* regulates cell migration in Drosophila, leading researchers to explore possible implications for similar adhesion proteins in human cell migration.

This research was funded in part by a National Science Foundation Career Award to Dr. Michelle Starz-Gaiano.

Poster 11

SPECTROPHOTOMETRIC DETERMINATION OF ACID DISSOCIATION CONSTANTS FOR ANTIBIOTICS

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Human-use and animal-use antibiotic pharmaceuticals have been widely detected all over the world in several sources of water including surface water, groundwater, and oceans. The negative impacts on the environment, due to the presence of antibiotics are rising, the foremost concern being antibiotic resistance. Several antibiotics have been declared critical to human use by World Health Organization, and the spread of resistance to such antibiotics is a serious public health concern. Hence, the study of the fate of antibiotics in the environment is critical. This work reports the spectrophotometrically determined acid dissociation constants (pKa) for 20 antibiotics including fluoroquinolones, sulfonamides, tetracyclines, macrolides, and ionophores. The pKa values describe the acid-base speciation for compounds in aqueous matrices, which affects a wide range of physicochemical properties and environmentally relevant behavior including adsorption, toxicity, and reactivity. In this study, antibiotic solutions at a concentration of 10 mg/L were buffered in the pH range of 2 to 11 with 10 mM phosphate buffer solutions, and the UV absorbance in the range of 200 to 900 nm was recorded. The data was then analyzed in MATLAB to generate contour maps. Since individual species of each antibiotic potentially shows distinct molar absorptivity behavior, the variation in the UV absorbance with a change in pH can be used to determine the pKa values. The spectrophotometrically determined pKa values were in agreement with those reported in the literature. Additionally, potentiometric titration was performed to validate results for antibiotics for which pKa values were available only from mathematical models. The results of this study demonstrate the applicability of spectrophotometric determination as a quick, inexpensive, simple and accurate method to study acid-base speciation of a wide range of antibiotics.

Temitope Ibitoye was supported, in part, by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program, UMBC, and the Meyerhoff Scholars Program.

Poster 12

THE ROLE OF DOPAMINE RECEPTOR 1 (D_1) AND *PPP1R1B*$^+$ BASOLATERAL AMYGDALAR (BLA) NEURONS IN FEAR EXTINCTION

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Fear extinction is the process by which an organism's fear response is diminished when they are repeatedly exposed to a conditioned stimulus. A key player in fear extinction is the BLA. Previous fear extinction studies in the BLA demonstrated that while neurons which previously responded to fear reduce their firing, additional distinct populations of BLA neurons are also recruited during fear extinction. Fear extinction is also thought to involve dopamine signaling in the BLA, based on the expression of dopamine receptor 1 (D_1) in the BLA, and pharmacological studies which implicated D_1 in extinction (Abraham et al. 2013). Therefore, in this study, we examined the role of D_1 in a distinct population of neurons recruited to the BLA during fear extinction in mice. Within the BLA there are two separate populations of neurons, *Ppp1r1b*$^+$- and *Rspo2*-expressing neurons, that define the posterior and anterior BLA, respectively. *Ppp1r1b*$^+$ neurons, mediate reward-related behaviors, whereas *Rspo2*$^+$ neurons mediate fear-related behaviors. Furthermore, these two populations have a reciprocal inhibitory relationship - when one is active the other is proportionally inactive. Here, we demonstrate that in response to fear extinction, *c-Fos* – an immediate early gene that correlates with neural activity - is expressed in the posterior BLA, which corresponds to the *Ppp1r1b*$^+$ neurons. Concurrently, *c-Fos* expression is reduced in anterior BLA, which corresponds to *Rpso2*$^+$ neurons. This suggests that the neurons that are recruited during fear extinction may include *Ppp1r1b*$^+$ neurons or a subset of them. In order to couple the function of D_1 to *Ppp1r1b*$^+$ neurons in extinction, we are currently developing genetic targeting strategies to knock down and to enhance D_1 expression in *Ppp1r1b*$^+$ neurons. This will allow us to examine the specific role of D_1 within *Ppp1r1b*$^+$ neurons during fear extinction. In doing so, we will also further validate the role of *Ppp1r1b*$^+$ neurons in fear extinction.

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Poster 13

DOES DIET MODULATE GENETIC INFLUENCES ON REPRODUCTION AND LIFESPAN?

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Natural selection reduces genetic variation at loci that affect fitness traits. This would seem to lead to a tendency toward genetic homogeneity within a population for genes that control these traits (survival and reproduction). One idea to explain the presence of variation at these loci is that a single gene has effects on multiple traits, possibly in opposite fitness directions. An example of this would be an allele that confers an advantage in early reproduction at a cost to lifespan. Alternatively, alleles that confer higher fitness in one environment may not do so in another; it is likely that both contribute to maintaining variation. In a previous study using *Drosophila melanogaster*, a number of candidate loci were identified that had different effects on reproduction and lifespan on different diets. We will test the hypothesis that these genes have environment dependent effects on fitness by knocking down the expression of candidate genes and examining their effect fitness traits on two diets. We will alter gene expression using RNA interference combined with the GAL4-UAS system in Drosophila. Female flies with reduced expression of genes implicated in these traits will be raised on both a low and high yeast diet (the main source of protein and cholesterol in fruit flies), and paired with a male. Reproduction will be measured by the number of eggs laid over a period of two days at one and five weeks of age, and lifespan from emergence from the pupal case until death. Control groups serve as a standard for comparison against which to draw conclusions about the effect, or lack thereof, of the experimental genes. If the genes do indeed have diet specific fitness effects, this information will lend itself to our understanding of the seemingly contradictory presence of genetic variation at fitness trait determining loci.

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Poster 14

UNDERSTANDING INDUCTION OF SUSPENDED ANIMATION IN ZEBRAFISH

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Deprivation of oxygen, or ischemia, is observed in stroke, heart attack and cancer, and leads to severe depletion of intracellular energy. Depletion of adenosine triphosphate (ATP), the major cellular energy source, is believed to be irreversibly damaging to living tissues. Some organisms have adaptive mechanisms that prevent them from completely expending ATP under low or zero oxygen conditions. These processes are not well understood, but a prevailing idea is that arrest of activity or "suspended animation" prevents complete depletion of ATP. Zebrafish embryos arrest under anoxia within thirty minutes, suggesting arrest is triggered possibly involving a key change in metabolites. A favored model for oxygen sensing supports that the decrease ATP and corresponding increase in adenosine monophosphate (AMP) serve as the proximal signal to trigger arrest. Working in collaboration with Dr. Young-Sam Lee at Johns Hopkins University, we are utilizing metabolic profiling, an unbiased approach, to identify rapidly changing metabolites after exposure to anoxia in Zebrafish. Interestingly, the levels of lactate, a byproduct of anaerobic respiration, change dramatically and may precede the previously reported changes in AMP:ATP ratio. Current experiments are attempting to elucidate a possible role of lactate in signaling developmental arrest, as well as identifying other key metabolites.

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Poster 16

PAVING THE WAY FOR REGENERATIVE MEDICINE: CURATING PLANARIAN EXPERIMENTS IN A CENTRALIZED MATHEMATICAL DATABASE

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For more than a century, scientists have been captivated by the regenerative capabilities of the planarian flatworm, which can regenerate a full body from almost any type of amputation. To understand the mechanisms controlling this extraordinary ability, research approaches based on surgical, pharmacological, and genetic manipulations have been used extensively to produce a huge dataset of experimental results disseminated through the literature. The rise of sophisticated machine learning algorithms and computational power has brought upon a novel way of studying these fascinating creatures. The Lobo Lab has developed a mathematical ontology for encoding regenerative experiments, together with an artificial intelligence method to automatically infer mechanistic models of regeneration. In this project, we have curated hundreds of additional experiments into a formal database, called Planform, which stores, in a mathematical language, thousands of planarian experiments and results performed in the past decade. The data includes the details of the experimental interventions, such as drug additions, genetic interference, and surgical manipulations, and their effects on the resultant morphologies. This curated dataset not only deal with the growth and shape of the worm, but also show how the presence, or the lack, of key genes, results in different patterns and morphologies in the worm. Planform is a freely-available, centralized collection of information that helps the scientific community search efficiently for experiments and morphologies published in the literature. More importantly, this resource is essential for the application of artificial intelligence methods to automatically reverse-engineer models that explain the regulatory mechanisms controlling the regeneration in these worms. The new dataset is already published and freely available in the dedicated website (http://lobolab.umbc.edu/planform), helping human scientists and the automated computational approach to find better models of planarian regeneration. All these efforts will pave the way for the next-generation applications in human regenerative medicine.

We thank the members of the Lobo lab and the planarian regeneration community for helpful discussions. This work is partially supported by the National Science Foundation (NSF) under award #1566077.

Poster 17

A COMPUTATIONAL METHOD FOR INFERRING MATHEMATICAL MODELS AND OPTIMAL TREATMENTS OF TUMOR SUB-CLONAL DYNAMICS

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Cancer is a disease arising from a variety of sub-clonal tumor cells dynamically interacting within themselves and the surrounding environment. This results in heterogeneous cancer phenotypes such as increased tumor volume and growth which are poorly understood. Sub-clonal tumor heterogeneity is a relatively new aspect of cancer, and its understanding is essential for the development of cancer therapeutics. It is shown that different sub-clones have varying impacts on overall tumor growth and their interactions are essential to maintaining the tumor proliferation. Sub-clones have been shown to result in variable phenotypes ranging from decreasing tumor volume to an extreme rise in tumor growth rates. To better understand the dynamics of sub-clonal tumor heterogeneity, we developed a computational framework to construct non-spatial, dynamic mathematical models of tumor heterogeneity. Our method uses high-performance computing to automatically infer models from the data, simulate them through time, and evaluate the in silico results in comparison to the results obtained from the experiments at the bench. The best-fitting model can accurately recapitulate tumor volume and clonal frequency data. Importantly, the reverse-engineered model can be used to predict the results of novel experiments, and hence determine the optimal clone or clones to target for intervention to make the tumor collapse. This project will vastly improve the efficacy of cancer therapies with the use of tumor-specific medication. Additionally, the inferred models may be used to accurately predict tumor growth over a period of time based solely off the genetic profile of the specific tumor. For cancer patients, instead of doctors using inefficient and risky trial and error technique of treatments, in silico testing for treatments using the patient specific inferred model will predict the best possible therapy.

We thank all the members of the Lobo Lab for the support and advice throughout the research project.

Poster 18

PROTEIN: RNA INTERACTIONS THAT NUCLEATE HIV-1 VIRAL ASSEMBLY

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36 million people are currently infected with human immunodeficiency virus (HIV), a retrovirus responsible for the onset of the acquired immunodeficiency syndrome (AIDS). Upon transmission, the virus invades $CD4^+$ T cells and integrates its proviral genome into the host genome leading to a life-long infection. During the viral life cycle, interactions between the unspliced viral RNA and its translated product, the Gag polyprotein, initiate the packaging of two copies of the HIV genome. Gag contains three structured domains: Matrix (MA), Capsid (CA), and Nucleocapsid (NC). The NC domain of Gag binds to regions of the 5'-leader (5'-L) within the dimeric HIV-1 genome to initiate genome packaging and viral assembly.

We seek to characterize the Gag-RNA interactions essential to genome packaging using a truncated 5'-L derivative and a hexameric NC protein. The basic unit of the immature viral shell is a hexamer of Gag; mutations at the hexameric interface significantly reduce Gag's selectivity towards dimeric viral RNA. We hypothesize that the hexameric structure of the CA domain contributes to the dimeric RNA genome selection. However, hexamer-hexamer interactions in the C-terminal Domain (CTD) of CA lead to protein aggregation and precipitation in the presence of RNA. To circumvent these problems, we have fused the NC domain of Gag to a hexameric protein scaffold, which mimics hexameric Gag but forms isolated hexamers and does not aggregate in solution. The truncated 5'-L contains only the necessary regions needed for NC binding and packaging. With these RNA and protein constructs, we aim to deduce the qualitative conditions, thermodynamic parameters, and structural information of these Gag-RNA interactions using electrophoretic mobility shift assays, isothermal titration calorimetry, X-ray crystallography, and cryo-electron microscopy. These studies will further our understanding of the mechanism of HIV genome selection, a step of the life cycle that can be targeted with therapeutics.

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Poster 19

MATRIX BINDING TO $tRNA^{LYS3}$ IN HIV-1 INFECTED CELLS IS pH DEPENDENT

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When entering a host cell, the HIV-1 RNA genome is reverse transcribed into double stranded DNA by reverse transcriptase using human $tRNA^{Lys3}$ as a primer. Packaging of virions starts with the recognition of unspliced viral RNA by Gag and GagPol proteins, which form a complex that is targeted to the plasma membrane (PM) by the matrix domain (MA) on Gag. This binding is mediated through the Highly Basic Region (HBR) and N-terminal myristoyl group on MA and phosphatidylinositol 4,5-bisphosphate [$PI(4,5)P_2$] on the PM. In addition to $PI(4,5)P_2$, MA binds specific tRNAs including $tRNA^{Lys3}$. MA mutant studies suggest that $tRNA^{Lys3}$ binds to the HBR, which may regulate MA binding to $PI(4,5)P_2$ in the PM. However, it is unclear whether the N-terminal myristoyl group, which exists in an equilibrium between sequestered and exposed conformations, impacts MA-$tRNA^{Lys3}$ interactions. Isothermal titration calorimetry (ITC) was used to titrate $tRNA^{Lys3}$into myristoylated (myrMA), unmyristoylated (unmyrMA), and exposure-deficient L8I matrix proteins.

NMR data shows that matrix is predominately in the sequestered form at pH 7, but decreasing the pH will shift the equilibrium toward the exposed conformation. MA's ability to bind $tRNA^{Lys3}$ is pH dependent, as ITC results showed that at pH 5.5, myrMA and L8I binds less strongly to $tRNA^{Lys3}$ than at pH 7. Additionally at pH 7, myrMA behaves like unmyrMA and L8I. This suggests that the myristoyl group is responsible for changes seen at different pHs. The difference seen at pH 5.5 suggests that $tRNA^{Lys3}$ cannot bind exposed myrMA or that myrMA multimerizes in solution and prevents $tRNA^{Lys3}$ binding. These proposed mechanisms can be verified by solving the structure of myrMA-$tRNA^{Lys3}$ complex in solution.

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Poster 22

GENE CLONING OF THE HIV-2 MATRIX PROTEIN

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In 1983, the human immunodeficiency virus (HIV) was discovered to be the leading cause of acquired immune deficiency syndrome (AIDS). HIV infects a type of T-lymphocyte cell critical to the immune system, and uses it as a means to spread and infect other cells, resulting in compromised immune function. There are two main subtypes of HIV: type 1 and 2 (HIV-1 and HIV-2, respectively). Although HIV-1 is responsible for the majority of AIDS infections, HIV-2 represents a significant number of cases in West Africa and is becoming increasingly prevalent in other areas. No cure for HIV exists, so research to better characterize HIV replication is necessary in order to identify novel drug targets. Assembly of the Gag polyprotein (Gag) to the plasma membrane is a plausible drug target. Gag assembles to the cellular membrane by the matrix protein (MA). HIV-2 MA requires the myristate, a fourteen carbon fatty acid, for its function. This myristate is linked to HIV-2 MA by the enzyme N-myristyltransferase (NMT). Previously, yeast NMT (yNMT) was used to prepare myristylated HIV-2 MA, but yNMT did not fully myristylate HIV-2 MA, resulting in the requirement for additional protein purification. This project aims to use human NMT (hNMT) to myristylate HIV-2 MA with the objective of preparing fully myristylated protein by performing gene cloning. In doing these analyses, ultimately myristylated HIV-2 MA may be prepared without the requirement for additional purification processes.

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Poster 23

A MACHINE LEARNING METHOD FOR DERIVING METABOLIC AND REGULATORY MODELS IN BACTERIAL SYSTEMS

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Cellulose, a major component of plant cell walls, is a remarkable polysaccharide. Its abundant availability makes cellulose a very good base material for the synthesis of environmentally sustainable hydrocarbon products like bioplastics and biofuels. Hence, the study of microorganisms that can degrade cellulose efficiently is of extraordinary importance. While there are experimental methods to elucidate the function of individual components of cellulose degradation pathways, creating a mechanistic model of the regulatory and metabolic networks with real predictive power is a very complex task for human scientists. Recent advances in machine learning and the availability of higher computational power make it possible to automate the task of deriving predictive models directly from biological experiments. We present here a novel method to automatically derive integrated metabolic and regulatory models using the experimental data from bacterial mutants and their resultant growth in different carbon sources. As a proof of concept, we applied our method to the bacterium *Cellvibrio japonicus*, which has a remarkable ability to completely degrade cellulose and other plant-cell wall polysaccharides. Based on an evolutionary algorithm approach, our method is able to reverse-engineer comprehensive predictive models of the regulation and metabolism of cellulose directly and automatically from the dataset of experiments. These results demonstrate the potential of such a method for inferring models of a wide range of complex biological processes and its applications in synthetic biology and biotechnology.

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Poster 24

STRUCTURE AND MECHANISM OF AN RNA THERMOSENSOR

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RNA thermosensors (RNATs) are non-coding RNA molecules found in the 5′-untranslated region (5′-UTR) of mRNAs and regulate the expression of the downstream gene as a function of temperature. RNATs are proposed to adopt a structure that occludes the ribosome-binding site (RBS) at low temperature, thus preventing translation. At elevated temperatures, the RBS is exposed, promoting translation. We are interested in the RNAT found in the 5′-UTR of prfA, a transcriptional activator that regulates the expression of a number of virulence genes in *Listeria monocytogenes*, which is an important human pathogen. Unlike well-characterized RNATs (4U, ROSE, and CSS), which gradually melt as a function of increasing temperature, the prfA RNAT utilizes a different mechanism, where there is a large functional change either permitting or inhibiting translation over a very narrow temperature range. Between 30 °C and 37 °C, there is no expression of PrfA, but at 38 °C there is significant amounts of PrfA expression. Using NMR spectroscopy we will probe the structure and mechanism of the prfA RNAT at different temperatures. Using a selective deuteration approach, we have obtained high-quality 1D proton and 2D proton-proton NOESY spectra of the 110-nt prfA RNAT at various temperatures. These preliminary spectra indicate that there is a large structural change over a narrow temperature window (3 °C). A detailed understanding of the structure and mechanism of the prfA RNAT will allow for the targeted design of a novel RNAT that functions at either higher or lower temperatures. Additionally, since PrfA controls a number of virulence genes in *Listeria monocytogenes*, it is a promising target for therapeutic development. The three-dimensional structure of the prfA RNAT will facilitate the design of small molecules that can bind to and "turn off" the prfA RNAT, even at elevated temperatures, which would normally promote translation.

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Poster 27

MUSIC AND MUSEUMS: AN INVESTIGATION INTO THE EFFECTS OF ACOUSTIC NOISE ON MUSEUM DISPLAYS AND ARTWORK

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Acoustic noise from social events that incorporate music can cause detrimental effects to museum objects by inducing vibration in these precious objects and the magnitude of the induced-vibration experienced by these objects is related to the intensity and frequency of the music along with the display environment. In this project we hypothesized that there is a correlation between the intensity of the acoustic noises at certain frequencies and the induced-vibration of museum display elements. Here, several glass object placed on a display were subjected to tones at controlled frequencies and intensities under numerous display conditions. The induced-vibrations were detected through the use of a wireless tri-axial accelerometer. The threat that these vibrations pose to museum objects can be modeled under multiphysics conditions to show that they are at risk of increased structural damage and stress.

Initial findings suggest that at intensities below 80 dB there is no significant evidence of a relationship between the vibration experienced and the display elements. Conversely, early trials suggest that at intensities exceeding 90 dB, changes in the vibration experienced inside the display case relate to the frequency of the tone being played, the presence of the Plexiglas cover and whether or not the display is freestanding.

We can infer that museum display elements do affect the vibration observed by the art objects and museums should account for the type of tones the art is exposed to when determining display environments. Future work will include a more extensive characterization of the effect of various intensities and frequencies of acoustic noise on the structures that support the artwork.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 28

ACOUSTIC INDUCED VIBRATION ANALYSIS OF GLASS ART OBJECT

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Museums display and preserve priceless pieces of cultural heritage however, music played during museum events could be endangering the very objects they are tasked with protecting. This project aims to characterize how art objects vibrate when subjected to acoustic stimulation at their resonant frequencies. This research investigates the effect of acoustic vibrations on glass objects using a tri-axial accelerometer. Vibration effects were modeled via the use of COMSOL Multiphysics and SolidWorks software.

The acceleration of the accelerometers was obtained to determine the vibration of the objects, the signal was then analyzed using the Fast Fourier Transform (FFT) to take the signal to the frequency domain. The data was also filtered and reconstructed in Matlab. This project aims to characterize how art objects vibrate when subjected to acoustic stimulation at their resonant frequencies.

Initial findings suggest a wine glass has three vibration mode shapes occurring at three distinct frequencies. At the first mode shape, the wine glass exhibited a bending behavior from side to side about the stem at 263.11 Hz, whereas at 660.12 Hz the top half of the wine glass expanded vertically illustrating the second mode shape. Lastly, the third mode shape exhibited an oscillating compression behavior at the lip of the glass. This third deformation appears to occur at the dominant resonant frequency 1212.9 Hz. Vibrations occurring at any of these three frequencies for extended periods of time can result in structural failure of the wine glass. In the future, the effect of the object's material, geometry, and defects on its vibration should be investigated.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 29

QUANTITATIVE ODDY TESTS OF MATERIALS USED FOR BOOK CONSERVATION, RESTORATION, DISPLAY, AND STORAGE

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A variety of materials are used to conserve, restore, store, and display books and paper including fabrics, adhesives, paper, and cleaning materials. These materials can off-gas harmful chemicals that can deteriorate the books and paper. The Oddy test, or the Accelerated Corrosion test, is used to determine if these materials might harm the books and paper they are supposed to protect. In this test, the materials are placed in a sealed container with copper, silver, and lead coupons. If corrosion of the metals is observed, it is assumed that the materials will also damage the books and paper and should not be used. Using the Walters Art Museum's Oddy Test Protocol, tests were run at Johns Hopkins University's Heritage Science for Conservation Laboratory on materials commonly used by the JHU conservators. Some modifications were made to the protocol including integrating Whatman #1 filter paper to test whether paper deterioration can be measured, comparing different polishing techniques on the copper and silver coupons, and integrating analytical techniques to detect corrosion. Before the test began, physical and chemical tests were performed on the sample materials and metal coupons to determine a baseline. These tests include mass, thickness, optical microscopy, Atomic Force Microscopy (AFM), colorimetry, and Infrared Spectroscopy. Corrosion is then measured 28 days after the start of the test, and these tests are still running. Once the testing is finished, we will repeat the baseline measurements and note any changes. In the future, we would like to integrate techniques such as Gas Chromatography (GC), High Performance Liquid Chromatography (HPLC), and Mass Spectrometry (MS) into the testing to measure and identify gas emission.

This project is supported by the Baltimore SCIART research experience for undergraduate students, a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore funded by the Andrew Mellon Foundation.

Poster 30

THE SECRET LIFE OF AN ANCIENT EGYPTIAN WEAVER: ADVANCEMENTS TO IDENTIFY DYES AND FIBERS ON AN ANCIENT EGYPTIAN BASKET

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A small, oval, coiled basket of the Ancient Egyptian New Kingdom Era (1550-1292 BCE) is on loan to the Johns Hopkins Archaeological Museum from the Eton College. The fibers and dyestuffs of the basket need to be identified to narrow its provenance and help link it to similar baskets identified during that era. This research aims to build a database of proposed dyes from Eton College including their historical background and their spectral, chemical, compositional, and anatomical properties as a step towards identification of the dyes. Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR) was performed on sample dyes to analyze their functional groups to be used for identification. X-Ray Photoelectron Spectroscopy (XPS) was used to identify metal elements found in the pigments representative of the dyes of interest. Scanning Electron Microscopy (SEM) was used to identify anatomical feature of fibers from the basket, thereby allowing us to identify the plant fiber used. Future research needs to create a replicated dye-fiber environment of the basket to compare to samples from the basket. They will both be analyzed using ATR-FTIR and XPS and then compared to each other for identification. Following this, conclusions can be drawn regarding what dyes are present, as well as a narrowing of its provenance.

This project is supported by the Baltimore SCIART research experience for undergraduate students, a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore funded by the Andrew Mellon Foundation.

Poster 31

GO FOR THE GOLD: AN INVESTIGATION INTO THE USE OF COSMETIC SPONGES FOR TARNISH REMOVAL FROM GILDED SILVER OBJECTS

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Since ancient times, cultures worldwide have been gilding objects to give them a metallic gold surface. Today art conservators are tasked with preserving these objects' integrity. Recent work at the Walters Art Museum revealed a problem for cleaning tarnished gilded silver objects. While cosmetic sponges have been used for the mechanical removal of silver tarnish, recent practice demonstrated that sponges remove thin gold layers just below tarnish on gilded silver objects, causing them to lose historic and aesthetic features. The goal of this study was to understand the effects of these mechanical conservation methods for tarnish removal, specifically by characterizing the sponge compositions, both on molecular and microscopic levels. Another aspect of this study was to understand whether or not extracts from the sponges were remaining on the object's surface after cleaning. We hypothesized that sponges with rougher texture would remove more gold and tarnish than those with smoother textures, and that solvents used to moisten sponges dissolved some sponge components, depositing them on the object surface. A variety of analytical techniques including Gas Chromatography (GC) and Inductively Coupled Plasma Mass Spectrometry (ICP:MS) as well as Scanning Electron Microscopy (SEM) with Energy-Dispersive X-ray Spectroscopy (EDS) and Fourier Transform-Infrared (FTIR) spectroscopy were used to study these problems. Our main finding so far is that sponges with greater roughness in their microscopic surface texture do remove more tarnish and gold from gilded silver object surfaces. Ongoing and future work will measure the abrasiveness of swabs as well as test the success of variations on the described cleaning techniques.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 32

SETTLING FOR SILVER: UNDERSTANDING THE INTERACTION OF ACIDIFIED THIOUREA SOLUTIONS AND THE SURFACES OF TARNISHED GILDED SILVER OBJECTS

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Tarnish is a challenge for silver preservation in applications from industrial electronics to jewelry. Aesthetically prized for its shine and color, silver's appearance is altered by tarnish layers, making its surface become dull and darker in color. For art conservators, traditional chemical cleaning methods for silver objects use an acidified thiourea solution. Despite best efforts to rinse this reactive solvent from the object's surface post-cleaning, museum staff have noticed that objects cleaned with thiourea re-tarnish at an accelerated rate. The goal of this study was to understand how thiourea solutions react with the surface of gilded silver objects and to characterize the complexes formed by this interaction. Our hypothesis is that thiourea is forming complexes with silver sulfides in the tarnish layer, and these may react more readily with the atmospheric environment. To study the potentially damaging effects of thiourea solutions on a valuable museum object, our laboratory recreated the object's surface by gold-plating silver coupons with electroless deposition. A variety of analytical techniques including Inductively Coupled Plasma Mass Spectrometry (ICP:MS) as well as Scanning Electron Microscopy (SEM) with Energy-Dispersive X-ray Spectroscopy (EDS) were used to study these problems. Our main finding so far is that in cleaning the coupons with multiple thiourea solutions separately prepared with three acids, different levels of pressure and mechanical effort are required for full tarnish removal. Ongoing and future work will analyze the coupon surfaces post-cleaning, as well as characterize the thiourea complexes formed on the surfaces of the coupons.

This project is supported by the Baltimore SCIART research experience for undergraduate students, which is a collaborative program between UMBC, Johns Hopkins University, and the Walters Art Museum in Baltimore. The program is funded by the Andrew Mellon Foundation.

Poster 33

UTILIZING SOLVATOCHROMIC DYES TO PROBE PHASE CHANGES IN STIMULI RESPONSIVE NANOGELS

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Stimuli responsive polymers have gained much attention due to their broad-ranging applications and have been considered as potential smart delivery systems for bioactive molecules. By building functionalized polymers that are thermally responsive, synthesizing novel solvatochromic dyes and covalently incorporating them into the polymer, one may be able to efficiently probe the "coil-to globular" phase transition that a smart polymer undergoes. Tracking the "swelling" behavior of these smart materials with solvatochromic dyes in different temperatures and solvent polarities can allow for the correlations between structure and function. In this research, the smart polymers are present as sub-micron sized hydrogels (cross-linked polymers) that we call nanogels. The absorption and fluorescence properties of the solvatochromic dye will be studied in solvents of varying polarities. In addition, fluorescence from the dye-labeled nanogels will be characterized above and below the lower critical solution temperature (LCST) to demonstrate that they can be used to probe real-time changes in the phase of a polymer.

The project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 38

DEVELOPING NANO-REACTION CHAMBER TO PROBE TRANSIENT MACROMOLECULAR COMPLEXES

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This project is focused on developing a novel method to examine weak, short-lived, protein-protein interactions in macromolecular complexes. A broad variety of signaling pathways, most interestingly those related to disease, contain such transient protein complexes. To study these interactions, we will trap molecules in vesicle "nano-chambers" and monitor them using a single molecule fluorescence microscope constructed in-house. Vesicles are nano-scale fluid filled sacs composed of a spherical lipid membrane separating the outside from the in. We designed vesicle pairs that fuse, mixing the contents stored inside to allow for controlled small volume mixing experiments. This new nano-reaction chamber approach is motivated by the need to overcome limits of conventional methodologies to study transient protein-protein interaction. The small volume of ~100nm diameter nano-vesicle allows for higher effective concentrations of the reactants mimicking the physiological conditions found in cells. By engineering a system where single molecules are trapped and probed in one location, it will be possible to examine not only equilibrium concentrations, but the dynamics of a specific protein-protein interaction.

We strive to prove that our system is capable of multiple rounds of controlled fusion, which would allow for sequential addition of multiple components to the reaction chamber under observation. Here, we present proof of the first step of fusion, an explanation of the data analysis software used, and the development of sequential fusion. Moving forward, once sequential fusion has been proven to occur, the project will then progress towards examining specific protein-protein interactions involved in signaling pathways present in cancer development.

We wish to acknowledge Mathew Law and Rishi Raval, UMBC computer science undergraduates for developing Matlab programs for acquiring and analyzing imaging data. The project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 39

UV RAMAN SPECTROSCOPY AS A POTENTIAL STANDOFF DETECTION TECHNIQUE

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Standoff detection techniques are needed to allow hazardous materials to be identified rapidly from a safe distance. One potentially useful standoff technique utilizes UV-Raman spectroscopy. A novel experimental configuration was implemented to generate Raman spectra for samples as a function of distance away from the collection optic. With this configuration, Raman spectroscopy was conducted using 213-nm light on samples of several common solvents. Identifiable spectra were generated with single laser pulses at distances approaching 5 meters. The experiment revealed an intensity drop off in collected Raman scatter inversely proportional to the distance between the sample and the collection optics. In order for spectra to be generated at 10 m, the target distance of the project, numerous pulses were averaged to achieve the desired signal-to-noise ratios. To improve on this performance the arrangement of the collection optics, the laser pulse intensity and the type of detection system were manipulated. The inclusion on a telescoping lens may prove to amplify the intensity of the signal.

The project is supported by the National Science Foundation Research Experience for Undergraduates (REU) Award No. CHE-1460653.

Poster 40

INDIUM PHOSPHIDE QUANTUM DOT-BASED FRET PROBE FOR THE ANALYSIS OF PHOSPHATASE ACTIVITY

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Dephosphorylation as it occurs in cells is vital to many biological processes. If the enzymes responsible for phosphorylation or dephosphorylation become damaged, the rate at which they activate proteins will be deregulated. This deregulation is linked to several health problems, some of which result in the death of the cell. In order to monitor the rate of phosphatase activity in cells, a probe would have to be water soluble, sensitive, accurate, and non-toxic. Fluorescence Resonance Energy Transfer (FRET) assays provide real-time spatially accurate molecular probes. Indium phosphide quantum dots, when applied to the FRET probe as the donor species, bring photostability and high sensitivity. They are a non-toxic alternative to the commonly studied cadmium-containing quantum dots. A polyethylene glycol derivative acts as a linker molecule and makes the probe water soluble. Suitable indium phosphide quantum dots and linker molecules were synthesized. A cap exchange modeling the substitution of the surface molecules on the quantum dots and the linker molecules was also successfully carried out. Research still remains to be done on the synthesis of the acceptor dye molecule and the orientation of the individual species within the probe.

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Poster 42

TENSOR PROPERTIES AND DECOMPOSITIONS IN DATA ANALYSIS

REU Site: Interdisciplinary Program in High Performance Computing
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A continuing effort to determine efficient ways to deal with large and high-dimensional data sets has led many to the area of multilinear algebra. With today's increasing computing power, it is now a more attractive option to make use of tensors to represent and analyze these data sets. Whereas matrices are two-way arrays with each element specified by two indices, tensors are N-way arrays with its elements specified by N indices. In this sense, tensors are higher-dimensional generalizations of matrices, and they can be sparse in many cases of data analysis.

We explore the properties of tensors as they are used to represent data, and take advantage of the ability to matricize them to apply readily known linear algebra techniques that apply to conventional matrices. We compare computations with tensors such as the Tucker decomposition to established techniques such as the singular value decomposition of matrices or principal component analysis. The Tucker decomposition attempts to express a tensor as a product of a potentially compressed tensor (known as the core tensor) and three factor matrices which are orthonormal. Many algorithms try to fit an Alternating Least Squares model to compute a plausible approximation. The objective is then to analyze the core tensor in hopes of obtaining a summary of the original data, and to find ways to compress it without losing meaningful information to obtain a simpler representation. Several areas and applications that have benefited from using tensors are psychometrics, chemical analysis, signal processing, and data mining. Data sets from different types of applications are used in our comparisons.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Darren Stevens II was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Jonathan Graf was supported by UMBC.

Poster 44

PERFORMANCE COMPARISON OF A TWO-DIMENSIONAL ELLIPTIC TEST PROBLEM ON INTEL XEON PHIS

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The Intel Xeon Phi is a processor with a theoretical peak performance of approximately 1 TFLOP/s in double precision. This project compares the performance of code on the Intel Xeon Phi. Specifically, we benchmark a reference code on two generations of the Intel Xeon Phi, code-named Knights Corner (KNC) and Knights Landing (KNL), and contrast to performance on one compute node with two CPUs. The second generation of Intel Xeon Phi, Knights Landing, just became available in Spring 2016. KNL uses MCDRAM memory, which is nearly 50% faster than the GDDR5 in the KNC version. KNL can have up to 72 cores interconnected by a 2D mesh network, whereas KNC only has on the order of 60 cores connected by a bi-directional ring bus. The KNL can be run as a processor or coprocessor, and can support a full stand-alone Linux OS. KNC can only be a coprocessor and can only support a Linux micro-OS.

The benchmark code solves a classical elliptic test problem, the two-dimensional Poisson equation with homogenous Dirichlet boundary conditions on a unit square domain. The partial differential equation is discretized by the finite difference method and the resulting system of linear equations with a symmetric positive definite system matrix solved by the conjugate gradient method. The same C implementation of the benchmark code with hybrid MPI+OpenMP parallelization is used on all hardware platforms.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Ishmail Jabbie was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Jonathan Graf was supported by UMBC. The authors would like to thank the Performance Research Laboratory, University of Oregon for providing access to the KNL hardware.

Poster 45

ELECTRICAL EXCITATION, CALCIUM SIGNALING, AND PSEUDO-MECHANICAL CONTRACTION IN CARDIOMYOCYTES: EXTENDING A PARTIAL DIFFERENTIAL EQUATIONS MODEL

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Calcium dysregulation is a significant cause of fatal cardiac arrythmias, but it is an incompletely understood phenomenon and difficult to predict. Heartbeat rhythm is governed by periodic membrane depolarizations causing the release of calcium ions into the cytosol of individual cardiomyocytes; the reaction of this calcium with contractile proteins triggers the overall contraction of the heart. These calcium wave patterns can be modelled as a system of coupled partial differential equations linking the excitation, signaling, and contraction of individual cardiomyocytes.

The starting point of this research is a model that includes the electrical system of the cell and establishes a one-way link from the electrical system to the chemical system. We extend the model to connect the chemical system to the electrical system and to incorporate a pseudo-mechanical component of calcium dynamics in cardiomyocytes. We extend the model further to include the impact of the efflux of calcium onto the electrical system.

A parallel implementation of a special-purpose numerical code using MPI is necessary to enable the long-time solutions of this large-scale system of partial differential equations. Numerical simulations examine the behavior of the system that arises from the feedback loops between the calcium system, the electrical system, and the pseudo-mechanical system.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Uchenna Osia was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Jonathan Graf was supported by UMBC.

Poster 46

THE INTERACTION OF CALCIUM AND METABOLIC OSCILLATIONS IN PANCREATIC β-CELLS

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Diabetes is a disease characterized by an excessive level of glucose in the bloodstream, which may be a result of improper insulin secretion. Insulin is secreted in a bursting behavior of pancreatic β-cells in the islets of Langerhans, which is affected by oscillations of cytosolic calcium concentration. We used the Dual Oscillator model to explore the role of calcium in calcium oscillation independent (CaI) versus calcium oscillation dependent (CaD) modes as well as the synchronization of metabolic oscillations in electrically coupled cells. We observed that voltage and calcium coupling result in increased synchronization and are more effective in CaD modes. Also increasing voltage coupling results in greater synchronization. Furthermore, we studied heterogeneous cellular bursting arrangements in the islets and their effects on synchronization. Calcium coupling has a larger impact on synchronization than voltage coupling, in the heterogeneous bursting scenarios. To better represent an entire islet, we altered previous code by further optimizing run-time and memory usage to allow for a greater number of cells.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Mary Aronne was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistant Janita Patwardhan was supported by UMBC.

Poster 47

DIMENSIONALITY REDUCTION USING SLICED INVERSE REGRESSION IN MODELING LARGE CLIMATE DATA

REU Site: Interdisciplinary Program in High Performance Computing
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This project aims at using a data-analytic tool called Sliced Inverse Regression (SIR) to reduce the dimension in the regression of monthly precipitation on historical data of several climate variables provided by Global Climate Models (GCM). The SIR approach enables us to identify a small number of linear combinations from a large list of predictor variables while still maintaining the prediction accuracy. Following SIR, we implement a simple non-parametric prediction method, the Nadaraya-Watson Estimator (NWE). NWE is adapted for a Tobit model in order to account for the semi continuous nature of the precipitation data to improve prediction accuracy.

We apply the SIR method on the data from the Missouri River Basin (MRB). We implement the methodology to data from the GCMs: MIROC5, HadCM3, and NCAR-CCSM4 with a temporal coverage of 1949-2010 at over 30,000 locations. The cluster Maya is used to parallelize the estimation by dividing the region into sub regions, each of which is assigned one node of the cluster. Some of the predictor variables that are included are precipitation, maximum/minimum temperature, sea-level pressure, relative humidity, and surface wind speed. Additional predictor variables are added to account for the spatial properties of the reduced dimensions. The results of the prediction carried out using SIR and NWE are compared to an alternate regression model to observe the accuracy of the results.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Danielle Sykes was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Poster 48

ENHANCED DATA EXPLORATION AND VISUALIZATION TOOL FOR LARGE SPATIO-TEMPORAL CLIMATE DATA

REU Site: Interdisciplinary Program in High Performance Computing
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This project builds on the research from past REU projects by enhancing a Graphical User Interface (GUI) for data exploration and visualization of spatio-temporal climate data from the Missouri River Basin (MRB) region. Teams from 2014 and 2015 REUs have built GUIs using the R software to facilitate the statistical downscaling process for precipitation and maximum/minimum temperatures using historical simulated data from the Global Climates Models (GCM) MIROC5 and HadCM3. Modeling attempts for temperature were largely accurate while precipitation proved more difficult to predict due to the semi-continuous distribution of rainfall. Therefore, our project seeks to complement predictive efforts by using visualizations to reveal spatio-temporal patterns such as underlying correlations and other trends in the data.

In this project several aspects of the GUI are enhanced by using the R package, Shiny, which allows greater control of the GUI design and thus will enable us to give more data visualization and exploration options. Specifically, the enhanced GUI enables an easy inter-comparison of MIROC5, HadCM3, and NCAR-CCSM4 in terms of prediction accuracy using bias, root mean-squared error (RMSE), and other metrics of interest for daily precipitation. Temporal trends and autocorrelation are determined through the use of time series plots, principal oscillation patterns (POPs), and sample autocorrelation function plots. Spatial correlation and patterns can be explored using contour plots, surface plots, and semivariograms. We will also provide calculation and visualization of cross-correlation matrices, empirical orthogonal functions (EOFs), and canonical correlation analysis (CCA).

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Poster 49

USING HISTORICAL DATA FOR RETROSPECTIVE PREDICTION OF RAINFALL IN THE MIDWEST

REU Site: Interdisciplinary Program in High Performance Computing
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The Missouri River Basin (MRB) is an important food-producing region in the United Stated and Canada. Climate variability and water availability affect crops production in this region. Past climate data have been recorded at various locations in the basin over a period of ten years. We use the data for a retrospective prediction of rainfall.

As the dimension of the data is relatively large, a sufficient dimension reduction approach is used to reduce the dimensionality of the data while preserving the regression information pertinent to rainfall. We use the nascent dimension reduction methodology called Minimum Average Deviance Estimation or MADE to reduce the dimensionality of the climate data. Since MADE is still a tool in development, we explored two of its intrinsic prediction methods and compared them to the Nadaraya-Watson prediction approach by a cross-validation method.

A parallel implementation of MADE and its prediction methods were carried out. A performance study was performed along with the application of the best prediction method to the MRB climate data.

These results were obtained as part of the REU Site: Interdisciplinary Program in High Performance Computing (hpcreu.umbc.edu) in the Department of Mathematics and Statistics at the University of Maryland, Baltimore County (UMBC) in Summer 2016. This program is funded by the National Science Foundation (NSF), the National Security Agency (NSA), and the Department of Defense (DOD), with additional support from UMBC, the Department of Mathematics and Statistics, the Center for Interdisciplinary Research and Consulting (CIRC), and the UMBC High Performance Computing Facility (HPCF). HPCF is supported by the U.S. National Science Foundation through the MRI program (grant nos. CNS-0821258 and CNS-1228778) and the SCREMS program (grant no. DMS-0821311), with additional substantial support from UMBC. Co-author Ephraim Alfa was supported, in part, by the UMBC National Security Agency (NSA) Scholars Program through a contract with the NSA. Graduate assistants Sai K. Popuri and Nadeesri Wijekoon were supported by UMBC.

Poster 50

THE IDENTIFICATION OF INSULIN THROUGH PROTEIN DIGESTION

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Insulin is the protein in human bodies that regulates sugar intake in the cells. Insulin levels are essential for individuals who live with diabetes because it prevents the body from producing insulin. Without being able to produce insulin, consequences may arise such as irregular blood glucose amounts, causing dementia, seizures, and even death. In this study, insulin is used as a model compound to explore novel approaches to improve protein characterization. The impact of this experiment is better characterization of insulin.

This experiment consists of taking insulin and breaking it down into polypeptides with the use of enzymes such as trypsin. High performance liquid chromatography with mass spectrometry is then used to separate and detect the polypeptides. Once all of the data is collected, it is then put into the bioinformatics software, Peaks 7. This processes all the spectra, and provides metrics which include sequence coverage of the protein. Along with the insulin sample, the protein bovine serum albumin (BSA) and water are also being digested to serve as controls in the experiment.

The first attempt to digest insulin was with trypsin alone. This digestion resulted in a 28% sequence coverage. The BSA and water controls received exceptional sequence coverages. BSA received a 75% sequence coverage, while the water control received a two percent sequence coverage. The sequence coverage for the insulin appears to be low because insulin is a glycosylated protein. This means that there are numerous glycans that are attached to the protein, making it difficult for the trypsin to make cleavages. To get a higher sequence coverage of the protein, PNGase is used to cleave the sugars followed by the enzymatic digestion.

I would like to acknowledge the Molecular Characterization and Analysis Complex (MCAC) for their monetary and educational support that allowed this experiment to be completed.

Poster 51

MATRIX BINDS SPECIFICALLY TO $tRNA^{Lys3}$

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Human immunodeficiency virus-1's (HIV-1) matrix domain (MA) of the Gag polyprotein targets Gag to the cell membrane through interactions between MA's highly basic region and phosphatidylinositol 4,5-bisphosphate [$PI(4,5)P_2$] on the cell membrane. Targeting to the plasma membrane is critical for the assembly of the virus. In addition to interacting with the plasma membrane, CLIP studies by the Bieniasz lab showed that MA specifically binds to certain tRNAs, including $tRNA^{Lys3}$, *in vivo*. Host $tRNA^{Lys3}$ acts as a primer for reverse transcription and also is packaged into budding virions. We confirmed that $tRNA^{Lys3}$ and MA form a complex *in vitro* using gel electrophoresis, and determined the thermodynamic properties of the interaction using isothermal titration calorimetry (ITC) to better understand how the interaction takes place. $tRNA^{IleGAT,}$ which was proven not to bind to MA through CLIP studies, was compared to $tRNA^{Lys3}$ using ITC. $tRNA^{Lys3}$ forms a one to one ratio with MA, while $tRNA^{IleGAT}$ forms a 0.5:1 ratio with matrix. Studying the interaction of HIV-1 MA and tRNAs will better our understanding of how these specific tRNAs regulate interactions with the plasma membrane. In the future we seek to determine the tRNA-MA complex structure, which could provide a target for future antiretroviral drugs for AIDS and HIV patients.

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Poster 53

MYRISTIC ACID'S EFFECT ON MYRISTOYLATION OF THE MATRIX PROTEIN

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Human immunodeficiency virus (HIV) is a serious global health problem that has resulted in 35 million deaths since the beginning of the epidemic. In the US alone it affects approximately 1.2 million Americans. In Maryland 1 out of 49 are at a risk for HIV in the population, meaning about 27.7 out of every 100,000 people. HIV has a matrix (MA) protein, which guides the Gag-genome complex to the plasma membrane of the cell to bind for assembly of new virions. We explored the necessity of supplemental myristic acid for myristoylation of HIV-1 MA protein. Ordinarily myristic acid is added during MA synthesis in *E. coli*, but this lowers the pH level, producing a small yield of protein. We hypothesized that if the *E. coli* cells in the media have sufficient native myristic acid, then the addition of myristic acid to the cells will not decrease the myristoylation rate in MA. If the myristic acid is not necessary, the yield will significantly rise, due to a more favorable environment for cells. To test this myrMA was expressed in *E. coli* cells with and without the addition of myristic acid, and purified through PEI precipitation, ammonium precipitation, cation exchange FPLC and size exclusion FPLC. Once the preparations were done, the myristoylation rate and protein yield was measured using hydrophobicity FPLC. Protein yield was confirmed with a Nanodrop spectrophotometer. Hydrophobicity FPLC showed that all matrix proteins were myristoylated. Without myristic acid the yield is 0.44 μmol and with myristic acid the yield was 0.27 μmol. In conclusion, we found that the addition of myristic acid produces a higher yield, but is not necessary for efficient myristoylation. Future protocols will include the addition of myristic acid.

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Poster 55

CHARACTERIZATION OF THE PROTEIN MYOGLOBIN

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Myoglobin is an iron and oxygen binding protein containing a single polypeptide with 154 amino acids. When muscle cells are in action they need large amounts of oxygen for respiration because of their demand for energy. Muscle cells use Myoglobin to speed up oxygen diffusion and act as an oxygen storage unit for times of extreme respiration. In this study, Myoglobin is used as a model compound to explore novel approaches to improved protein characterization. The goal of this project is to perform a protein digest, changing various factors in each trial, to optimize the reaction and instrumentation to provide the highest protein sequence coverage.

This experiment used a high performance liquid chromatography (HPLC) system with mass spectrometry. HPLC is a technique used to separate various compounds in solution, where it is then passed through a column in order to separate each component. The mass spectrometer will ionize the samples then fragment and detect their mass. Once the data from the sample has been collected Peaks 7 Database provides the bioinformatics of the sample giving sequence coverage. Factors such as digestion time, amount, and the enzymes used, were optimized in order to provide the highest protein sequence coverage. The first step in the experiment involved making a Bovine Serum Albumin (BSA) and water control, to ensure the instrument and digestion are working properly. Next, the experimental protein sample Myoglobin was prepared using enzymatic digestion.

The first attempt at the Myoglobin digest used a 1:40 ratio of Trypsin. This digest resulted in 82% of protein sequence coverage of Myoglobin. As research continues, the optimization of Myoglobin will be used to find what will provide the highest protein sequence coverage.

I would like to thank Baltimore Youthworks Summer Jobs Program for funding my experience at the Summer Biomedical Training Program. I would also like to thank MCAC for allowing me to have this great learning experience and for the instrumentation.

Poster 56

THE ROLE OF APONTIC IN CELL MIGRATION AND STEM CELL DYNAMICS

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The dynamics of cell migration and stem cell differentiation are two topics of particular interest because they are normally tightly controlled but, when unchecked, often play roles in pathological conditions. The migratory border cells of the Drosophila ovary and the stem cell niche of the Drosophila testis, serve as well characterized systems for study of both migration and stem cell differentiation. What we learn in this context is likely to be relevant in many different animals, including humans.

In the fruit fly ovary and testis, a molecular cascade ending in transcription, known as the JAK/STAT signaling pathway, is involved in these two distinct but essential cellular processes. This study focuses on a protein, Apontic, that is present in this molecular pathway. Previous literature showed that Apontic plays a role in suppressing cell migration and motile cell recruitment by regulating STAT activity within Drosophila ovaries. Also, in testes, Apontic appears to promote differentiation by antagonizing STAT activity. The mechanism by which STAT and Apontic regulate each other is yet to be elucidated in testes. Here, we look at the MicroRNA 284 (mir284) as a possible means by which STAT down regulates Apontic activity in both the ovaries and the testis.

In addition, we also looked to another protein, Zfh1, that is required for stem cell maintenance in the testes, as a possible regulator of Apontic levels in the stem cell niche. Finally, we sought to mathematically represent the theoretical change in Zfh1 levels using differential equations based on the proposed molecular cascade. We used these equations to develop an understanding of possible cross repression between Apontic and Zfh1.

This work was funded in part by an Undergraduate Biology and Mathematics (UBM) Research Award from the National Science Foundation (NSF), Grant No. DBI 1031420. Program Directors: Dr. Jeff Leips[1] and Dr. Nagaraj Neerchal[2] and an NSF CAREER AWARD to MSG.

Poster 57

5′ START SITE HETEROGENEITY OF THE HIV-1 RNA AND ITS EFFECT ON STRUCTURE AND FUNCTION

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The 5′ Leader (5′-L) of the human immunodeficiency virus-1 (HIV-1) RNA genome is highly conserved and constantly in an equilibrium between the monomer and dimer conformations. In the monomer conformation, the RNA is preferentially translated into proteins necessary for reproduction, while in the dimer conformation, the RNA is packaged as the genome for a new virion. The exact start site of the RNA has not been listed consistently in the literature in the past years. It was found that *in vivo*, there exists a mixed population of capped viral RNA with start sites that begin with one, two, or three guanosines (Cap1G, Cap2G, and Cap3G, respectively). This discrepancy had a profound effect on the folding patterns of the RNA, as it was observed using native gel electrophoresis Cap1G 5′-L favored the dimer conformation, whereas the Cap2G and Cap3G preferred the monomer conformation. This difference in start sites therefore influences the structure and function of the RNA. We used nuclear magnetic resonance spectroscopy to determine the exact structural mechanism by which start site differences direct this change. Using specific nucleotide- and site- specific labeling schemes, we were able identify a sensitive signal that is unique to the Cap2G construct only. Assigning signals in the full 5′-L is difficult due to the numerous signal overlap. To overcome this problem and assign the residue that the sensitive signal belongs to, we constructed smaller oligo controls of the full 5′-L. Our future works include making oligo control constructs of the TAR hairpin with different start sites to compare the signals.

This research was funded by NIH/NIGMS grant *1P50GM103297*, and was conducted at the Howard Hughes Medical Institute at UMBC with support in part by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. Matthew Orellana was supported, in part, by the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program, UMBC, and the Meyerhoff Scholars Program. We would like to thank our principal investigator Michael Summers for allowing us this opportunity to work in the lab, our graduate student Joshua Brown for his mentorship and guidance, and our lab members for their support.

Poster 58

CRISPR/CAS9-MEDIATED GENOME EDITING FOR FLUORESCENCE SINGLE-CELL MICROSCOPY

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Dysregulated glucose metabolism is an emerging hallmark of cancers. We have investigated the spatiotemporal role of human liver-type phosphofructokinase (PFKL) in glucose metabolism under fluorescence single-cell microscopy. According to our preliminary data, we hypothesize that PFKL is a scaffold to other enzymes involved in human glucose metabolism. We have aimed to develop a genome-edited cell line expressing endogenously-tagged PFKL by knocking in a gene encoding an enhanced green fluorescent protein (EGFP), using the Clustered Regularly Interspaced Short Palindromic Repeats/Caspase 9 (CRISPR/Cas9) technology. Currently, we have prepared a nuclease plasmid containing a Cas9 nuclease and a guide RNA sequence pinpointing the genomic locus for EGFP insertion, and a donor plasmid containing PFK homology arms and EGFP is in progress. We anticipate that these plasmids will be transfected into human breast cancer Hs578T cells to incorporate the EGFP tag into the C-terminal region of the genomic PFKL gene via a homology-directed DNA repair system. Development of this cell line will allow us to investigate the scaffold hypothesis of PFKL and further the importance of its scaffold role in spatiotemporal regulation of glucose metabolism.

This investigation was supported, in part, by a MARC Undergraduate Student Training in Academic Research (U-STAR) National Research Service Award (NRSA) Institutional Research Training Grant (2 T34 GM008663) and a Chemistry-Biology Interface Training Grant (NIH/NIGMS T32GM066706) from the National Institutes of Health, National Institute for General Medical Sciences, and the AACR-Bayer Innovation and Discovery Grant.

Poster 59

SCREENING SMALL MOLECULE LIGANDS WITH THE CORE ENCAPSIDATION SIGNAL OF HIV-1 RNA AS A POTENTIAL DRUG TARGET

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Over 1.2 million people in the United States are infected with the human immunodeficiency virus type 1 (HIV-1). Current treatments target proteins that play important roles in various stages of the HIV-1 life cycle, but due to the high mutation rate of the virus, these drugs can only work for so long. One alternative is to develop therapeutics that target functional RNA elements within the highly-conserved 5′-untranslated region (UTR).

The core encapsidation signal (CES) was identified as a region within the 5'-UTR that is capable of directing packaging of the virus's dimeric genome. In the absence of this RNA element, HIV-1 virions cannot efficiently package their genomes, and therefore cannot produce infectious virions. The important role the CES plays makes it a potential drug target, and therefore the three-dimensional structure of this RNA was recently determined. Our research focuses on understanding how ligands bind to and modulate the CES structure. We use techniques such as nuclear magnetic resonance (NMR) spectroscopy and isothermal titration calorimetry (ITC) to characterize the sites of ligand binding and affinity. SOFAST HMQCs were performed on free and ligand bound CES and the resulting spectra were compared. Ligands that resulted in changes in the HMQC spectrum relative to that of free CES were identified as hits and further screened by ITC.

Out of 82 molecules, we identified 24 molecules as hits. We are currently using ITC to identify the binding affinity of these 24 small molecules. While these ligands bind to CES, it is not known whether they function as inhibitors of the genome packaging step of the HIV-1 replication cycle. Based on our experimental data, in vivo studies will be performed to further examine these effects. Our findings will aid in the development of a new drug that specifically targets the RNA genome.

This research was supported by NIH grant #5R01GM042561, and was conducted at the Howard Hughes Medical Institute at UMBC as part of the Howard Hughes Medical Institute's Precollege and Undergraduate Science Education Program. We would like to thank and acknowledge Dr. Michael Summers for providing the opportunity to participate in this competitive research, lab members who assisted in this process, the Hargrove Lab at Duke University for providing ligands for the project and the Meyerhoff/HHMI program for their support.

Poster 60

OVEREXPRESSION OF DUAL FUNCTION FRUCTOSE-1,6-BISPHOSPHATASE/ SEDOHEPTULOSE-1,7-BISPHOSPHATASE (DFS) TO IMPROVE GROWTH IN *CHLAMYDOMONAS REINHARDTII*

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Algal biofuels are an environmentally sustainable alternative to currently used and diminishing fossil fuels because they can be obtained directly from biomass derived from carbon dioxide (CO_2) and sunlight. Increasing the photosynthetic activity of algae can increase their growth rate and biomass. One way to increase photosynthetic activity is to improve the Calvin cycle, a photosynthetic pathway of enzymatic reactions that convert CO_2 and the energy of sunlight into sugars. Dual-function fructose-1,6-bisphosphatase/sedoheptulose-1,7-bisphosphatase (DFS) is a cyanobacterial enzyme that works to regenerate ribulose-1,5-bisphosphate (RuBP) in the regeneration phase of the Calvin cycle. Previously others found that overexpressing this cyanobacterial protein that possesses two Calvin cycle enzyme activities, could significantly improve plant biomass production. The goal of this project is to determine whether overexpressing this dual-function enzyme has the same effect in algae. We have generated *C. reinhardtii* transformants that contain the coding region for DFS under the control of *psbD* and *psbA* 5' and 3' regulatory sequences, respectively, integrated into the chloroplast genome. We analyzed the expression of this protein in transformants by western blot and found that the cyanobacterial protein is expressed. We will proceed by comparing the growth of these transformants with the wild type strain of *C. reinhardtii*. If expression of DFS leads to increased growth rate, then we would conclude that DFS carries out one or more rate-limiting steps in the Calvin cycle. If that is the case, we ultimately will overexpress DFS in a biotechnology production organism like *Chlorella*, in hopes of improving it as a biofuel-producing organism.

These results were obtained as a part of the Research Experience and Mentoring (REM) program in the Department of Biological Sciences at the University of Maryland Baltimore County. This program is funded by a grant (REM supplement to NSF-EFRI-1332344) from the National Science Foundation (NSF) Directorate for Engineering (ENG) Office of Emerging Frontiers in Research and Innovation (EFRI).

Poster 61

ASSIGNING THE SECONDARY STRUCTURE OF THE HIV-1 MONOMER-DIMER CONFORMATIONS

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The human immunodeficiency virus-1 (HIV-1) is a pandemic that affects thirty-seven million people worldwide, resulting in over 1.2 million AIDS-related deaths yearly. In order to attack this retrovirus and reduce the amount of deaths associated with HIV, we must first look at the HIV-1 replication cycle. During the late phase of the retroviral replication cycle, the 5′ Leader (5′-L) can remain as a monomer or base pair with another 5′-L molecule to form a dimeric complex. There is currently no drug therapy that targets this highly conserved portion of the viral RNA. In this monomer-dimer equilibrium, the monomer allows the RNA genome to be translated into Gag-pol, while the dimer is responsible for assembling an RNA-protein complex to be packaged into new virions. To further understand its function, we plan to characterize the secondary structure of the two conformations using nuclear magnetic resonance (NMR) spectroscopy. However, studying large RNAs by NMR is difficult because only four residues are present, thus resulting in limited chemical shift dispersion. We overcame this obstacle by using fragmentation techniques. Fragmentation uses smaller, synthesized hairpins that resemble portions of the longer stem loop. The NMR data of these fragments can be overlaid with the data from the full length 5′-L to assign and confirm the existence of structural elements. This method allowed us to confirm several structural elements in both the monomer and the dimer conformation. Our future work includes assigning the bottom of the TAR hairpin and the polyA stem loop in the dimer as well as confirm the U5: DIS interaction and the U5: AUG interaction in a native monomer and dimer construct, respectively.

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Poster 62

STRUCTURAL COMPARISON OF TRUNCATED AND FULL-LENGTH FELINE IMMUNODEFICIENCY VIRUS MATRIX PROTEIN BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

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The human immunodeficiency virus (HIV) remains a global health issue and warrants further research to address resistance to current treatment. To combat this issue, an animal model is necessary for understanding the processes that facilitate successful replication. Cats offer potential because the feline immunodeficiency virus (FIV) shares similar features to HIV. One of these features includes the trafficking of the Gag polyprotein to the plasma membrane, a process that is dependent on the N-terminal matrix (MA) domain. MA is comprised of a specific, six amino acid myristylation sequence that serves as a site for recognition and binding of a myristate moiety. Previous research has revealed that most mammals share a common myristylation signal, however FIV MA diverges from this pattern. Our research investigates the purpose of this unique myristylation signal by better characterizing the structure and function of the native FIV MA using nuclear magnetic resonance (NMR) spectroscopy. FIV MA features an unstructured, non-functional C-terminus, and truncation of this region has provided better stability, solubility, and higher yields compared to the full length (FL) FIV MA, ultimately resulting in better NMR spectra. FIV MA FL is most stable at pH 7, whereas solubility of truncated FIV MA was optimized at pH 8. In order to ensure that this change in pH did not significantly change the structure of FIV MA, NMR data was collected on FIV MA FL at pH 8 for comparison to spectra at pH 7. By making these comparisons between the truncated and full length samples, this work can provide insight on methods that facilitate collection of long-term NMR experiments using a more soluble, stable, and highly concentrated FIV MA.

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Poster 64

STRUCTURAL ELUCIDATION OF THE REV-RRE COMPLEX IN HIV-1

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HIV-1 is a virus that leads to acquired immune deficiency syndrome, also known as AIDS. It is highly pathogenic, with approximately 2 million new cases every year, and up to 40 million people currently infected. The RRE and its binding partner the Rev protein are important for viral replication, as they are needed to help transfer viral RNA out of the nucleus.

The main goal of our research is to discover the structure of the RRE. Using a computer program known as Mfold, we have created several secondary structure predictions. Using NMR we have evaluated the full length RRE as well as specific fragments of that sequence. Comparing the NMR spectra from those fragments to the spectrum from the full length RRE, we are able to validate certain portions of our predicted RRE structure.

Another current objective in our research is to purify the Rev protein, which we overexpressed in *E.coli*. We are optimizing the purification process and will eventually analyze the protein using a range of methods, so that we can investigate and analyze the protein's structure as well as its interaction with the RRE.

Knowledge of the structures of the RRE and Rev protein, and how they interact, may allow therapeutics to be developed to target this stage of viral replication.

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Poster 66

PROBING INTRAMOLECULAR INTERACTIONS IN THE HIV-1 5′-LEADER DIMERIC CONFORMATION

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The human immunodeficiency virus (HIV-1) is the causative agent of acquired immunodeficiency syndrome (AIDS), which was associated with 1.1 million deaths in 2015. The late phase of HIV-1 replication cycle is characterized by the equilibrium between the monomer and dimer conformations of the 5′ Leader (5′-L) in the RNA genome. Our model predicts that in both conformations, a hallmark interaction occurs with the Unique 5 region (U5) which characterizes the respective conformations; in the monomer, the U5 region is bound to the Dimer Initiation Site (DIS), and in the dimer, the AUG hairpin. The dimer is essential for virus reproduction, it binds to nucleocapsid and acts as the genome for a new virion during packaging. We synthesized a construct with modification that locked it into the dimeric conformation but prevented intermolecular dimerization. We called this construct locked dimer (LD). Using nuclear magnetic resonance (NMR) spectroscopy is particularly challenging for large RNA such as the 5′-L or LD. We overcame that obstacle by probing a small oligo control which mimics the chemical environment for the U5:AUG interaction. We then compared the spectrum from this oligo to the LD construct and found that the signals overlapped, confirming the existence of the U5:DIS interaction in LD. We next plan to compare these spectra with the native 5′-L. If the spectra overlap, that will be the first evidence of the U5:AUG interaction in the native dimeric 5′-L.

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Poster 68

A MATHEMATICAL AND COMPUTATIONAL FRAMEWORK FOR DISCOVERING MODELS OF SHAPE AND FORM REGENERATION

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Regenerative medicine aims to repair, rebuild, and restructure new tissue in an injured or amputated organism to fully restore functionality. Remarkably, planarian worms have the ability to regenerate a complete body, including new organs such as the brain, eyes, pharynx with the correct size and position, from almost any amputated piece. Understanding the mechanisms by which planarian flatworms regenerate can revolutionize medical techniques and treatment. Current models of planarian regeneration explain the emergence of appropriate body region patterning during regeneration, but no model or appropriate modeling technique exists to explain the restoration and allometric re-scaling of form and shape that occurs and are essential for planarian regeneration. In this work, we have combined a mathematical and computational approach for the discovery of mechanistic models of large-scale tissue regeneration and growth. We have developed a novel mathematical formalism based on partial differential equations to model full-body tissue regeneration. Importantly, this modeling framework includes cell density and growth and is able to describe mechanistic genetic networks controlling the restoration of shape and forms. In addition, we have integrated this new formalism into an artificial intelligence methodology for the automated reverse-engineering of quantitative models directly from experimental data. As a proof of concept, we have applied our novel framework to infer the mechanisms responsible for the allometric restoration of body shape in amputated trunk-pieces of planarian worms. Using a dataset of planarian experiments and their resultant morphologies, we have discovered a suitable, dynamic genetic model that accurately recapitulates the regeneration of shape and form in planarian worms after surgical amputations. This work paves the way for the understanding of how shape and form is restored through a regenerative process, an essential step towards the much sought-after tissue regeneration applications in human medicine.

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Poster 70

SYNTHESIS OF FLEX-BCX4430 – A POTENTIAL TREATMENT FOR EBOLA

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Ebola is a filovirus which was first identified in the Zaire Ebola Outbreak of 1976. Its mortality rate can be up to 90%, and after the recent outbreak during 2014 in West Africa, more focus has been placed in research to treating the virus. Current treatments being explored include therapeutic antibodies, peptide entry inhibitors, and nucleoside antivirals. One potential drug which has shown promise in treating the virus is the nucleoside analogue BCX4430. BCX4430 is an adenosine nucleoside analogue that has shown to inhibit the RNA-dependent RNA polymerase (RdRp) of the Ebola virus, which then halts the replication process of the virus.

As is typical with many antiviral treatments, the possibility for mutations in the viral enzyme binding site can lead to the development of resistance. In order to combat the adaptations the virus can make, we have designed a flexible nucleoside analogue with a carbon-carbon bond connecting the pyrrole and the pyrimidine of the "split" purine ring system. It provides an extra degree of freedom within the bicyclic purine ring, and will impart flexibility to the scaffold of BCX4430. This creates a BCX4430 analogue (Flex-BCX4430) with the ability to reposition itself in the enzyme binding site, and may improve the recognition between the enzyme and the nucleoside, leading to better binding. It may also provide the analogue with the ability to overcome resistance mutations in the binding site of the Ebola virus by allowing it to engage in alternative interactions with the enzyme active site. The goal of the current project is to synthesize the sugar of the Flex-BCX4430 starting with D-ribose, and the progress to date will be reported herein.

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Poster 72

PREPARATION AND PURIFICATION OF HIV-1 RNA 5' LEADER FOR GEL ELECTROPHOERESIS AND NMR STUDIES

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The human immunodeficiency virus (HIV) attacks the immune system and affects 5,753 people a day, which adds to about 2.1 million people every year. The reason why the 5' monomeric leader is so important is because it is the most conversed region of the whole genome. To study the HIV RNA we first have to create the RNA. We start with the trial transcription. In the trial transcription we create small mixtures of varying amounts of the reactants in order to find the best conditions that will create the most RNA. We then pick the mixture that produced the most RNA and create a large-scale version. After we create the large-scale version and complete the *in vitro* transcription we start the purification process. We prepare a large gel, which will separate by-products and the T7 enzyme used in the *in vitro* transcription reaction. Once the gel is finished running we place the gel under UV light, which exposes the region of gel that contains our desired RNA. We then cut the gel into pieces and place them into an elutrap electroelution system. The elutrap separates the RNA from the pieces of gel. Finally, the RNA will be washed with high purity salts and autoclaved Millipore water. After the RNA is purified it can be used in gel electrophoresis and nuclear magnetic resonance experiments to study the properties of the HIV-1 5' leader RNA.

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Poster 73

GENE CLONING OF HUMAN N-MYRISTYLTRANSFERASE

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The human immunodeficiency virus (HIV) is an immunosuppressant retrovirus that is a worldwide epidemic. The development of treatment for HIV has been hindered by a lack of an adequate animal model. Cats are infected by a similar retrovirus called the feline immunodeficiency virus (FIV) that elicits a similar disease course in cats as HIV does in humans, thus the FIV/feline system is a viable animal model. The Gag polyprotein (Gag) is a major structural protein of HIV and FIV that targets to the membrane for production of new virions, and better characterization of FIV assembly may lead to development of a novel therapy for HIV. Matrix (MA), the N-terminal domain of Gag, mediates this assembly to the cell membrane. The myristate, a saturated fatty acid that anchors MA to the plasma membrane, is linked to the N-terminus of MA and is critical to the assembly process. Myristylation is mediated by the enzyme N-myristyltransferase (NMT), a process which requires NMT recognition of the substrate MA myristylation signal. FIV MA has a unique myristylation signal compared to other feline and mammalian proteins, and a better comprehension of the advantages of such a unique signal could help to further characterize the function of FIV MA. The current methods to prepare FIV MA involve modifications for protein purification, which may influence studies of FIV MA function. The aim for this project is to prepare human NMT in a protein expression vector by means of gene cloning, and, ultimately, to express and purify the protein. This work would facilitate preparation of unmodified, myristylated FIV MA for analysis of structure and function.

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Poster 80

TONGUE CURVATURE OF /S/ DURING "A SOUK."

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During the speech task "A Souk," the tongue elevates to produce the /s/ sound and a curvature is created in the anterior portion of the tongue surface. To produce the /s/ sound, the tongue tip creates an apical (tongue tip up) or laminal (tongue tip down) movement. As a result, differences in tongue tip shape may capture the difference in /s/ type shape observed subjectively on MRI and X-Ray. Using CineMRI, points were taken from a time frame with the maximum /s/ contact. These points were used to obtain tongue curvature quantities. The goal of this research is to study the shape of the tongue's curvature measurements in order to evaluate quantitative differences in tongue's maximum contact for /s/ in controls and post-glossectomy patients.

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Poster 84