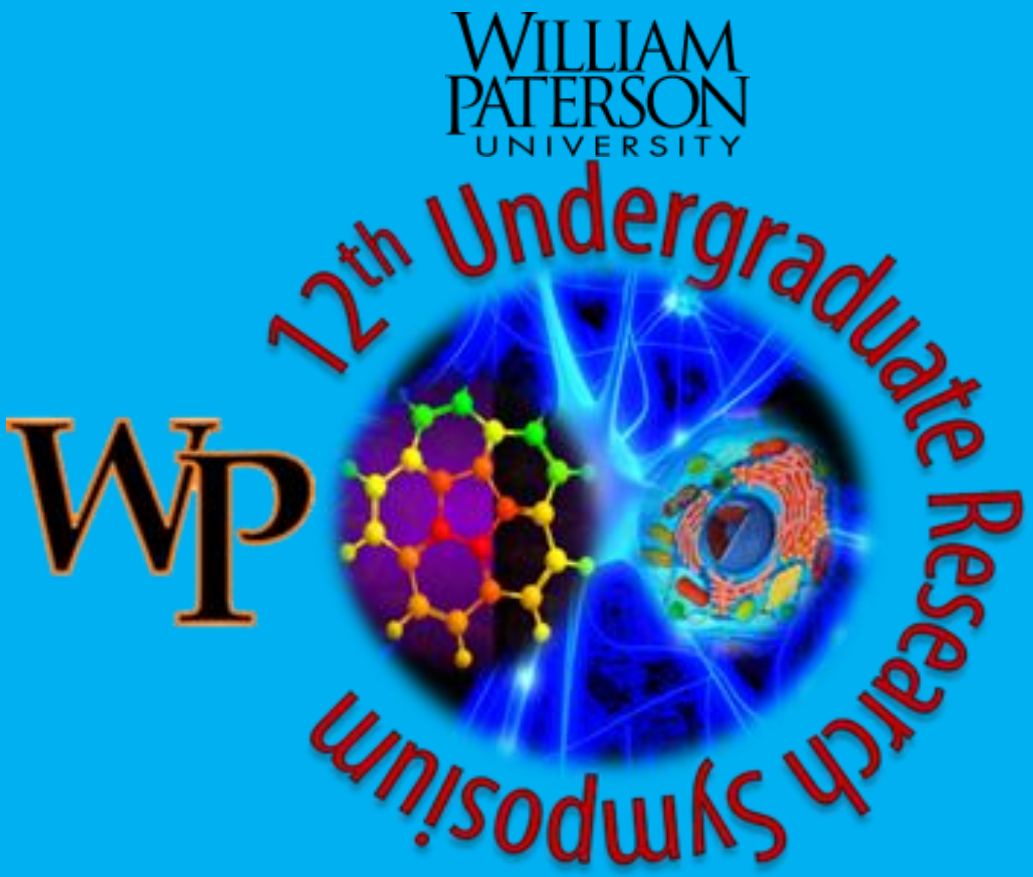

William Paterson University

Biological and Chemical Sciences

Program and Abstracts

Undergraduate Research Symposium

Saturday, April 14, 2018

300 Pompton Road, Wayne, NJ 07470

WPSTEMRESEARCH

Table of Contents

Entrée	Subject	Page
1	"Few Words from Organizers"	2
2	Plenary Abstracts and Speaker Profile	4
	Organizing Committee	6
3	Schedule of Events and Posters	7
4	Poster Abstract	24
5	Author/Faculty Information	139
6	Participating Institutions	143

"FEW WORDS FROM ORGANIZERS"

Few activities are as rewarding as research to the motivated students as well as faculty mentors. In addition to the acquisition of invaluable research skills, students learn how knowledge is created and experience the excitement of the "eureka moment". To celebrate undergraduate achievements, a research symposium has been held since 2007 on the WPUNJ campus for students in biological, chemical and environmental sciences. This symposium provides an opportunity to the students to showcase their talents and share their research achievements with their peers from about Thirty-Four universities from the Tri State area.

We would like to welcome all of you to an exciting 12th year of the Undergraduate Research Symposium at William Paterson University of New Jersey. This is an example of a budding community of undergraduate researchers. We want to thank all of the students from past and current who participated in the symposium and shared their research with us. We also want to thank all of the research mentors who have made it possible by investing their time, knowledge, resources and energy, so that undergraduates gain their first hand research experiences.

We express our gratitude to all of our student volunteers who show great enthusiasm and worked very hard to make this symposium a success.

We are very much obliged to Professor Rigoberto Hernandez, Johns Hopkins University for accepting our invitation as our keynote speaker and investing her valuable time to be with us.

This symposium could not have been successful without the moral support and continuous help from our Deans, Dr. Sharma and Dr. Fuller-Stanley, who worked very diligently with us so that everything is put together in a professional manner. Our special thanks also due to Dr. Sandy DeYoung (Emeritus Dean), under whose direction and guidance this symposium was initiated.

We also want to thank Dr. David Slaymaker and Dr. Bhanu P. S. Chauhan (Chairs of the Biology and the Chemistry Departments) for their continued support. As well as the office of Institutional Advancement and the Alumni Association for partly financing the event in various capacities.

The symposium of this magnitude could not have been possible without the support we get from Dr. Warren Sandmann, Provost & Vice President of Academic Affairs.

Finally yet importantly, we extend our gratitude to President Kathleen Waldron for her leadership who continuously encouraged us and inspired us with her ideas to make this symposium a great success.

ORGANIZERS:
Dr. Jaishri Menon
Dr. Bhanu P. S. Chauhan

Plenary Speaker

Professor Rigoberto Hernandez

Gompf Family Professor & Director of (OXIDE) Johns Hopkins University

PLENARY ABSTRACT

"Benign by Design from the Nanoscale to the Human Scale"

Abstract:

The nanoparticles we make today to address problems in energy and human health will enter the environment tomorrow. But will they be benign or will they lead to deleterious downstream effects to our environment? The Center for Sustainable Nanotechnology is developing and benchmarking design principles for sustainable nanoparticles. Our group contributes the theoretical and computational frameworks to bridge the molecular scale structure and motion to macro and meso scale behavior of nanoparticles in heterogeneous environments. This includes contact with model membranes and other constituents found in the cellular matrix.

About Professor Rigoberto Hernandez

Dr. Rigoberto Hernandez is the Gompf Family Professor in the Department of Chemistry at the Johns Hopkins University as of July 2016, and remains as the Director of the Open Chemistry Collaborative in Diversity Equity (OXIDE) since 2011. Before Hopkins, he was a Professor in the School of Chemistry and Biochemistry at Georgia Tech, and Co-Director of the Center for Computational Molecular Science and Technology he co-founded. He holds a B.S.E. in Chemical Engineering and Mathematics from Princeton University (1989), and a Ph.D. in Chemistry from the University of California, Berkeley (1993). (Hernandez was born in G ü inez, Havana, Cuba but was raised and educated in the United States of America since he was in primary school. He is a U.S. citizen by birthright.

Dr. Hernandez is the recipient of a National Science Foundation (NSF) CAREER Award (1997), Research Corporation Cottrell Scholar Award (1999), the Alfred P. Sloan Fellow Award (2000), a Humboldt Research Fellowship (2006-07), the ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences (2014), the CCR Diversity Award (2015), the RCSA Transformative Research and Exceptional Education (TREE) Award (2016), and the Herty Medal (2017). He is a Fellow of the American Association for the Advancement of Science (AAAS, 2004), the American Chemical Society (ACS, 2010), and the American Physical Society (APS, 2011). In 2015-2016, he was a Phi Beta Kappa Visiting Scholar. At Georgia Tech, he served as the first Blanchard Assistant Professor of Chemistry (1999-2001), the first Goizueta Foundation Junior Rotating Faculty Chair (2002-07) and a Vasser Woolley Faculty Fellow (2011-13).

His recent board memberships include the National Academies Panel within the Army Research Laboratory Technical Assessment Board (2005-2011), the National Academies Board on Chemical Sciences and Technology (2007-2010), the Telluride Summer Research Conference Board of Directors (2007-09), the NIH Study Section on Molecular Structure and Function B (MSFB, 2009-2013), the Research Corporation Cottrell Scholars Advisory Committee (member 2011-15, and chair 2016-17), the DOE Committee of Visitors (Division of Chemical Sciences, Geosciences and Bio-sciences, 2014) and the American Chemical Society Board of Directors (2014-2019).

Dr.Hernandez's research programs are currently funded by the NSF through a single-investigator grant and the CCI Center for Sustainable Nanomaterials. The OXIDE effort is cofunded by the NSF, DOE and NIH.

Research Interests

Dr. Hernandez' s research area can be broadly classified as the theoretical and computational chemistry of systems far from equilibrium. This includes a focus on microscopic reaction dynamics and their effects on macroscopic chemical reaction rates in arbitrary solvent environments. His current projects involve questions pertaining to the diffusion of mesogens in colloidal suspensions and liquid crystals, the structure and dynamics of assemblies of Janus and other patchy particles, fundamental advances in transition state theory, design principles for sustainable nanotechnologies and the dynamics of protein folding and rearrangement.

SYMPOSIUM ORGANIZING COMMITTEE

ORGANIZERS

Dr. Jaishri Menon

Dr. Bhanu P. S. Chauhan

Committee Members

Dr. Jean Fuller-Stanley

Dr. Michael Peek

Dr. Eileen Gardner

Dr. Jeung Woon Lee

Dr. Carey Waldburger

Dr. Pradeep Patnaik

Dr. Yalan Xing

Dr. Parminder Kaur

Dr. Jay Foley

Dr. Mihaela Jitianu

Dr. Emily Monroe

Dr. Mukesh Sahni

Ms. Karyn Lapadura

SCHEDULE OF EVENTS

7:30 am– 8:30 am	Registration, Breakfast, & Poster Setup University Commons 171 A/B
8:30 am – 8:45 am	Welcome and Opening Remarks President Kathleen Waldron Ballroom
9:00 am – 11:00 am	POSTER SESSION A, Ballroom Behavior: B1 – B7 Cell & Molecular Biology & Genetics I: CMB 1 – CMB 9 Ecology, & Environmental Science I: EE 1 – EE 7 Genetics: G 1 – G 7 Miscellaneous: MISC 1 – MISC 5 Analytical Chemistry: AC 1 – AC 9 Nanochemistry: NC 1 – NC 7 Organic Chemistry: OC 1 – OC 8
11:15 am – 12:45 pm	LUNCH – Wayne Dining Hall
1:00 pm – 2:00 pm	PLENARY TALK - Ballroom Dr. Rigoberto Hernandez Gompf Family Professor of Chemistry & Director of (OXIDE) Johns Hopkins University “Benign By Design: From The Nanoscale To The Human Scale”
2:00 pm – 4:00 pm	POSTER SESSION B , Ballroom Cell & Molecular Biology II: CMB 10 - CMB 18 Ecology, & Environmental Science II: EE 8 – EE 15 Microbiology: MB 1 – MB 9 Physiology: P 1 – P 8 Biochemistry: BC 1 – BC 9 Polymer & Materials Chemistry: PMC 1 – PMC 7 Theoretical & Physical Chemistry: T&PC 1 – T&PC 8
4:15 pm – 4:30 pm	Refreshments, Coffee & Cake - Ballroom
4:30 pm – 5:00 pm	AWARDS CEREMONY, Ballroom

Poster Session: Behavior

JUDGES: Dr. Kendall Martin*
Dr. Matthew Marcello

Poster#	Title, Author(s), Affiliation(s)	Page#
B1	**THE IMPACT OF SELECTIVE DELETION OF CANNABINOID CB2 RECEPTORS IN THE NEURODEVELOPMENT OF DAT-C*nr2* NAD CX3CR1-C*nr2* TRANSGENIC MICE; *Mariam Hammouda,*** Ana Canesco, Norman Schanz, & Dr. Emmanuel Onaivi; Department of Biology, William Paterson University, Wayne, NJ	24
B2	**BIOLOGY OF DESIRE: NEUROTRANSMITTER MEDIATED BEHAVIOR IN CHERRY SHRIMP: *Molly Mancuso, Carla Granda, Louis Durosier*** & Dr. Josh Stout, School of Natural Sciences, Fairleigh Dickinson University, Teaneck, NJ	25
B3	**A STUDY OF CELL PHONE DEPENDENCY: *Leandro Martelino*** & Dr. Gaby Fahmy; Department of Biology, Felician University, Lodi, NJ	26
B4	**THE EFFECTS OF MODULATION OF A POTASSIUM CHANNEL ON SOCIAL BEHAVIOR AFTER A TRAUMATIC BRAIN INJURY: *Jose Munoz*** & Dr. Sonya Bierbower; Department of Biology, William Paterson University, Wayne, NJ	27
B5	**BEHAVIORAL MODIFICATIONS FOLLOWING DELETION OF TYPE 2 CANNABINOID RECEPTORS IN DOPAMINE NEURONS: *Tameh Rohani,*** Branden Sanabria, Ana Canseco-Alba, Norman Schanz, Liu Qing-Rong, DX, & Dr. Emmanuel Onaivi; Department of Biology, William Paterson University, Wayne, NJ	28
B6	**THE ROLE OF CANNABINOID CB2 RECEPTORS IN COGNITIVE FUNCTION OF DAT-C*nr2* CONDITIONAL KNOCKOUT MICE: *Bernadin Rollanda,*** Ana Canseco-Alba, & Dr. Emmanuel Onaivi; Department of Biology, William Paterson University, Wayne, NJ	29
B7	**HORMONAL CONTROL OF CUTANEOUS DRINKING IN THE CHACOAN HORNED FROG (*CERATOPHRYS CRANWELLI*): *Michelle Foster*** & Dr. Joseph Agugliaro; Department of Biological & Allied Health Services, Fairleigh Dickinson University, Florham Campus	109

***Coordinator**

Poster Session: Cell & Molecular Biology I

JUDGES: Dr. Carey Waldburger*
Dr. Edith Myers
Dr. Gaby Fahmy

Poster#	Title, Author(s), Affiliation(s)	Page#
CMB1	**THE EFFECT OF HIGH LIGHT INTENSITY ON TOXIC AND NONTOXIC STRAINS OF *KARENIA BREVIS:*** ***Alan Abboud, Belal Almouallem***, & Dr. Emily Monroe; Department of Biology, William Paterson University, Wayne, NJ	30
CMB2	**STRUCTURAL STUDY OF THE *SLERT* LONG NON-CODING RNA:** ***Christina Ashby[1]***, & Dr. Shuang Li[2]; Department of Sociology, Pre-Med, Pace University, NY, NY[1]; Institute of Diabetes, Digestive & Kidney Diseases (NIDDK) National Institute of Health, Bethesda, MD[2]	31
CMB3	**LEAD EXPOSURE: HOW MUCH IS TOO MUCH? – A STUDY OF EFFECT OF LEAD ON NERVE GROWTH FACTOR REGULATED EMBRYONIC DORSAL ROOT GANGLION NEURODEVELOPMENT:** ***Christopher Cowie, Jeffrey Finch,*** & Dr. Yungcui Li; Department of Biology, University of Hartford, West Hartford, CT	32
CMB4	**TESTING THE ENHANCER-PROMOTER HYPOTHESIS IN *SACCHAROMYCES CEREVISIAE:*** ***Megan Deschaine***, Ahmad Abu Hardian, Sarah Elkamhawy & Dr. James Arnone; Department of Biology, William Paterson University, Wayne, NJ	33
CMB5	**CHANGES IN HYPOTHALAMIC HORMONE LEVELS AFFECTING ADDICTION AND NOCICEPTIVE RESPONSES:** ***Mohamed Eita***, Sandy Cheng & Dr. J.W. Lee; Department of Biology, William Paterson University, Wayne, NJ	34
CMB6	**SYSTEMATIC CHARACTERIZATION AND CONSERVATION OF ADJACENT GENE CO-REGULATION IN FUNGI:** ***Reem Eldabagh, Nelson Mejia***, Rachael Barret, Dr. Jay Foley*, & Dr. James Arnone; Department of Chemistry*, Department of Biology, William Paterson University, Wayne, NJ	35
CMB7	**STRUCTURE-FUNCTION ANALYSIS OF MKL1 IN MEGAKARYOCYTOPOIESIS:** ***Nicole Eskow***, Dr. Vanessa Scanlon, & Dr. Diane Krause; Department of Laboratory Medicine, Yale University, New Haven, CT	36
CMB8	**DESIGN OF AN IMMUNOGENIC AND ANTI-EGFR RNA THERAPEUTIC TO ALTER RNA AND PROTEIN EXPRESSION IN GLIOBLASTOMA MULTIFORME:** ***Sarah Falotico,*** Nicole Sivetz, Peter Nekrasov & Dr. Martin J. Hicks; Department of Biology, Monmouth University, West Long Branch, NJ	37
CMB9	**CDK5: THE CONNECTION BETWEEN ALZHEIMER'S DISEAST AND DIABETES:** ***Kevin Mora***, & Dr. Ann Aguanno; Department of Natural Sciences, Marymount	38

	Manhattan College, New York, NY	

***Coordinator**

Poster Session: Ecology & Environmental Science I

JUDGES: Dr. Michael Peek*
Dr. Michael Sebetich
Dr. Nicole Davi

Poster#	Title, Author(s), Affiliation(s)	Page#
EE1	**ANALYSIS OF BIODIVERSITY OF DEAD WOOD-INHABITING FUNGI IN THE NORTH AND SOUTH NEW JERSEY USING DNA-BARCODING:** ***Eve Bell, Lothar Vidal,*** & Dr. Maria Shumskaya, School of Natural Sciences, Kean University, Union, NJ	39
EE2	**ENVIRONMENTAL EVALUATION OF MID-ATLANTIC COASTAL WETLANDS:** ***Ksawery Biskup, Austin Degen***, & Dr. Michael Griffiths; Department of Environmental Science, William Paterson University, Wayne, NJ	40
EE3	**NUTRITIONAL REQUIREMENTS OF BEAN BEETLES (*CALLOSOBRUCHUS MACULATUS)* AND A "MENU" OF BEANS THAT "SELECT" FOR OVIPOSITION AND EMERGENCE RATES:** ***Diana Chaimov, Myar Drandish***, Alvin Sanchez & Dr. Kathleen A. Nolan; Department of Biology, St. Francis College, Brooklyn, NY	41
EE4	**GENETIC ANALYSES REVEAL THE POSSIBLE DESCRIPTION OF A NEW DEEP-SEA SPECIES IN THE GENUS *CONGER*:** ***Dominique Cheb Terrab[1],*** Dr. Andra M. Quattrini[2], & Dr. Katriina L.Ilves[1]; Department of Biology, Pace University, New York, NY[1], F.W. Olin Science Center, Harvey Mudd College, Claremont, CA[2]	42
EE5	**THE EFFECTS OF ETHINYL ESTRADIOL ON *DAPHNIA MAGNA* POPULATION DYNAMICS AND BODY LENGTH:** ***Alicia Cole***, & Dr. James Salierno, Department of Biological & Allied Health Sciences, Fairleigh Dickinson University, Madison, NJ	43
EE6	**PHENOLOGY OF HONEYBEE COLONIES AND THEIR KEY POLLEN PLANTS IN THE URBANIZED NEW JERSEY LANDSCAPE:** ***Trevor Courtright*** & Dr. David Gilley, Department of Biology, William Paterson University, Wayne, NJ	44
EE7	**EFFECTS OF WASTEWATER TREATMENT EFFLUENT ON POPULATION BIOLOGY OF THE FRESHWATER AMPHIPOD, *GAMMARUS FASCIATUS:*** ***Marialaina Nissenbaum*** & Dr. James Salierno; Department of Biology & Allied Health Services, Fairleigh Dickinson University, Madison, NJ	45

***Coordinator**

Poster Session: Genetics

JUDGES: Dr. David Slaymaker*
Dr. James Salierno
Dr. Megan Phifer-Rixey
Dr. Robert Benno

Poster#	Title, Author(s), Affiliation(s)	Page#
G1	**CHARACTERIZATION OF DIADINOXANTHIN DE-EPOXIDASE ENZYME IN *KARENIA BREVIS:* *Yuliana Cruz Herrera*** & Dr. Emily Monroe; Department of Biology, William Paterson University, Wayne, NJ	46
G2	**THE EFFECTS OF NITROGEN LIMITED ENVIRONMENTS ON THE DINOFLAGELLATE *KARENIA BREVIS:* *Rita De Almeida[1]*** & Dr. Emily Monroe[2]; Department of Environmental Science[1] & Department of Biology[2], William Paterson University, Wayne, NJ	47
G3	**EVALUATING THE FUNCTION OF GENES IMPLICATED GLIOBLASTOMA MULTIFORME (GBM) FORMATION USING *C. ELEGANS:* *Agata D. Durda*** & Dr. Matthew R. Marcello; Department of Biology, Pace University, New York, NY	48
G4	**ANALYZING THE FUNCTION OF THE CAENORHABDITIS ELEGANS GENE MO5D6.S, AN ORTHOLOG OF HUMAN T-COMPLEX PROTEIN 11 (TCP11), IN SPERM FUNCTION AND FERTILITY:** ***Amber Jacob, Danielle Cooley***, Emily Lopez, & Dr. Matthew Marcello; Department of Biology, Pace University, New York, NY	49
G5	**SYSTEMATIC IDENTIFICATION AND CONSERVATION OF ADJACENT GENE PAIRINGS IN FUNGI:** ***Christopher Monzo,*** Matthew So, Nelson Mejia, Rachael Barret & Dr. James Arnone; Department of Biology, William Paterson University, Wayne, NJ	50
G6	**OSTEOARTHRITIS INDUCED BY *HAS2* GENE KNOCKOUT OF CARTILAGE:** ***Kyle Murphy, Kyle Vaccaro,*** Kemar Edwards & Dr. Yingciu Li; Department of Biology, University of Hartford, West Hartford, Ct	51
G7	**REGULATION OF DNA REPAIR PATHWAYS TO ENSURE GAMETE QUALITY:** ***Aidan Nowakowski, Richard Monsky***, Julia Laibach, Carolyn Turcotte, Erika Rosenkrause, Dr. Paula Checchi & Dr. Nicolas Andrews; Department of Biology, Marist College, Poughkeepsie, NY	52

***Coordinator**

Poster Session: Miscellaneous

JUDGES: Dr. Ana Canseco-Alba*
Dr. Maria Vogt

Poster#	Title, Author(s), Affiliation(s)	Page#
MISC 1	**USING A CELL CULTURE-BASED MODULE TO TRAIN RESEARCH STUDENTS:** ***Julia Furnari*** & Dr. AnnAguanno; Department of Natural Sciences, Marymount Manhattan College, New York, NY	53
MISC 2	**THE URBAN ECOSYSTEM: A FIRST-YEAR COURSE TO BOOST COHORT FORMATION AND STEM RETENTION:** ***Emma Kamen*** & Dr. Alessandra Leri; Department of Natural Sciences, Marymount Manhattan College, New York, NY	54
MISC 3	**CHARACTERIZATION OF PLASMA SOURCE USED TO ACCELERATE WOUND HEALING OF THE TADPOLE *XENOPUS LAEVIS**:** ***Samantha Nieves***, Dr. Jaishri Menon and Dr. Kevin Martus, Department of Biology, William Paterson University, Wayne, NJ	55
MISC 4	**COMPARISON OF MICROFLUIDIC PDMS AND SILICON DEVICES THROUGH CRYO-ELECTRON MICROSCOPY:** ***Manasi Soman*** & Dr. Sandip Kaledhonkar; Department of Molecular, Biophysics and Biological Science, Columbia University, New York, NY	56
MISC 5	**THE USE OF A CELL CULTURE-BASED MODULE IN A BIOLOGY COURSE:** ***Brandon Tran*** & Dr. AnnAguanno; Department of Natural Sciences, Marymount Manhattan, College, New York, NY	57

***Coordinator**

Poster Session: Analytical Chemistry

JUDGES: Dr. Yalan Xing*
Dr. Gene Hall
Dr. Ish Kumar
Dr. Suresh Sahni

Poster#	Title, Author(s), Affiliation(s)	Page#
AC 1	**PROVING "PROOF" BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY:** ***Cristian Arias*** & Dr. Maria Vogt; Department of Chemistry, Bloomfield College, Bloomfield, NJ	58

AC 2	**HIGH-YIELD RECOMBINANT PRODUCTION HYPOXIA-INDUCIBLE FACTOR PROLYL-HYDROXYLASE DOMAIN PROTEIN 3: A KEY REGULATOR OF THE HYPOXIC RESPONSE SYSTEM:** ***Michelle Currie, Kayla Schardien*** & Dr. Nathaniel Nucci; Physics Department, Rowan University, Glassboro, NJ	59
AC 3	**DETERMINATION OF CRITICAL MICELLE CONCENTRATION OF AEROSOL-OT USING FLUORESCENCE SPECTROSCOPY:** ***Katerina Djambazova, Pragun Tuladhar, John Schaffer***, ***Alexa Hacopian*** & Dr. Loraine Tan; Department of Chemistry, Ramapo College of New Jersey, Mahwah, NJ	60
AC 4	**OPTIMIZATION OF A FLUORESCENCE ASSAY TO TEST INHIBITION OF PROLYL-HYDROXYLASE DOMAIN PROTEINS:** ***Thomas Fasano, Nakoa Webber***, Jacob Zangaro, Pamela Gallo & Dr. Nathaniel Nucci; Department of Translational Biomedical Sciences, Rowan University, Glassboro, NJ	61
AC 5	**ADSORPTION OF ACETAMINOPHEN ON ACTIVATED CARBONS FROM CASHEW NUT SHELLS:** ***Alexandra Geczo*** & Dr. Svetlana Bashkova; Department of Chemisry & Pharmaceutical Science, Fairleigh Dickinson University, Madison, NJ	62
AC 6	**IN SEARCH OF TRANS FFATS IN HYDROGENATED VEGETABLE OILS:** ***Oscar Jossue Gutierrez-Zuniga*** & Dr. Maria Vogt; Department of Chemistry, Bloomfield College, Bloomfield, NJ	63
AC 7	**AN INFRARED SPECTROSCOPIC ANALYSIS OF SHRINK—RAPPED PLASTICS TO FACILITATE SORTING IN RECYCLING PLANTS:** ***Ashley Pavia*** & Dr. Alessandra Leri; Department of Natural Sciences, Marymount Manhattan College, New York, NY	64
AC 8	**CHROMATOGRAP[HIC ANALYSIS OF AMPHETAMINES IN BIOLOGICAL SAMPLES:** ***Lauren Reilly*** & Dr. Elmer-Rico Mojica; Department of Chemistry & Physical Sciences, Pace University, New York, NY	65
AC 9	**GREEN SYNTHESIS OF POLYHODANINE MICROSPHERES AND ITS APPLICATION FOR THE ADSORPTION OF ORGANIC DYE:** ***[1] Yousif Saleh,*** [1]Anjali Gaba**,** [2]Qiaxian Johnson , [1]Dr. Moni Chauhan, and [2]Dr. Bhanu Chauhan; [1] Department of Chemistry, Queensborough Community College Of CUNY, Bayside, NY [2]Department of Chemistry, William Paterson University of New Jersey, Wayne, NJ	66

***Coordinator**

Poster Session: Nanochemistry

JUDGES: Dr. Parminder Kaur*
Dr. Joseph Baker
Dr. Wooseok Ki
Dr. Maria Shumskaya

Poster#	Title, Author(s), Affiliation(s)	Page#
NC 1	**SHAPE AND SIZE CONTROL OF SILVER NANOPARTICLES:** ***Roshena Harty, Zachary Mosley*** & Dr. Bhanu P. S. Chauhan, Department of Chemistry, William Paterson University, Wayne, NJ	67
NC 2	**SINGLE NANOPARTICLE INVESTIGATION FOR HYDROGEN EVOLUTION REACTION:** ***Jordyn Janusz*** & Dr. Glen O'Neil; Chemistry Department, Montclair State University, Montclair, NJ	68
NC 3	**FORMATION OF GELS USING DIFFERENT AMINO GROUPS INCORPORATED WITH NANOPARTICLES AND MULTI-WALLED CARBON NANOTUBES:** ***Gurjeet Longia***, Qiaxian John, & Dr. Bhanu P. S. Chauhan, Department of Chemistry, William Paterson University, Wayne, NJ	69
NC 4	**CATALSE ENCAPSULATED IN NANOSIZED MATRICES CAN BE USED IN SKIN CARE:** ***Karina Magro-Machado***, Faith Adams & Dr .Mihaela Leonida; School of Natural Science, Fairleigh Dickinson University, Teaneck, NJ	70
NC 5	**VARIOUS APPLICATIONS OF RHODANINE AND METAL COMPLEXEX:** ***Viven Musli***, Gurjeet Longia, Qiaxian Johnson & Dr. Bhanu P. S. Chauhan; Department of Chemistry, William Paterson University, Wayne, NJ	71
NC 6	**ELECTROCHEMICAL EXPLORATION OF GRAPHENE OXIDE:** ***Alexandra Rodriquez*** & Dr. Glen O'Neil; Department of Chemistry, Montclair State University, Montclair, NJ	72
NC 7	**PROBING THE PROPERTIES OF IONIC LIQUID MIXTURES WITH SINGLE-WALLED CARBON NANOTUBES:** ***Rawlric Sumner,[1]*** Katelyn Urena,[1] Fei Li,[1] Sharon Lall-Ramnarine,[1] James Wishart,[2] and Dr. Tirandai Hemraj-Benny[1] ; [1]Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY [2]Chemistry Division, Brookhaven National Laboratory, Upton, NY	73

***Coordinator**

Poster Session: Organic Chemistry

JUDGES: Dr. Jay Foley*
Dr. Moni Chauhan
Dr. Tirandai Hemraj-Benny
Dr. Alfred Castro
Dr. Edward Salaski

Poster#	Title, Author(s), Affiliation(s)	Page#
OC 1	**NON-PRECIOUS METAL CATALYZED OXIDATIVE ESTERIFICATION OF ALLYLIC SP³ -CARBON FOLLOWED BY *IN-SITU* REDUCTION:** ***Brenda Calalpa***, ***Tatiana Hapatsha,*** Sarafina Cartelli & Dr. Parminder Kaur; Department of Chemistry, William Paterson University, Wayne, NJ	74
OC 2	**A RECYCLABLE SOL-GEL CTALYZED APPROACH: EFFICIENT ONE POT SYNTHESIS OF *a,a* Di-HALOGENATED KETONES:** ***Justin Domena***, Carlos Chong, Qiaxian Johnson, Dr. Yalan Xing, & Dr. Bhanu P. S. Chauhan; Department of Chemistry, William Paterson University, Wayne, NJ	75
OC 3	**COPPER CATALYZED HOMOCOUPLING AND HETEROCOUPLING OF TERMINAL ALKYNES:** ***Maria Katrina Holganza***,Suzanne Elfarra, & Dr. Yalan Xing; Department of Chemistry, William Paterson University, Wayne, NJ	76
OC 4	**Mn-TERPYRIDINE CATALYZED DEHYDROGENATIVE ACCEPTORLESS COUPLING OF AMINES AND ALCOHOLS TO GIVE ALDIMINE:** ***Laura Lopez***, Brenda Calalpa, Giovanni Berrera, & Dr. Parminder Kaur; Department of Chemistry, William Paterson University, Wayne, NJ	77
OC 5	**IDAZOLES SYNTHESIS: ACCELERATING CYCLIZATION VIA MANIPULATION OF ELECTRON DENSITY:** ***Tran Nguyen*** & Dr. Edward Salaski; Department of Chemistry, Fairleigh Dickinson University, Madison, NJ	78
OC 6	**A NOVEL SYNTHETIC METHOD FOR THE PREPARATION OF (2H)-INDAZOLES:** ***Melissa Rock*** & Dr. Edward Salaski; Department of Chemistry & Pharmaceutical Sciences, Fairleigh Dickinson University, Madison, NJ	79
OC 7	**SYNTHESIS OF DAUMONE ANALOGS AND ANTI-AGING ACTIVITY STUDY:** ***Chiara St. Amant,[a] Mansi Patel,[a]*** Claudia Kim,[a] Maria K. Holganza,[b] Dr. James Arnone,[b,*] Dr. Yalan Xing,[a,*] Dr. Xiaofan Liu,[c] and Dr. George O'Doherty[c] [a] Department of Chemistry, William Paterson University of New Jersey. Wayne, NJ; [b] Department of Biology, William Paterson University of New Jersey. Wayne, NJ; [c] Department of Chemistry and Chemical Biology. Northeastern University, Boston, MA	80

OC 8	**VISIBLE LIGHT INDUCED ALKYNE FUNCTIONALIZATION:** ***Juan Torres***, John Lee, & Dr. Yalan Xing; Department of Chemistry, William Paterson University, Wayne, NJ	81

***Coordinator**

Poster Session: Cell & Molecular Biology II

JUDGES: Dr. Pradeep Patnaik*
Dr. Ann Aguanno
Scott Hofsess

Poster#	Title, Author(s), Affiliation(s)	Page#
CMB 10	**THE COORDINATION OF GENE EXPRESSION VIA GENOMIC CLUSTERING:** ***Maria Katrina Holganza***, Alanna Nolan, Irvin Gamarra, Exequiel Sisso, Dr. Jay Foley* *Dr. James Arnone; Department of Chemistry*, Department of Biology, William Paterson University, Wayne, NJ	82
CMB 11	**THE EFFECT OF CD44 ON REDD1 IN BREAST CANCER:** ***Sharon Mowla*** & Dr. Kyle Murphy; Department of Biochemistry & Microbiology, Rutgers University, New Brunswick, NJ	83
CMB 12	**SYNTHESIS OF A MINI-REPORTER CONSTRUCT TO TEST GENE TRANSFER OF RNA THERAPEUTICS:** ***Koushik Muralidharan***, Arbaz Khan, Kerianne Fuoco, Hemangi Patel & Dr. Martin J. Hicks; Department of Biology, Monmouth University, West Long Branch, NJ	84
CMB 13	**EFFECT OF A6 PEPTIDE ON CD44 IN OVARIAN CANCER:** ***Elizabeth Reynolds*** & Dr. Kyle Murphy; Department of Biochemistry & Microbiology, Rutgers University, New Brunswick, NJ	85
CMB 14	**EXOSOMES FROM HPV NEGATIVE CERVICAL CANCER CELLS NEGATIVELY AFFECT NORMAL CELL GROWTH:** ***Andrea Silva***, Emily Barkley, Alaina Kaiser, & Dr. Christina Zito; Department of Biology & Environmental Sciences, University of New Haven, West Haven, CT	86
CMB 15	**DELIVERY OF THERAPEUTIC RNA MOLECULES TO ALTER EPIDERMAL GROWTH FACTOR RECEPTOR EXPRESS IN GLIOBLASTOMA MULTIFORME:** ***Nicole Sivetz[1]***, Sanjana Akula[2], Anjali Chakradhar[3], Ester Teper[2], Lucy Zou[4], Sarah Falotico[1], Peter Nekrasov[1], & Dr. Martin J. Hicks; [1]Department of Biology, Monmouth University, West Long Branch, NJ; [2]Biotechnology High School, Freehold, NJ; [3]High Technology High School, Middletown, NJ; [4]East Brunswick High School, East Brunswick, NJ	87
CMB 16	**THE ROLE OF BRaf IN AhR SIGNALING AND**	88

	MELANOMA PROGRESSION: ***Ariadna Uribe*** & Dr. Kyle Murphy, Department of Biochemistry & Microbiology, Rutgers University, New Brunswick, NJ	
CMB 17	**IDENTIFYING PATHWAYS WITH SIGNALS OF GLOBAL REGULATION LINKED TO ENVIRONMENTAL ADAPTATION IN HOUSE MICE:** ***Sebastian Vera[1]***, Katya Mack[2], Michael Nackman[2], & Dr. Michael Phifer-Rixey[1]; Department of Biology, Monmouth University, West Long Branch, NJ[1]; The Museum of Vertebrate Zoology, University of California Berkeley, Berkeley, CA[2]	89

***Coordinator**

Poster Session: Ecology & Environmental Science II

JUDGES: Dr. Karen Swanson*
Dr. Ilena Boucher
Dr. Roy Messaro

Poster#	Title, Author(s), Affiliation(s)	Page#
EE 8	**SURVEY OF SPIDER FAUNA AND DNA BARCODE IDENTIFICATION ON WILLIAM PATERSON UNIVERSITY CAMPUS:** ***Aldrick Espinosa*** & Dr. Joseph Spagna; Department of Biology, William Paterson University, Wayne, NJ	90
EE 9	**NAUTILOID CEPHALOPODS FROM GLACIAL ERRATIFCS: EVIDENCE FOR LAG DEPOSIT FORMATION IN THE RICKARD HILL FACIES OF THE SAUGERTIES MEMBER OF THE SCHOHARIE FORMATION (LOWER DEVONIAN-LATE EMSIAN), HELDERBERG MOUNTAIN REGION, NEW YORK STATE, U.S.A.:** ***Christie Kline[1], Cling Mautz[1]***,Harry Maisch IV[2], Rebecca Chamberlain[3], John Chamberlain[2-4], and Dr. Martin Becker[1]: Department of Environmental Science, William Paterson University, Wayne, NJ[1]; Doctoral Programs in Earth &Environmental Sciences & Biology, City University of NY Graduate Center, NY, NY[2]; Department of Biology, College of Staten Island, Staten Island, NY[3]; Department of Earth & Environmental Sciences, Brooklyn College, Brooklyn, NY[4]	91
EE 10	**VARIATION IN REPRODUCTIVE TRAITS AMONG HOUSE MICE ADAPTED TO DIFFERENT CLIMATES IN THE AMERICAS:** ***Tiffany Longo[1]***, Mallory Ballinger[2], Dr. Nachman[2], & Dr. Phifer- Rixey; Department of Biology, Monmouth University, West Long Branch, NJ[1]; Museum of Vetebrate Zoology, University of California,, Berkeley, CA[2]	92
EE 11	**THE EXTINCTION OF THE MEGATOOTHED SHARK *OTODUS MEGALODON: EVIDENCE FROM CLUPED ISOTOPE THERMOMETRY (CIT):*** ***Allison Neumann[1],***	93

	***Chelsia Clarke*[1]**Drew Pedersen[1], Christi Kline[1], Clint Mautz[1], Robert Eagle[2], Harry Maisch[3], Aradhna Tripati[2], Dr. Michael Griffiths[1] and Dr. Martin Becker[1]; Department of Environmental Science, William Paterson University, Wayne, NJ[1]; UCLA Atmospheric & Oceanic Sciences, Los Angeles, CA[2]; Doctoral Program in Earth and Environmental Sciences, CUNY Graduate Center, NY, NY[3]	
EE 12	**A PRELIMINARY STUDY OF MICROPLASTICS AND MICROFIBERS AT THE MOLLY ANN BROOK, NJ: *Richard Plattel***, Eric Howard, Dr. Nicole Davie & Dr. Martin Becker; Department of Environmental Science, William Paterson University, Wayne, NJ	94
EE 13	**INSECT BIODIVERSITY AT HIGH MOUNTAIN PRESERVE: *Karisa Quimby, Elika Moallem*** & Dr. Joseph Spagna; Department of Biology, William Paterson University, Wayne, NJ	95
EE 14	**DNA EXTRACTION FROM ATLANTIC STURGEON SPINE AND FIN TISSUE: *Brian Reiss***, Dr. Dunton, & Dr. Phifer-Rixey; Department of Biology, Monmouth University, West Long Branch, NJ	96
EE 15	**CREATING AN AXENIC CULTURE OF THE TOXIC DINOFLAGELLATE *KARENIA BREVIS,* AND COMPARING ITS GROWTH RATE AND BREVETOXIN PRODUCTION TO XENIC CULTURES OF *K. BREVIS:* *Tehreem Tahir*** & Dr. Carey Waldburger; Department of Biology, William Paterson University, Wayne, NJ	97

***Coordinator**

Poster Session: Microbiology

JUDGES: Dr. Emmanuel Onaivi*
Dr. Sonya Bierbower
Dr. Joseph Agugliaro

Poster#	Title, Author(s), Affiliation(s)	Page#
MB 1	**RECOVERY OF DNA AND RNA FROM MICROORGANISMS IN WATER SAMPLES: *Catherine Dougherty*** & Dr. Sara Reynolds; Department of Biological & Allied Health Sciences, Fairleigh Dickinson University, Madison, NJ	98
MB 2	**QUANTIFICATION OF FECAL *AKKERMANSIA MUCINIPHILA* AS AN INDICATOR FOR A HEALTH GUT-MUCIN COMMUNITY: *Sofia Gomez***, Marjory Bustamante, Jennifer Louis, Marissa Angelucci, Nicholas Mully, Dr. Kendall Martin & Dr. Emmanuel Onaivi; Department of Biology, William Paterson University, Wayne, NJ	99
MB 3	**QUANTIFICATION OF PATHOGENIC FECAL BACTERIA OF NEW YORK CITY SIDEWALKS: *Marjan***	100

	Khan & Dr. Alessandra Leri; Department of Natural Sciences, Marymount Manhattan College, New York, NY	
MB 4	**DISCOVERY OF A MARINE BACTERIA WITH A WIDE SPECTRUM ANTI-BACTERIAL ACTIVITY: *Jenique Klinkerth***, Sonam Dosanjh, Carol Ellameh & Dr. Meriem Bendaoud; Department of Biology, New Jersey City University, Jersey City, NJ	101
MB 5	**DESIGNING NEW INHIBITORS FOR MYCOBACTERIUM TUBERCULOSIS USING BIOINFORMATIC SOFTWARES: *Eujin Lim***, Dr. Phalguni Ghosh, Dr. Sutapa Ghosh, Dr. Brian Lavey, & Dr. Rowley; Department of Natural Science, Middlesex County College, Edison, NJ	102
MB 6	**KIRBY-BAUER DIFFUSION SUSCEPTIBILITY TEST RESULTS FROM BSL1 BACTERIA IN THE MICROBIOLOGY TEACHING LABORATORY: *Angela Nuno*** & Dr. Sara Reynolds; Department of Biological & Allied Health Sciences, Fairleigh Dickinson University, Madison, NJ	103
MB 7	**SYNTHESIS OF UNIQUE LUBRICANTS MADE OF EXOTIC BUTTERS INFUSED WITH INDEGENOUS OILS TO PROMOTE INHIBITION OF BACTERIA AND PROTECTION AGAINST UV RADIATION:*Rudra Persaud*[1]** Keanna McLeod[2], Karin Melkonian[2], and Dr JaimeLee Rizzo[1] , Department of Chemistry and Physical Sciences, Pace University, New York, NY [1] C.W. Post, Long Island University, Brookville, NY [2]	104
MB 8	**STRONG ANTIMICROBIAL ACTIVITY DISPLAYED BY NEWLY SYNTHESIZED HYDROXAMIC ACIDS AND THEIR ANALOGS: *Stephanie Ramiez***, Sonam Dosanjh, Lina Marcella Henao, Destini Beauregard, Dr. Robert Aslanian & Dr. Mereiem Bendaoud; Department of Biology, New Jersey City University, Jersey City, NJ	105
MB 9	**EVALUATION OF *IN VIVO* TOXICITY OF NB1207, A NOVEL SYNTHETIC ANALOG OF miR-1207-3p: [1]*Tamara Gillot***, [1]Fayola Levine, and [1,2]Dr. Olorunseun O. Ogunwobi; [1]Department of Biological Sciences, Hunter College of The City University of New York; [2]Joan and Sanford I. Weill Department of Medicine, Weill Cornell Medicine, Cornell University	106

***Coordinator**

Poster Session: Physiology

JUDGES: Dr. James Arnone*
Dr. Sara Reynolds
Dr. Yingcui Li

Poster#	Title, Author(s), Affiliation(s)	Page#
P 1	**INVOLVEMENT OF HYPOTHALAMIC NEURONS IN**	107

	CONTROLLING MIDBRAIN NOCICEPTIVE NEURONS: A NEUROANATOMICAL EXAMINATION: ***Sandy Cheng***, ***Dara Buendia,*** Janice Yalong, Dara Buendia & Dr. J.W. Lee; Department of Biology, William Paterson University, Wayne, NJ	
P 2	**CREATINE MONOHYDRATE INCREASES RESISTANCE TO REACTIVE OXYGEN SPECIES (ROS) IN *CAENORHABDITIS ELEGANS:*** ***Kevin Dager*** & Dr. Ilene Boucher; Department of Natural Sciences, Felician University, Lodi, NJ	108
P 3	**Changed category**	**----**
P 4	**PLASMA EXPOSURE AND TAIL REGENERATION: THE INTERPLAY OF CALCIUM WITH MITOCHONDRIA AND PEROXISOMES:** ***Ma Veronica Holganza***, Dr. Kevin Martus & Dr. Jaishri Menon; Department of Biology, William Paterson University, Wayne, NJ	110
P 5	**THE EFFECTS OF TRICLOSAN ON *CAENORHABDITIS ELEGANS* SURVIVAL, REPRODUCTION, AND MOVEMENT:** ***Noel Khamis*** & Dr. Edith M. Myers; Department of Biology, Fairleigh Dickinson University, Madison, NJ	111
P 6	**SEASONAL VARIATION IN LOCOMOTOR PERFORMANCE OF GTHE RUBBER BOA (*CHARINA BOTTAE*):** ***Christine Macri*** & Dr. Joseph Agugliaro; Department of Biological & Allied Health Sciences, Fairleigh Dickinson University, Madison, NJ	112
P 7	**TESTING OF INNATE IMMUNITY STIMULATIONAS A METHOD TO AMELIORATE AD PATHOLOGY IN NON-HUMAN PRIMATES:** ***Margish Ramani '***, Xuewei Pei[1], Akash Patel[1], Pramod Nehete[2], Bharti Nehete[2], Elizabeth Cho[1], Dr. Lawrence Williams[2], Dr. Henrieta Scholtzova[1], & Dr.,Thomas Wisniewski[1]; Department of Neurology, New York University School of Medicine, New York, NY[1]; Department of Veterinary Sciences, UT MD Anderson Cancer Center, Bastrop, TX[2]	113
P 8	**THE ROLE OF CANNABINOID 2 RECEPTOR IN MODULATING MICROGLIA ACTIVATION AFTER A TRAUMATIC BRAIN INJURY:** ***Maria Zamora***, Ana Canseco-Alba & Dr. Sonya Bierbower; Department of Biology, William Paterson University, Wayne, NJ	114

***Coordinator**

Poster Session: Biochemistry

JUDGES: Dr. Mihaela Jitianu*
Dr. Matthew Marcello
Dr. Maria Shumskaya

Poster#	Title, Author(s), Affiliation(s)	Page#
BC 1	**SUSTAINED RELEASE OF HISTAMINASE ENCAPSULATED IN NANOCOMPOSITES MAY BE BENEFICIAL IN TREATMENT OF SKIN ALLERGIES:** ***Faith Adams, Jessica Maldonado***, & Dr. Mihaela Leonida; School of Natural Sciences, Fairleigh Dickinson University, Teaneck, NJ	115
BC 2	**CANNABINOID INTERACTION WITH THE CB1-RECEPTOR:** ***Josh Alb***, Dr. Phalguni Ghosh, Dr. Sutapa Ghosh & Dr. Brian Lavey; Department of Natural Sciences, Middlesex County College, Edison, NJ	116
BC 3	**CONVENTIONAL FMOC SOLID-PHASE SYNTHESIS, BIOCONJUGATION AND CHARACTERIZATION OF CANCER-TARGETING PEPTIDES:** ***Andrieh Darwich***, Adah Beck, Claudia Heller, Niki Rana, Mariana Phillips, Christopher Cultrara & Dr. David Sabatino; Department of Chemistry & Biochemistry, Seton Hall University, South Orange, NJ	117
BC 4	**INVESTIGATING IONIC LIQUID EFFECTS ON TRP-CAGE STABILITY:** ***Mattheus De Souza[1]***, Alexanndra J. Heyert[2], Gerrick E. Lindberg[2], and Dr. Joseph L. Baker[1] Department of Chemistry, The College of New Jersey, Ewing, NJ; Department of Chemistry and Biochemistry, Northern Arizona University, Flagstaff, AZ	118
BC 5	**EXPLORING THE ROLE OF DISULFIDE BONDS IN A COMP/DNA COMPLEX:** ***Maria Fairfield***, Keyur Patel & Dr. Joseph Baker; Department of Chemistry, The College of New Jersey, Ewing, NJ	119
BC 6	**ETHYLENEDIAMINETETRAACETIC ACID AS AN INHIBITOR OF ALKALINE PHOSPHOTASE:** ***Fernando Gomez*** & Dr. Alfredo Castro; Department of Natural Science, Felician University, Lodi, NJ	120
BC 7	**EXAMINATION OF BORIC ACID DERIVATIVES AS ANGIOTENSIN CONVERTING ENZYME INHIBITORS:** ***Kristina Neri,*** Dinesh-Amram Choudhary, Uday-Kiran Bijja, & Dr. Ish Kumar; School of Natural Sciences, Fairleigh Dickinson University, Teaneck, NJ	121
BC 8	**BINDING INTERACTION OF NANOCERAMICS (METAL OXIDES) WITH HUMAN SERUM ALBUMIN:** ***Tyler Nolan***, & Dr. Elmer-Rico Mojica; Department of Biology and Department of Chemistry & Physical Sciences, Pace University, New York, NY	122
BC 9	**ENZYME CATALYST FOR POLYSTYRENE:** ***Nazila Yekanifard*** & Dr. David Snyder; Department of Chemistry, William Paterson University, Wayne, NJ	123

***Coordinator**

Poster Session: Polymer & Materials Chemistry

JUDGES: Dr. Parminder Kaur*
Dr. Gene Hall
Dr. Maria Vogt
Dr. Dmytro Kosenkov

Poster#	Title, Author(s), Affiliation(s)	Page#
PMC 1	**3 D PRINTING OF NANOMATERIALS FOR APPLICATIONS IN MEDICINE AND CATALYSIS** ***Natasha Ampomah***, ***Jaquill Peppers,*** Qiaxian Johnson, & Dr. Bhanu P. S. Chauhan; Department of Chemistry, William Paterson University, Wayne, NJ	124
PMC 2	**NiO-Al_2O_3 OXIDES FROM SOL-GEL SYNTHESIZED TAKOVITES:** ***Laura Kuhlman[1], Shayma Embaby[1]***, Dr. Andrei Jitianu[2], Dr. Mihaela Jitianu[1]**;** [1]William Paterson University of New Jersey, Department of Chemistry, Wayne, NJ; [2]Lehman College, CUNY, Department of Chemistry, Davis Hall, West, Bronx, NY	125
PMC 3	**TAILORABLE MESOPOROUS SOLGELS CATALYZED BY HALOSUCCINAMIDES:** ***Gurpreet Longia***, Noor Eldabagh, Justin Domena, Qiaxian John, Dr. Yalan Xing & Dr. Bhanu P. S. Chauhan; Department of Chemistry, William Paterson University, Wayne, NJ	126
PMC 4	**STRUCTURE-BASED DESIGN OF MOLECULARLY IMPRINTED POLYMERS FOR G-QUADRUPLEX NUCLEIC ACIDS:** ***James Mizvesky, Arielle Golod,*** & Dr.Mohammed Elshaer; Department of Chemistry & Pharmaceutical Sciences, Fairleigh Dickinson University, Madison, NJ	127
PMC 5	**DEVELOPMENT OF NANOPOROUS THIN FILM SEMICONDUCTORS FOR SUN-DRIVEN WATER SPLITTING APPLICATIONS:** ***Anastasia Morozova, Anthony Bautista***, & Dr. Wooseok Ki; School of Natural Sciences, Chemistry Program, Stockton University, Galloway, NJ	128
PMC 6	**SYNTHESIS OF BORAN-FUNCTIONALIZED POLYMERS FOR CATALYSIS APPLICATIONS:** ***Mah Noor***, Fernando Vidal Pena, & Dr. Frieder Jaekle; Department of Chemistry, Rutgers University, Newark, NJ	129
PMC 7	**PREPARATION AND PROPERTIES OF PROPYL MODIFIED ORGANIC-INORGANIC HYBRID GLASSES:** ***Medine Sahin[2]***, Anhay Hernandez[2], Jennifer Guzman[1], Dr. Mihaela Jitianu[2], Dr. Lisa C. Klein[3] and Dr. Andrei Jitianu[1]; [1]Department of Chemistry, Lehman College, CUNY, Bronx, NY; [2]Department of Chemistry, William Paterson University of NJ, Wayne, NJ; [3]Department of Materials Science and Engineering, Rutgers University,	130

	Piscataway, NJ	

Poster Session: Theoretical & Physical Chemistry

JUDGES: Dr. Jay Foley*
Dr. Yalan Xing
Dr. Suresh Sahni
Dr. Alessandra Leri

Poster#	Title, Author(s), Affiliation(s)	Page#
T&PC 1	**COARSE-GRAINED MODELING AND SIMULATION OF TYPE IV PILI:** ***Bryan Bogin*** & Dr. Joseph Baker; Department of Chemistry, the College of New Jersey, Ewing, NJ	131
T&PC 2	**INHIBITION STUDIES OF NCI MOLECULES ON MMP-1 ENZYME BY FLUOROMETRIC ASSAY METHOD:** ***Dinesh-Amaram Choudhary, Syeda Fatima***, Raymong Rusak & Dr. Ish Kumar; School of Natural Sciences, Fairleigh Dickinson University, Teaneck, NJ	132
T&PC 3	**ANALYSIS OF EXCITATION ENERGY TRANSFER IN PIGMENT-PROTEIN COMPLEXES WITH PyFREC SOFTWARE:** ***Julia Farnan, Grant Gillan***, Yana Kholod & Dr. Dmytro Kosenkov; Department of Chemistry & Physics, Monmouth University, West Long Branch, NJ	133
T&PC 4	**DYNAMICS OF TYPE IV PILI IN PERIODIC SIMULATIONS:** ***Rebecca Goncalves*** & Dr. Joseph Baker; Department of Chemistry, The College of New Jersey, Ewing, NJ	134
T&PC 5	**SIMULATING PILIN/DNA INTERACTIONS WITH MOLECULAR DYNAMICS:** ***Keyur Patel*** & Dr. Joseph Baker; Department of Chemistry, The College of New Jersey, Ewing, NJ	135
T&PC 6	**MOLECULAR DYNAMICS SIMULATION ON A MIXED SOLVENT SYSTEM:** ***Eshaan Soman[1]*** and Dr. Jannette Carey[2]; Hillsborough High School, Hillsborough, NJ; [2]Department of Chemistry, Princeton University, Princeton, NJ	136
T&PC 7	**HOPPING-TYPE MODIFICATIONS OF QUANTUM INTERFERENCE CONDITIONS IN NANOSCALE THERMAL JUNCTIONS:** ***Hunter Tonn*** & Dr. Kamil Walczak; Department of Chemistry & Physical Sciences, Pace University, New York, NY	137
T&PC 8	**THE CAGE EFFECT: IONIC LIQUIDS MODIFY MEMBRANCE PERMEABILITY:** ***Kristen C. Vogt,[1]*** Alexanndra J. Heyert,[2] Gerrick E. Lindberg,[2] and Dr. Joseph L. Baker[1] [1]Department of Chemistry, The College of New Jersey, Ewing, NJ; [2]Department of Chemistry and Biochemistry, Northern Arizona University, Flagstaff, AZ	138

THE IMPACT OF SELECTIVE DELETION OF CANNABINOID CB2 RECEPTORS IN THE NEURODEVELOPMENT OF DAT-*Cnr2* AND CX3CR1-*Cnr2* TRANSGENIC MICE

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There are two major cannabinoid receptors (CB1Rs and CB2Rs) that are part of the endocannabinoid system in the periphery and central nervous system (CNS). CB1Rs are highly expressed and well characterized in the CNS compared to CB2Rs. The aim of this study was to determine the developmental profile following cell-type specific deletion of CB2Rs in microglia and dopaminergic neurons in Cx3cr1-*Cnr2* and DAT-*Cnr2* conditional knockout (cKO) mice in comparison to the wild type (WT) C57BL/6J controls. As our recent studies demonstrated that the DAT-*Cnr2* cKO mice exhibit spontaneous hyperactivity characteristic of hyperdopaminergic response, we also investigated and tested the hypothesis that the DAT-*Cnr2* cKO mice may represent a model of attention deficit hyperactivity disorder (ADHD).

The neurodevelopmental profile of the three strains of mice were determined daily from postnatal day 1 (PND1) to weaning postnatal day (PND21). Ultrasonic vocalizations (USVs) in the neonates were taken from PD1 to PD10. Body weights, physical development (incisors eruption, ear and eye opening), and general activity of the pups were measured and recorded until PND21. A separate group of DAT-*Cnr2* cKO and WT adolescent mice (PD30 $\pm$ 2) were treated acutely with amphetamine (2.0 mg/kg) or the vehicle alone intraperitoneally (i.p.), and their performance in the open field test were evaluated. We report that the USV rates at 60-80 hertz were higher in the DAT-*Cnr2* and Cx3cr1-*Cnr2* cKO mice than in the WT mice. The DAT-*Cnr2* cKO mice gained weight more slowly and were hyperactive in the open field test compared to the Cx3cr1-*Cnr2* cKO and WT mice. The 2.0 mg/kg amphetamine produced a significant increase in motor activity in the WT, and a striking significant reduction in motor activity of the DAT-*Cnr2* cKO mice in the open field test. Taken together the results suggests that CB2 cannabinoid receptors in microglia and dopamine neurons are involved in neuro-immune cross-talk in neurodevelopment, and that the DAT-*Cnr2* cKO mice may be a useful model for the investigation of the components of the endocannabinoid system as possible therapeutic targets in ADHD.

BIOLOGY OF DESIRE: NEUROTRANSMITTER MEDIATED BEHAVIOR IN CHERRY SHRIMP

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Dopamine is the neurotransmitter associated with love, lust, disease, and addiction. Dopamine is a chemical signal linked to the reward system in both vertebrate and invertebrate organisms. The reward system is also associated with seeking behavior, or mediated movement toward a certain target. To discover the neurophysiologic effect of dopamine on invertebrates, a behavioral approach was taken, with the selected model organism as *Neocaridina davidi*, commonly referred to as the "Cherry Shrimp." The neurobiology of all organisms is strikingly similar, regardless of how advanced or simple the organism appears. Invertebrates and vertebrates contain many of the same neurotransmitters, with functions that are nearly identical in nature. Dopamine is present in both vertebrates, invertebrates, and even some protists. Majority of vertebrates contain a structure known as the blood-brain barrier, which excludes exogenous chemicals and materials from entering the brain. It is unclear as to whether or not invertebrates, specifically crustaceans, contain a highly permeable blood-brain barrier or lack one altogether. Behavioral research allows for an indirect measure of the neurophysiologic effect that dopamine has on Cherry Shrimp, specifically by observing movement after exogenously dosing the organisms. Dopamine, Haloperidol, Glutamate, Glucose, and Insulin were used as the molecules of desire. The hypothesis in this study is that the exogenous neurotransmitters and chemicals given to the shrimp are capable of passing through their exoskeleton and into their brain tissue, resulting in the observed behavior. Dopamine reveals an inhibition of movement, whereas Haloperidol partially restores movement. Glutamate stimulates movement. Glucose was shown to inhibit movement and Insulin, at natural levels, had no effect. Glucose combined with Dopamine partially restored movement, similar to the effects of Dopamine and Haloperidol. The aim of this study is to understand the neurobiology at a relatively simple evolutionary level, which can later be applied to the evolution of neurotransmitters of all organisms.

A STUDY OF CELL PHONE DEPENDENCY

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Cell phone dependency is a modern issue that is growing in relevance as more and more people utilize mobile technology. Cell phones have now become integral to how people operate on a daily basis. These devices have become an extension of self, so that separation from the device can cause panic, stress, anxiety, irritability, and to a greater extent psychological symptoms similar to substance addiction. This research, aptly titled "Could Cell Phone Addiction Be a Diagnostic Condition in the Future: A Study on Cell Phone Dependency" aimed to determine various levels of user dependency on cell phone device, as well as determine whether or not unavailability of the device resulted to a difference in vital readings (blood pressure) as a result of changes in the subject's emotions such as panic, stress, anxiousness, nervousness, or agitation.

This study was two parts: First, male and female participants were requested to complete a 42-item Questionnaire which established their level of use. The Questionnaire, *please see attached,* has been reviewed and approved for use by Professor Richard Burnor, Chairperson of Felician University's Institutional Review Board (IRB) for the Protection of Human Subjects. There was no specific age group for this study so as to capture a wider population. By not limiting to a specific age group, i.e. school age, working population, or older adults, the study was also able to analyze whether or not age was a factor for this emerging behavioral addiction.

Second, in order to enable the researcher to determine the correlation between the subject's level of use and dependency on his/her cell phone device, the subjects were requested to give up his/her device. Vital readings (blood pressure) were taken while the subject was still in possession of the device. There was an 8 hour window when the subject's device was taken away. A second blood pressure reading was then taken after the 8 hour period and before the device was returned. This process was able to determine whether or not unavailability of the device or what we can call the "period of withdrawal" has caused the subject's blood pressure to rise, as a result of a change of his/her emotion such as stress, anxiousness, nervousness, or agitation while the cell phone was not in his/her possession.

From data collected from 80 subjects, it was determined that the level of dependency for school age population (between the ages of 12 and 21) was significantly higher as 95% of the subjects responded that they "felt uncomfortable and "lost" without their device; were agitated if they cannot look up information on their device; were scared if their cell phone ran out of battery; were anxious that important messages were sent to their device; and were also nervous that friends or family members could not reach them." The subjects vital readings confirmed their feelings of anxiousness, agitation and nervousness as their blood pressure rose, with readings ranging from 125/80 to 138/90 after the 8-hour period of withdrawal from the device. 90% of the subjects were female. The working population (between the ages of 27 and 48) were somewhat neutral in their responses with a mix of high to medium dependency level; while the older adults (between the ages of 50 and 65) were merely passive in their responses. The data collected determined that, among the school age population, the cell phone gave rise to problems that affected daily life and enabled a behavioral addiction.

THE EFFECTS OF MODULATION OF A POTASSIUM CHANNEL ON SOCIAL BEHAVIOR AFTER A TRAUMATIC BRAIN INJURY

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Traumatic Brain Injury (TBI) is the result of a sudden or violent blunt impact to the head, which is commonly caused by car accidents, assaults, falls, or even war. Our brain is responsible for controlling movements, thoughts, sensations, behaviors, and communication throughout our body, injury to this vital organ can bring about a varied range of cognitive, sensory, behavioral symptoms and in severe case can be fatal. More than 200,000 cases of TBI are reported a year and with no specific treatment method any advancement in neuro-protective measures can mean huge improvements in preventive and therapeutic procedures. This research aims to target variables that naturally help the brain fight off neuro-degradation after a TBI, specifically using "M-Type" Potassium (K+) Channels. By modulation of Potassium Ion Channels it is hoped to see an increase in its neuroprotective role in the brain and how it effects varying serveries of trauma. TBI can be broken into two components, primary and secondary injury. Primary injury is irreversible as it refers to the damage suffered as a result of blunt force, penetrating, or blast trauma. Primary injuries cause significant amount of permanent damage to the brain due to destruction of brain tissue, brain injury due to skull fragmentation, and laceration of cerebral blood vessels. The secondary injury of TBI is the result of prolonged metabolic processes leading to cell death and worsening damage to the brain far beyond the primary injury. One specific aspect of secondary injury being looked at in this study is the intracellular biochemical cascades pouring into the neuron in response to the primary injury, this overstimulation of chemicals can lead to excitotoxity and programmed cell death

BEHAVIORAL MODIFICATIONS FOLLOWING DELETION OF TYPE 2 CANNABINOID RECEPTORS IN DOPAMINE NEURONS

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The endocannabinoid system (ECS) consists of two major types of cannabinoid receptors (CB1Rs and CB2Rs), their endogenous ligands endocannabinoids (eCBs), and their synthesizing and degradation enzymes. There is increasing global awareness and interest in the use of marijuana and cannabis products – which contain multiple ligands for both CBRs – for therapeutic (epilepsy and pain management, for example) purposes. CB1Rs, the most abundant G-protein coupled receptors (GPCRs) in the mammalian brain have been well characterized. The functional neuronal expression of CB2Rs has been the subject of controversy and debate, but current research indicate that the expression of CB2Rs in neurons and immune cells are involved in mental and neurological disorders. However, the cell type-specific mechanisms are unclear since the available CB2R gene knockout mice are constitutive and partial germline knockouts and are not suitable for tissue- and cell type – specific studies at molecular, pharmacological, and behavioral levels. Therefore, we generated *Cnr2*-floxed mice that were crossed with DAT-*Cre* mice, in which the recombinase expression is under dopamine transporter gene (DAT) promoter control to generate CB2R conditional knockout mice in midbrain DA neurons in DAT-*Cre*-*Cnr2*-Lox transgenic mice.

By using a novel highly-sensitive RNAscope *in situ* hybridization method, we detected clear CB2R mRNA expression in VTA DA neurons in wildtype control and DAT-*Cnr2* heterozygous mice, but not in the homozygous DAT-*Cnr2* cKO mice. We then characterized the DAT-*Cnr2* cKO mice in a battery of behavioral test systems. We report that the deletion of CB2Rs in dopamine neurons enhances motor activities, modulates anxiety-like and depressogenic-like behaviors and reduces the rewarding properties of alcohol and cocaine. Our data also reveals for the first time that CB2Rs are involved in the tetrad assay induced by cannabinoids which had been largely associated with CB1R agonism. The GWAS secondary analysis indicate that the CNR2 gene is associated with Parkinson's disease and substance use disorders. We conclude that CB2Rs in dopaminergic neurons play an important role in the modulation of psychomotor behaviors, anxiety, depression, and pain sensation and in the rewarding effects of alcohol and cocaine.

THE ROLE OF CANNABINOID CB2 RECEPTORS IN COGNITIVE FUNCTION OF DAT-*Cnr2* CONDITIONAL KNOCKOUT MICE

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The endocannabinoid system (ECS) encompasses cannabinoid receptors (CB1Rs and CB2Rs), endogenous cannabinoids (endocannabinoids), and their synthetic and degradation enzymes. Dopamine (DA) is a neurotransmitter that is involved in several physiological and behavioral processes, including the modulation of cognitive function such as learning and memory. In order to gain a better understanding of the role of the CB2Rs in cognitive function, experiments were performed in DAT- *Cnr2* conditional knockout (cKO) mice with selective deletion of CB2Rs in dopamine neurons in comparison to C57BL/6J wild type (WT) control mice.

In this study, we used two models of cognitive function: Novel Object Recognition (NOR) and Social Recognition Task (SRT). NOR is a model for learning and episodic memory; it is based on mice ability to discriminate between familiar and unfamiliar objects and address possible learning deficits. SRT evaluates general sociability and addresses learning deficits by the recognition of an old and a new intruder mouse. In addition, we used the Open Field test to assess exploration and habituation of both strains of mice in a novel environment. The results showed that the WT mice habituated to their environment and displayed less locomotor activity/exploratory behavior whereas the DAT-*Cnr2* cKO mice maintained their characteristic hyperactive exploratory behavior. In the SRT we found that the DAT-*Cnr2* cKO mice displayed less social interaction time and poor recognition index compared with the WT mice. In the NOR test the exploration time by the DAT-*Cnr2* cKO mice were more than the exploration time of the WT mice. Furthermore, the DAT-*Cnr2* cKO mice discrimination index was lower than that of the WT control mice. These results demonstrated that DAT-*Cnr2* cKO mice displayed learning deficits and concluded that cannabinoid CB2 receptors plays a role in the mouse models of cognitive function.

THE EFFECT OF HIGH LIGHT INTENSITY ON TOXIC AND NONTOXIC STRAINS OF *KARENIA BREVIS*

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Karenia brevis causes negative human health and environmental impacts through the production of brevetoxins. Recent studies suggest that brevetoxins play a role in non-photochemical quenching and protection from photooxidative stress as the toxin binds to photosystem II in the chloroplast. This study tested the hypothesis that high light intensity will affect the growth rate, photosynthetic efficiency, and the gene expression of both the toxic (KB) and nontoxic (NT-KB) strains of *K. brevis*, and that NT-KB will be more sensitive to the light stress. To test this hypothesis, one-liter cultures were grown in modified *f*/2 media in 36 ppt seawater at 25 ^{o}C under 16:8 hours light cycle with an initial light intensity of ~ 55 µmol photons $m^{-2}s^{-1}$. The cultures were then exposed to the high light treatment of ~ 100 µmol photons $m^{-2}s^{-1}$ at mid-log with samples taken for protein and toxin analysis before (T0) and three days after the treatment (T3). Growth rate of *K. brevis* was not affected by the high light treatment in either strain. Growth rates of the toxic strain were 0.54 divisions/day and 0.56 div/day for control and high light-treated cultures, respectively. Similarly, the growth rates of the nontoxic strain were 0.54 div/day and 0.55 div/day for control and high light treated cultures. However, toxic *K. brevis* cultures maintained a higher photosynthetic efficiency than the nontoxic strain cultures. Throughout the log and stationary phase, the average photosynthetic efficiency for the toxic strain was 0.498 and 0.550 in control and high light treatments, respectively. Under high light treatment, NT-KB had a lower photosynthetic efficiency than the control with a photosynthetic efficiency of 0.371 for control cultures and 0.238 for high light treated cultures. Furthermore, NT-KB did not maintain a typical stationary phase. In the completion of this experiment, we will analyze the protein abundance of a polyketide synthase (PKS) involved in the production of brevetoxin in both strains using western blot. Total brevetoxins in samples will also be measured using a brevetoxin ELISA to determine the effect of high light intensity on the toxicity of *K. brevis*. Data obtained thus far supports previous studies that the production of brevetoxins may serve a protective role from photooxidative stress in *K. brevis.* Examining the effect of light intensity on *K. brevis* will help us understand how light stress may increase the production of brevetoxin and the ultimate role of brevetoxin in maintaining the survival of *K. brevis.*

STRUCTURAL STUDY OF THE *SLERT* LONG NON-CODING RNA

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*SLER*T (snoRNA-ended lncRNA that enhances pre-ribosomal RNA transcription) RNA is a long noncoding RNA (lncRNA) as defined by a length of over 200 nucleotides (nts) that do not encode proteins, and whose purpose is to regulate gene expression. *SLERT* RNA is a newly discovered RNA in the already young study of lncRNAs; as such, its domain architecture and molecular structure are still unknown. This study will attempt to characterize the three-dimensional structure of *SLERT* RNA through Polymerase Chain Reaction (PCR) and in vitro transcription to produce specific nucleotide lengths (both the full length 694nt sequence and 143nt fragment), followed by biophysical characterizations. Since this is a noncoding RNA, and others have been shown to contain bulges, interior loops, hairpin loops, and multiloops, it is hypothesized that *SLERT* will contain a similar structure.

A panel of molecular biology techniques including PCR and in vitro transcription were used to create the RNA sample. Purification techniques such as size exclusion chromatography were used to isolate pure RNA. Through small- and large-scale transcription, and refolding tests, whether or not the RNA sample forms its proper, folded conformation was evaluated. Magnesium ions play a vital role in *SLERT* RNA folding, because the backbone of RNA are negatively charged, so during the refolding process they would repel each other, unless cations such as Mg2+ can bridge and neutralize the excessive negative charged placed in close proximity. With a proper cationic magnesium concentration, the *SLERT* would be able to properly refold as opposite charges attract each other. In denaturing gels, it was found that 6-8% acrylamide gels worked best.

Through analysis of *SLERT* RNA folding using native gels and size-exclusion chromatography, we have achieved good folding and isolation of the better-behaved *SLERT* 143nt fragment, and set up crystallization trials against a diverse chemical library to coax its crystallization. Future steps involve studying the interaction between the *SLERT* RNA with its RNA-binding protein, DDX21 (DExD-Box Helicase 21), which binds the 143nt fragment of the *SLERT* RNA to provide an alternate to trying to crystallize the full-length SLERT

LEAD EXPOSURE: HOW MUCH IS TOO MUCH?
-A study on Effect of Lead on Nerve Growth Factor Regulated Embryonic Dorsal Root Ganglion Neurodevelopment

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Lead is a naturally occurring element whose toxicity in humans has been documented throughout history. Lead is widely present in our environment due to its natural occurrence in addition to human activities that have introduced it into the general environment such as the use of leaded gasoline, outdated pipes and paint. The dangers of lead poisoning include developmental delays, memory loss, neurological changes and even death at high concentrations. Fetal neurodevelopment that has been exposed to lead toxic environments, either through maternal ingestion or maternal lead bone migration, is one aspect that is underdeveloped in current literature. Being a 2+ ion (Pb2+), lead easily mimics and takes the place of Calcium (Ca2+) interfering with its many roles in the human body including bone structure, cell signaling and nerve function. In this study, we tested lead's effect on a nerve precursor, Dorsal Root Ganglions (DRGs); clusters of nerves that will develop into the sensory nervous system, found on the dorsal root of the spinal nerve in embryos. Using one tenth of the FDA approved safe level of lead (15 parts per billion) we have found significant differences in tissue morphology, cell proliferation, and tissue differentiation, in response to NGF (neuronal growth factor) promoted process in cultures between treated groups ($p<0.5$). It is the mission of this research to shed light on lead poisoning and its dangerous ramifications on embryonic development.

Tests run on the DRGs had a consistency of running three distinct cultures: a negative control in which extracted ganglion were developed in culture media, a positive control which had DRGs in culture media and Nerve Growth Factor (NGF) (200 ng/ml), and finally an experimental group which consisted of ganglions grown in culture media with both NGF and lead. Subsets of the lead experiments have also been run in which the concentrations of lead varied between 0.1 uM/L, 0.3 uM/L, 0.5 uM/L, and 1uM/L of lead to examine different dose responses. Experiments thus far have revealed a substantial morphological difference between lead treated ganglions and untreated ganglions. Changes in axon growth, ganglion shape, dead cells within the ganglion, and new neurite outgrowth have all been observed ($p<0.5$). Software such as Image J, Cellsens, and Zen have been used to collect images of the ganglions on 1-5 day regimens as well as analyze the images, along with statistical analysis through T-tests and ANOVA.

TESTING THE ENHANCER-PROMOTER HYPOTHESIS IN *SACCHAROMYCES CEREVISIAE*

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Transcriptional regulation in eukaryotes is a multi-faceted process. The role of spatial positioning – the linear arrangement of genes along the chromosome – is correlated with transcriptional coordination of genomic 'neighborhoods' that have correlated expression. It has been observed that some sets of functionally related genes exist as clusters that are spread throughout the genome. This arrangement has been found to result in coordinating the expression of these functional clusters, termed adjacent gene co-regulation. One potential mechanism that could underlie this phenomena is that of the enhancer-promoter hypothesis. Our work is focused on testing this hypothesis in *S. cerevisiae* using a series of strains that contain a *HIS3* reporter gene that is separated by spacers, of varying length, from a galactose inducible reporter. This study aims to test the effects of induction of the *HIS3* gene in two different genomic neighborhoods.

CHANGES IN HYPOTHALAMIC HORMONE LEVELS AFFECTING ADDICTION AND NOCICEPTIVE RESPONSES

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The dopaminergic system has been well characterized as playing a major role in addiction and nociceptive behaviors in rodents and human. The neural circuitry connecting the prefrontal, hypothalamic, midbrain and medullary noradrenergic pathways shows the complex interplay between many brain nuclei involved in expression of addiction and pain experiences. In this study we examined the level of dopaminergic protein synthesis in C57BL/6J mice using immunohistochemistry and western blot. Brains were harvested at postnatal and adulthood stages, homogenized in buffer and kept frozen until used for western blot analysis. Additional brains were stained using immunohistochemistry to localize and quantitate the number of adrenergic neurons. Our data showed that the adrenergic system is expressed since early neonatal stage and peaks during early post-natal stage. These cells were found distributed throughout the hypothalamic nuclei.

SYSTEMATIC CHARACTERIZATION AND CONSERVATION OF ADJACENT GENE CO-REGULATION IN FUNGI

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There are multiple regulatory systems that exist for modulating gene expression in response to specific developmental and environmental conditions. It is essential that cells orchestrate gene expression for the specific niche that they occupy, and this oftentimes requires the regulated expression of large sets of genes. Previously it has been observed that spatial positioning influences transcription; including, for example, in the rRNA and ribosome biogenesis (RRB) and ribosomal protein (RP) gene sets. It has been previously reported that both gene families included a disproportionate number of immediately adjacent gene pairs – both gene families can be found clustered directly adjacent to another member of the same family. In both gene families this arrangement resulted in a tighter transcriptional coordination among adjacent paired genes compared to the unpaired genes within each regulon. This arrangement was functionally dissected for one RRB gene pair *(MPP10-MRX12*), which demonstrated a dependency of maintaining the proper genomic arrangement to allow for a shared promoter to regulate the pair. Furthermore, this non-random genomic distribution has been seen in a handful of functionally related gene families and many of these functional pairings are conserved across divergent fungal lineages. However, to date the significance of these observations have not been extended in a systematic way to characterize how prevalent and significant the role of adjacent gene co-regulation is in transcriptional regulation. To further our understanding of adjacent gene co-regulation, we analyzed genome wide expression profile data of related gene families under five stressors (heat shock, MMS, H_2O_2, nitrogen starvation, and glucose depletion) for the RP, nitrogen metabolism, carbohydrate metabolism, response to toxins and heat shock gene families (among others). We calculated the Pearson's correlation coefficient to determine the transcriptional coherence of the functional pairs to the singletons within each family. Using Python, we wrote code to allow us to determine the transcriptional response for every combinatorial possibility that could have evolved. To our surprise, it appears that there is not an overall transcriptional advantage to functional pairing of genes in *S. cerevisiae* – although there are specific conditions that appear to be more important, and thus could be the driving force behind this phenomena (e.g. the response of the nitrogen metabolism genes to nitrogen starvation). This analysis was extended to divergent fungal lineages, to allow for comparison of newer evolved pairings to more ancestral pairings. Our results demonstrate that the longer two genes have co-existed as neighbors, the tighter their transcriptional response is to broad stress and nutritional responses. Follow up analysis shows that there are a significant fraction of functionally related gene sets that have a non-random distribution throughout the genome – and that the functionally clustered members exhibit a tighter transcriptional co-regulation than unpaired members of the same set in about 75% of these instances.

STRUCTURE-FUNCTION ANALYSIS OF MKL1 IN MEGAKARYOCYTOPOIESIS

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MKL1 (megakaryoblastic leukemia 1) is a myocardin family protein that mediates megakaryocytopoiesis through SRF (serum response factor) transcriptional coactivation. Previous research demonstrates that MKL1-deficient mice produce significantly fewer mature polyploid megakaryocytes. MKL1 is involved in the reciprocal t(1;22) chromosomal translocation found in acute megakaryoblastic leukemia (AMKL). This translocation results in the production of the RBM15-MKL1 fusion protein, which encompasses every functional domain encoded by each individual gene. To elucidate the leukemogenic mechanisms of RBM15-MKL1, further studies must be done to understand how the conserved domains of RBM15 and MKL1 function in megakaryocytopoiesis. This project investigates the roles of the MKL1 domains in megakaryocytopoiesis by deleting each individual domain in megakaryocyte progenitors undergoing differentiation. Stable HEL (human erythroleukemia) cell lines with inducible expression of wild-type MKL1 and MKL1 domain deletion constructs have been established. These cells differentiate and undergo endomitosis upon exposure to 12-O-tetradecanoylphorbol 13-acetate. The effects of the domain deletions on this polyploidization will be analyzed by flow cytometry. In parallel studies, fetal liver cells of MKL1 knockout and MKL1/MKL2 double knockout mice will be transduced with retrovirus encoding the MKL1 deletion constructs and assessed by flow cytometry. Preliminary results in HEL cells show that MKL1-mediated polyploidization is not inhibited in the absence of the leucine zipper dimerization domain or the SAP domain, suggesting that megakaryocytic maturation may occur independent of these domains. Future studies will investigate the potential involvement of the MKL1 SAP domain, whose function remains unknown, in the RBM15-MKL1-induced development of AMKL.

DESIGN OF AN IMMUNOGENIC AND ANTI-EGFR RNA THERAPEUTIC TO ALTER RNA AND PROTEIN EXPRESSION IN GLIOBLASTOMA MULTIFORME

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The most common and lethal malignancy of the central nervous system (CNS) is glioblastoma multiforme (GBM). Due to the blood brain barrier (BBB) and the relatively immunologically privileged status of the CNS, clinical strategies have not improved the standard of care. Epidermal growth factor receptor (EGFR), a type of tyrosine kinase receptor, has been found to be overexpressed in as much as 60% of GBM tumors. Upon binding of its cognate ligand, EGFR promotes tumor growth and proliferation. The glioma-specific antigen, interleukin-13 receptor alpha variant 2 (IL13Rα2) is highly immunogenic, attracting cytotoxic Tcells to the tumor microenvironment.

Therapeutically, delivery of this antigen to the tumor has the potential to bypass the BBB and reactivate the immune system toward GBM. In the current study, we have designed and cloned an immunogenic pre-trans splicing RNA molecule (iPTR) against EGFR. In a GBM tissue culture model, we measure the RNA and protein expression of the iPTR and compare to multiple anti-EGFR RNA therapies. In addition, we are developing assays to use ELISA to measure changes in EGFR protein expression. Genetic delivery of our highly immunogenic IL13Rα2 peptide using the iPTR has the potential to redirect the immune system to recognize and induce apoptosis in GBM cells.

CDK5: THE CONNECTION BETWEEN ALZHEIMER'S DISEASE AND DIABETES

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Type 2 diabetes mellitus (T2DM) and Alzheimer's disease (AD) are two of the fastest growing diseases in the United States. T2DM is a complex, onset disorder affecting the sensitivity of pancreatic beta cells to insulin. AD is a neurodegenerative disorder causing a decline in cognitive ability that is associated with two neuropathological hallmarks; neurofibrillary tangles (NFTs) comprised of hyperphosphorylated tau, and plaques comprised of aggregated amyloid beta proteins. Recent evidence suggests that insulin deregulation in the brain may play a role in the pathology of AD. Cyclin dependent kinase 5 (CDK5) is a member of the cyclin dependent kinase family that is unusual in that it is predominantly active in terminally differentiated neurons. CDK5 has been shown to be required for proper central nervous system development and for neuronal patterning and migration. Aberrant activation of CDK5 has been implicated in several neurodegenerative diseases, including Alzheimer's Disease, where its deregulation contributes to the formation of neurofibrillary tangles, among other protein aggregation and misfolding events. CDK5 has recently been associated with insulin exocytosis in the pancreas. An emerging correlation between Type II diabetes and AD suggests a connection between insulin deregulation and neurodegeneration. As CDK5 is active in both tissues, it represents a possible common feature in these two pathologies. To study this connection, our lab uses the neuronal cell line model, PC12. We transdifferentiate these cells using growth factors, then assess the extent of differentiation via qualitative and quantitative methods in the presence or absence of CDK5 chemical inhibitors. We also quantify the morphological changes that arise in response to neurotrophic factors using digital photomicroscopy. Our results indicate that aberrant CDK5 activity contributes both to alterations in neuronal architecture and changes in CDK5's kinase activity, confirming the effectiveness of our chemical inhibitors in altering CDK5 activity. Using this model, we have now begun to examine the role of normal and aberrant CDK5 activity on the response of differentiated neuronal-like PC12 cells to varying concentrations of glucose and insulin in culture. Since a number of reports suggest that dysfunction in cerebral glucose metabolism and deregulation of brain insulin signaling are early abnormalities in AD, this model system provides a means to examine the potential role of CDK5 as a link between AD and Type II diabetes.

ANALYSIS OF BIODIVERSITY OF DEAD WOOD-INHABITING FUNGI IN THE NORTH AND SOUTH NEW JERSEY USING DNA-BARCODING

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Dead wood provides habitats to preserve biodiversity in ecosystems including forest, urban, and rural areas. It protects the soil against erosion and aids in water retention, and provides an ecological niche for fungi, bacteria, plants and animals. Dead wood fungi perpetuate a healthy eco-environment by decomposing and detoxifying forest waste and renewing the soil. We hypothesize that the removal of dead wood in urbanized areas results in a decrease of dead wood fungi species diversity thus impacting the stability of the urban ecosystem. Most of the dead wood fungi are cryptic, so the DNA barcoding technique is utilized to identify fungal species across the parks, forests and urban areas in NJ. In this study, the analysis of 94 samples of fungi collected from Meadowood Park and Belleplain State Forest representing both northern and southern areas of the state is presented. The data is catalogued and the information is available online at iNaturalist.org. Here, we discuss the species richness in areas that remove dead wood in comparison to the areas that allow the wood to decompose naturally, and the role of park management in urban biodiversity

ENVIRONMENTAL EVALUATION OF MID-ATLANTIC COASTAL WETLANDS

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Industrial and urban pollutants have been changing the ecosystems on which many organisms depend. This study focuses on the effects modern anthropogenic activities have had on mid-Atlantic coastal wetlands. Pollution and other environmental factors that alter an ecological system are readily preserved in the water and sediments, along with the organisms that inhabit the wetland. For example, diatoms are microscopic siliceous algae widely used as indicators of environmental conditions in aquatic ecosystems. Because of their high ecological sensitivity and silica shell that gets preserved and accumulates in bottom sediments, they are one of the most valuable tools to infer past environmental conditions from core sediments in both lacustrine and coastal environments. However, whilst some work has been done to develop diatom transfer functions in mid-Atlantic estuaries and marshes—namely, relating diatom species to ecological conditions—we still lack a robust understanding of how the abundances of the different species vary within the ecosystems. What's more, there are still uncertainties in the transfer functions themselves, which calls for additional geochemical tracers to help constrain these relationships. Therefore, to help reduce these uncertainties we have analyzed the diatom assemblages from seven spatially distributed locations in New Jersey coastal wetlands which extend from Raritan Bay to the north, to Cape May to the south. To better assess the link between diatoms and ecological conditions, we also examined total phosphorus, nitrogen, and carbon, along with mineral grain size in the various locales across the NJ shoreline. Results from this study will not only improve the diatom transfer functions, but also allow us to trace the diatom composition over time and identify reference assemblages that existed in the Bay over the past few centuries. Such data are not only important for understanding how the structure and function of biological communities is changing as a result of human impacts, but are also useful for establishing biological indicators of ecosystem health.

NUTRITIONAL REQUIREMENTS OF BEAN BEETLES (*CALLOSOBRUCHUS MACULATUS*) AND A "MENU" OF BEANS THAT "SELECT" FOR OVIPOSITION AND EMERGENCE RATES

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Bean beetles have increasingly been used as a model organism to study genetics and the effects of nutrition and artificial selection on survival. They require only mung beans, an incubator set to between 25-30^{o} C, and a source of humidity in the incubator. The bean beetles do not (normally) fly, except under certain circumstances, which make them easier to handle than *Drosophila melanogaster*. The females lay their eggs, which are similar in size and shape to sesame seeds, on mung beans, as well as other types of beans. The larvae hatch out of the eggs but burrow into the beans, and emerge out of the beans 3-4 weeks later. Bean beetles will lay their eggs on other types of beans such as black beans, adzuki, kidney, and black-eyed peas as well as mung beans (USDA data is available for all beans). Our hypothesis is that there will be differential rates of egg-laying on various types of beans, and that the emergence rate of an adult beetle will be different among beans. For a control of 277 mung beans, after week one, 43 beans contained eggs and 19 beans had emergence holes. However, the bean beetles are short-lived, and only live 10-14 days. There were two males and two females alive after week one. After five weeks, 188 beans contained eggs, and 89 beans had emergence holes. On a group of mixed beans (32 black beans, 27 adzuki beans and 354 mung beans, no eggs were observed on any types of beans; however, 13 emergence holes were seen on mung beans only. After five weeks, there were 141 eggs on the black beans, 77 eggs on adzuki beans and 105 eggs on the mung beans. However, there were only 33 emergence holes on mung beans only. Fifteen females and seven males were alive. The results allow us to accept the hypothesis that there is differential egg laying, emergence rates and, ultimately, survival rates of adults based on beans chosen for egg-laying (oviposition). What is interesting to us is that there were many more adult survivors on a mixed "menu" of beans that were offered to the beetles.

GENETIC ANALYSES REVEAL THE POSSIBLE DESCRIPTION OF A NEW DEEP-SEA EEL SPECIES IN THE GENUS *CONGER*

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The deep-sea currently represents one of the most underexplored ecosystems. Surveys show that it is the habitat to much of Earth's biodiversity that is yet to be discovered. Here we present evidence of a potential new deep-sea eel species in the genus *Conger*. Five individuals collected in the Gulf of Mexico at ~300 meters depth have been initially identified as *Conger oceanicus* based on morphological similarity. However, COI sequences revealed significant genetic differences (~8%) that describe the potential existence of a new species. Additional genetic and morphological tests are ongoing to better support the COI data. This study emphasizes the importance of gathering barcoding data and using a genetic library as a starting point for evolution and biodiversity investigation.

THE EFFECTS OF ETHINYL ESTRADIOL ON *DAPHNIA MAGNA* POPULATION DYNAMICS AND BODY LENGTH

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Ethinylestradiol (EE_2) is a common constituent of birth control pills and acts as an estrogen agonist in the human body. EE_2 is released into fresh water river systems across the globe due to inadequate wastewater treatment. Currently, effects of EE_2 on aquatic ecosystems are poorly understood and the increased usage of birth control pills calls for a need to research this potentially dangerous toxin on aquatic life. The goal of this study was to evaluate the effects of chronic sub-lethal EE_2 exposure on population dynamics and body size in the aquatic micro crustacean, *Daphnia magna*. Our hypothesis stated that *Daphnia* exposed to EE_2 would display alterations in population density, growth rate, and body size. In a series of bioassays, we exposed *Daphnia* to a range of EE_2 concentrations to determine lethal and sub-lethal toxicity. An acute 72-hour LC_{50} dose-response bioassay was conducted in which *Daphnia* were exposed to 0, 1, 2.5, and 5 ppm of EE_2 with freshwater and solvent (ethanol) controls. Using these results, we further studied the effects of chronic, sub-lethal EE_2 exposure (0, 0.5 and 1 ppm with freshwater and ethanol controls) for 20 days on population growth, growth rate, and body size for 2 generations. The 72-hour LC_{50} was determined to be 3.11 ppm. The ethanol control treatment displayed the greatest population growth, and growth rate, by the end of the chronic exposure followed by both concentrations of EE_2 and the freshwater control. In addition, we found that *Daphnia* exposed to EE_2, across the 2 generations, displayed reduced body sizes when compared to controls. We believe the results are due to ethanol acting as a potential stressor on *Daphnia,* increasing population growth rate through increased reproduction. Further, EE_2 exposure possibly counteracted the stressing effects of ethanol by producing population growth rates higher than the water controls but less than the ethanol controls. However, the current mechanisms by which EE_2 acts on *Daphnia* physiology and reproduction are unknown. These results support the hypothesis that prolonged exposure of EE_2 to *Daphnia* populations can influence population dynamics and decrease the quality of offspring.

PHENOLOGY OF HONEYBEE COLONIES AND THEIR KEY POLLEN PLANTS IN THE URBANIZED NEW JERSEY LANDSCAPE

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Honeybees can be used as bioindicators of landscape health as their success is dependent upon the quality of their environment. Honeybees' role in pollination in both natural and agricultural environments is critical for successful management; understanding bee health and foraging with relation to the phenology (cyclical patterns) of important plants is imperative. Four colonies from the rooftop apiary of WPUNJ were utilized in this study. Colonies were fitted with traps for pollen collection and Broodminder scales to track colony growth. Identification of major pollen sources paired with colony data provides insight as to which species are important throughout the foraging season. Honeybees utilized 17 species but were reliant upon just two for half of their pollen needs, and another four species for an additional 35% percent. Colony growth was constant up until 5 July, supported by *Rhus typhina* (staghorn sumac), thereafter growth plateaued and colonies were sustained by *Lythrum salicaria* (purple loosestrife) and others.

EFFECTS OF WASTEWATER TREATMENT EFFLUENT ON POPULATION BIOLOGY OF THE FRESHWATER AMPHIPOD, *GAMMARUS FASCIATUS*

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Wastewater treatment plants (WWTP) are located along rivers and designed to remove contaminants, pharmaceuticals, and excess nutrients before returning the water to the environment. In addition, recycled wastewater is one of the main sources of fresh drinking water due to growing population density and industrial needs. The goal of this research was to evaluate the potential effects of wastewater treatment effluent on the population biology of the amphipod, *Gammarus fasciatus*. The hypotheses stated that population density, body size, and gender ratios of gammarids located at and below the source of wastewater effluent introduction will differ compared to the population located upstream (reference site). During the late summer and fall of 2018 (Sept. to Nov.), bimonthly samples were collected with a kick net, in duplicate, from three sites on the Whippany River in Morris County NJ: upstream (reference), at the treatment site WWTP outflow (effluent), and downstream. At the same time, abiotic conditions (pH, temperature, depth, and dissolved oxygen (D.O.)) were measured. Amphipods were then fixed in ethanol until processing. Lateral and ventral photos of all individuals were recorded through the use of a dissection scope with a digital camera. Body and antennae length were measured in mm and gender was confirmed, if possible, by the presence of brood plates (female) or genital papillae (male). The density, size, and the number of juvenile (< 4mm) and adult (> 4mm) amphipods were compared across the 3 locations. There was a trend of higher total density and number of adult amphipods located in the effluent and downstream samples compared to the upstream location. Juvenile amphipod density declined over time from September to November regardless of location. There was an observed pattern of population cycling among the sampling periods for adult and overall populations at all locations. Total and adult amphipod body length increased over time with no effect by location. Gender identification for the majority of the amphipods was inconclusive and further research is required to determine gender. The increased population density of amphipods located at and downstream of the WWTP may be due to excess nutrients and increased organic matter. Knowledge regarding amphipod populations changes due to WWTP input can be valuable when accessing effects of anthropogenic activities on aquatic ecosystems.

CHARACTERIZATION OF DIADINOXANTHIN DE-EPOXIDASE ENZYME IN *KARENIA BREVIS*

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Karenia brevis is a toxic dinoflagellate that can form harmful algal blooms (HABs) that negatively impact the environment, economy, and human health. These HABs occur in the Gulf of Mexico as a result of rapidly increasing concentrations of *K. brevis* and the production of potent neurotoxins, the brevetoxins. Previous experiments have localized brevetoxin to the chloroplast, suggesting its role in non-photochemical quenching (NPQ). This photoprotective mechanism is regulated by the xanthophyll cycle, which involves the conversion between carotenoids, diadinoxanthin and dinoxanthin, via the enzyme diadinoxanthin de-epoxidase (DDE). Previous studies suggest the xanthophyll cycle is not functioning properly in a non-toxic *K. brevis* (NT-KB) strain, which could be due to a mutated DDE in NT-KB. The goal of this project is to characterize DDE in *K. brevis* and to determine if it is in fact mutated in NT-KB. Additionally, expression of DDE in toxic and nontoxic K. brevis will be analyzed after exposure to light stress. Six potential DDE candidates in a toxic strain of *K. brevis* were identified using a diatom DDE to search against a *K. brevis* translated transcriptome database. The candidates were then searched against the nonredundant database in NCBI using Blastp. The top hit for each candidate was violaxanthin de-epoxidase (VDE), a homolog of DDE, with significant E-values ranging from $1.05E^{-131}$ to 0. A multiple sequence alignment performed with two characterized diatom VDEs showed two *K. brevis* candidates contain 12 of the 13 previously identified conserved active sites, two of which are essential for enzymatic activity. These data suggest that both candidates are functional DDE enzymes in *K. brevis*. These sequences have been used to design primers for amplification and sequencing of DDE in NT-KB. DDE expression will also be analyzed in toxic and NT-KB after exposure to light stress to determine if the genes are differentially regulated in the two strains. Analysis of DDE in NT-KB will determine if the problem observed in the xanthophyll cycle in NT-KB is the results of a dysfunctional DDE enzyme or the results of a process upstream of enzyme activity in the xanthophyll cycle. Characterization of DDE in both strains will provide additional evidence for the functional role of brevetoxins in *K. brevis* in NPQ.

THE EFFECTS OF NITROGEN LIMITED ENVIRONMENTS ON THE DINOFLAGELLATE *KARENIA BREVIS*

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Karenia brevis is a toxic dinoflagellate that causes harmful algal blooms in the Gulf of Mexico where it causes detrimental effects on humans and death of marine life due to the production of potent neurotoxins. In nitrogen-limited environments, *K. brevis* has been shown to have a decrease in growth rate which led to the increase in production of brevetoxins; however, the effects of N-limitation on gene expression and the effects on the nontoxic strain remain unknown. This study examines the effect of N-limitation on growth, toxicity and PKS protein abundance on both toxic and nontoxic strains of the dinoflagellate, *K. brevis*. Four replicates of control (N-replete) and N-limited cultures were monitored for growth and photosynthetic efficiency every other day for the entire experiment. At mid-log phase, four replicate cultures of each treatment were sampled for brevetoxin and protein analysis. N-replete cultures for the toxic strain showed steady growth during log phase with a growth rate of 0.76 div/day. The N-limited cultures had a slower growth rate during a longer period of 0.46 div/day. N-replete cultures reached stationary phase on day 9, and N-replete cultures began to quickly decline on day 11. N-limited cultures had a slightly lower photosynthetic efficiency which suggests these cultures to be more stressed than the N-replete cultures. The N-replete nontoxic cultures had a faster growth rate of 0.53 div/day until day 8 and the N-limited nontoxic cultures had a growth rate of 0.31 div/day until day 10. There were no differences in photosynthetic efficiency between treatments for the nontoxic strain. Both N-replete and the N-limited nontoxic cultures started with a low photosynthetic efficiency, stabilized to a healthy state on day 6, and then started to become stressed after day 8. Current results are consistent with published data as nitrogen limitation in both toxic and non-toxic strains showed a decrease in growth rate. Further studies will examine the effects of nitrogen limitation on toxicity and PKS protein abundance. This study increases our understanding of environmental factors that affect toxicity at the cellular and molecular level.

EVALUATING THE FUNCTION OF GENES IMPLICATED GLIOBLASTOMA MULTIFORME (GBM) FORMATION USING *C. ELEGANS*

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The purpose of this study is to identify which orthologs of Glioblastoma multiforme (GBM) genes present in *Caenorhabditis elegans (C.elegans*) play a role in cancer development, through the analysis of cell division. The study is interested in genes that are known to play a role in the development of GBM. *C.elegans* is an ideal organism for studying genes and proteins in humans because both possess many genes in common, some of which may be associated with the development of cancer in humans. *C. elegans* is a valuable model system that can give crucial insights into how cell division is controlled and to understand how misregulation of cell division can lead to cancer. For the methods, we will identify which genes implicated in GBM development are also present in *C. elegans.* RNA inference (RNAi) experiments in *C. elegans* will be conducted, which will enable the disruption of gene function to determine the role of those genes. After the RNAi experiments, an assay will be conducted to see if cell division is disrupted by looking at embryo development. During embryo development, the cell must maintain the proper regulation of the cell cycle if not the embryo will not develop properly, which is similar to the errors that are seen in many cancers. These experiments will allow us to determine mechanistically what parts of the cell cycle are being affected and pinpoint the essential proteins that are linked to these abnormalities. This project will help elucidate how changes in genes could affect cell function that could ultimately cause cancer.

ANALYZING THE FUNCTION OF THE CAENORHABDITIS ELEGANS GENE M05D6.2, AN ORTHOLOG OF HUMAN T−COMPLEX PROTEIN 11 (TCP11), IN SPERM FUNCTION AND FERTILITY

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Human t−complex protein 11 (TCP11) is a testis−specific gene product that is hypothesized to be necessary for proper sperm capacitation, acrosome reaction, and sperm morphology. M05D6.2 is the Caenorhabditis elegans ortholog of human TCP11. Our goal is to use the investigation of M05D6.2 gene function to understand the role of TCP11 in human reproduction. C. elegans have two sexes: hermaphrodite and male. Sperm from both hermaphrodites and males must undergo proper sperm activation, which includes processes similar to sperm capacitation and acrosome reaction in mammals, in order to migrate to and fertilize the egg. We have used RNA interference (RNAi) to disrupt the gene function of M05D6.2 in C. elegans. Hermaphrodites subject to M05D6.2 RNAi−treatment show no reduction in fertility. However, when male C. elegans are subject to M05D6.2 RNAi−treatment our preliminary results indicate that they have a significant decrease in fertility, despite making a normal number of sperm. We have generated three transgenic C. elegans strains using CRISPR/Cas9 genome editing (a deletion mutant, a mutant mimicking mutations found in infertile male patients, and a GFP−tagged version of the protein) to further characterize M05D6.2 function and localization. We are also investigating C. elegans strains with single nucleotide polymorphisms (SNPs) in the gene to characterize the function of specific residues in the TCP11 domain.

SYSTEMATIC IDENTIFICATION AND CONSERVATION OF ADJACENT GENE PAIRINGS IN FUNGI

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It is known that spatial positioning influences transcription; for example, it has been found that the clustering of functionally related genes increases their transcriptional co-regulation compared to unpaired members of the same family. This relationship has been extensively characterized for both the rRNA and ribosome biogenesis (RRB) and the ribosomal protein (RP) regulons, and this has been functionally dissected within the RRB family – where clustering results in adjacent gene co-regulation. While a non-random spatial distribution was observed in several other functionally related gene families, there has been little follow up characterization as to how wide spread this phenomena may be. Thus, the significance and prevalence of these observations has not yet been fully studied. To test how extensive this spatial arrangement was, we performed an exhaustive expansion to characterize the genomic distribution of all gene families using the G.O. Slim categorizations using *Saccharomyces cerevisiae* as a model. Of these 138 functional classifications, we observed a non-random distribution 27% of the time. Within this subset, the functional clustered genes exhibited tighter transcription through the cell cycle compared to their singleton counterparts approximately 75% of the time. The identified clustered gene pairs in *Saccharomyces cerevisiae* were compared with a widely divergent yeast species to characterize the extent of conservation of spatial positioning. Conservation of *Saccharomyces cerevisiae* functional gene pairings were observed across all species analyzed, however, there are both new and old pairings seen. This suggests the functional clustering of genes, which could allow for adjacent gene co-regulation, is a widespread phenomenon in yeasts and potentially eukaryotes.

OSTEOARTHRITIS INDUCED BY *HAS2* GENE KNOCKOUT OF CARTILAGE

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Osteoarthritis (**OA**), also known as degenerative joint disease, is the most common form of arthritis affecting over 26 million people in the US. It is characterized by the degradation of articular cartilage cells leading to joint dysfunction usually in the hips, hands, knees and spine. This debilitating disease has limited palliative care options and there are no effective treatments to date, because its genetic causes are unknown. The goal of our study is to determine one of the primary genetic causes of OA. The central dogma of molecular biology is an explanation of the flow of genetic information within a biological system. The *Has2* gene codes for a major enzyme that produces hyaluronic acid, which is a glycosaminoglycan in the articular cartilage matrix. Using *Has2* gene knockout in joint cartilage prevents the production of hyaluronic acid.

In this study, we used an inducible cell specific Cre-LoxP conditional transgenic mouse model to look into the genetic role of *Has2* for the development of OA. The AgcCreERT2-loxP system was chosen to target the *Has2* gene at multiple stages within the life cycle of a mouse. To generate this system, the following mouse models were used: agcCreERT2, tdTom, and *Has2*LoxP. PCR and 4-OH Tamoxifen cultures were used to sustain and verify the lines over the course of the experiment. A reporter line, tdTom red fluorescent protein, was used to assess cell specific articular cartilage targeting efficiency and specificity. This preliminary data strongly suggests that a single gene (*Has2*) is responsible for the pathogenesis of OA. The correlation of *Has2* to OA would be the first proven link between a single gene and the development of OA. Based on its genetic causes, the results of our study could be used to develop a novel treatment for OA. This would be an application of the Central Dogma of Biology for potential improvement of palliative care options.

This research was supported by ANRF (American National Research Foundation) research award to YL, the faculty fellowship award by The Women's Advancement Initiative, advancing each woman's potential in the HCW tradition at the University of Hartford to YL, Dean's research student and faculty funds for KM, KV, KE and YL of College of Arts and Sciences, University of Hartford.

REGULATION OF DNA REPAIR PATHWAYS TO ENSURE GAMETE QUALITY

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Meiotic recombination requires the formation and repair of genome-wide, programmed double-stranded breaks (DSBs). Repair of meiotic DSBs requires homologous recombination (HR), an error-free repair pathway required for crossover formation. Accordingly, error-prone pathways such as non-homologous end joining (NHEJ) are not favored during meiosis due to their propensity for generating mutations and their inability to form chiasmata. How error prone repair pathways are suppressed during meiosis is not well understood. Here, we demonstrate a role of for Mi2, the core ATPase subunit of the NuRD chromatin remodeling complex, in coordinating the repair of DSBs and maintaining genomic stability through multiple mechanisms. Our data reveal that the conserved Mi2 homologs CHD-3 and LET-418 promote HR, though in their absence, NHEJ is engaged as a secondary DNA repair mechanism to prevent persisting damage in gametes. In support of this, our findings indicate that a population of DSBs are repaired via NHEJ in situations with compromised LET-418 activity. We have molecular evidence wherein *let-418* mutants have elevated expression of several NHEJ components, indicating a role for NuRD in the transcriptional regulation of repair genes during meiosis. Intriguing, our data also reveal that loss of LET-418 leads to upregulation HR machinery, which we attribute to increased genomic stress in mitotically dividing germ cells, and we are currently investigating the causes and consequences of this. As these genes involved in these processes are highly conserved throughout eukaryotes, our findings have implications for understanding how Mi2 may contribute to the prevention of human disease states such as infertility and cancer.

USING A CELL CULTURE-BASED MODULE TO TRAIN RESEARCH STUDENTS

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Undergraduate biology students routinely conduct authentic scientific research. At PUI institutions lacking graduate programs like ours, undergraduates often participate in laboratory-based research early in their academic career, well before they have acquired the requisite lab skills and foundational concepts necessary for success at the bench. To address this, in 2013 our lab developed and published a research training program for undergraduates that relies on structured, skills-based activities and peer mentoring. Recently we developed and published a laboratory teaching module for use in sophomore-level cellular and molecular biology course, that uses cell culture-based experiments to teach core concepts in cell signaling and cell cycle control. The ease and success of this teaching module led our research group to modify our traditional research training program and use this teaching module instead to train our newest undergraduate researchers. This teaching module employs the mouse mammary tumor (MMT) cell line to model breast cancer and includes activities designed to teach fundamental concepts while developing experimental design and analysis skills. Specifically, students learn to grow and characterize animal cells in culture and test the effects of traditional and non-traditional chemotherapy agents on cell proliferation. Students determine the optimal cell concentration for plating and growing cells, learn how to prepare and dilute drug solutions, identify the best dosage and treatment time course of anti-proliferative agents, and ascertain the rate of cell death in response to various treatments. The module employs both a standard cell counting technique using a hemocytometer and a novel cell counting method using microscopy software. The experimental procedure lends to open-ended inquiry as students can modify critical steps of the protocol, including testing homeopathic agents and over-the-counter drugs. Here we report an evaluation of the effectiveness of a pilot program that used this teaching module to train undergraduate researchers. Freshman and sophomore level research students performed the teaching module over a twenty week period during the 2017/2018 academic year. The students worked as a team and were mentored by an upper level undergraduate researcher in our lab. Students also met twice weekly with the lab PI. Assessment of student learning relied on evaluation of the initial skill and knowledge base of the students by the PI and student mentor, followed by weekly evaluation of achievement of learning objectives specific to the teaching module and research training. Assessment instruments included written, oral and practicum along with actual experimental results. Our initial findings strongly suggest that this educational module, which requires students to use the scientific process to apply foundational concepts while developing laboratory and experimental skills, is a highly effective means of training undergraduate researchers.

THE URBAN ECOSYSTEM: A FIRST-YEAR COURSE TO BOOST COHORT FORMATION AND STEM RETENTION

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In the United States, the attrition rate of undergraduate science, technology, engineering and math (STEM) students is notoriously high; over 50% of first-year STEM students either change their major or fail to earn a degree, which is significantly higher than the attrition rate among non-STEM majors. This high STEM attrition is unique to the U.S., and reducing STEM attrition has become a national priority, as there is predicted to be a shortage of 1 million STEM-trained professionals in upcoming years. Academic studies suggest several factors characteristic of U.S. undergraduate STEM programs that contribute to this phenomenon. These factors include the traditional lecture-based teaching style and resulting social isolation, a lack of role models, hyper-competitive peer environments, the "sink or swim" culture during the first year, and overall low grades in STEM courses, particularly compared with other disciplines.

At our small urban liberal arts campus, we recently introduced a field trip-based course into the curriculum as a requirement for all first-year science majors. This course, entitled *The Urban Ecosystem*, focuses on how New York City functions as an ecosystem and explores various aspects of science and technology using New York as a case study. We used unconventional teaching methods such as field trips, original research projects, social media, student collaboration and peer mentorship to explore this topic and to attain our two objectives; integration into our urban campus and decreasing STEM attrition. Field trips included visits to aqueducts and reservoirs to learn about the history and evolution of urban water supply, a local recycling facility to learn about urban waste management, a wastewater treatment plant to learn about water quality issues, a green roof on a convention center to learn about green infrastructure, and Central Park to learn about biodiversity and water quality in NYC.

We have analyzed two years of quantitative and qualitative data from surveys and evaluations by participants in this course to assess the effectiveness of our integrated methods. We have found that students have benefited from the social bonding aspects of the course in particular, and we link the success of this freshman seminar with record retention in our Biology majors. Ultimately, the results will allow us to examine the broader impact of incorporating an interactive first-year seminar course into undergraduate STEM curricula and will contribute to enhancing retention in STEM programs at the undergraduate level.

CHARACTERIZATION OF A PLASMA SOURCE USED TO ACCELERATE WOUND HEALING OF THE TADPOLE *XENOPUS LAEVIS**

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A plasma source used in a collaborative study that produced accelerated healing of wounds in the tadpole species *Xenopus laevis* has been analyzed. The discharge source operated with Helium gas at a flow rate of 50sccm that passed through a quartz tube. A copper electrode was attached to the outer surface of the tube at a point 5.0cm from the end of the tube. Attached to the electrode was an AC power supply operating at 32kHz and 12kV. The optical emissions were analyzed using a high-resolution spectrometer coupled to an CCD detector. The spectra indicated that molecular nitrogen was present in both the neutral and ionized states. Emissions from the radical OH were observed both inside and extending outside of the quartz tube. The emission profile was used to calculate the vibrational temperature and it was found to be 3500±350K. The rotational temperature was determined from a fitting of the Second Positive System transition at 337nm to a Boltzmann distribution and it was found to be 375±50K. The current was measured by monitoring the ground connection from a metal plate that was placed adjacent to the exit aperture of the quartz tube using a current transformer. When the plasma was "on" the signal consisted of an additional component superimposed on the sinusoidal background wave. The height of this current pulse decreased with distance from the exit aperture of the quartz tube.

COMPARISON OF MICROFLUIDIC PDMS AND SILICON DEVICES THROUGH CRYO-ELECTRON MICROSCOPY

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Time-Resolved (TR) cryo-electron microscopy (cryo-EM) is an imaging technique to photograph the structure of biomolecules. Beams of electrons are directed at biomolecules that have been frozen in solution. A microfluidic device is used to mix two reacting biomolecules. Afterward, the biomolecules are sprayed onto a grid and frozen by plunging the grid into a cryogen, and eventually imaged through cryo-EM.

However, the silicon devices used during cryo-EM are often expensive and difficult to manufacture. This study examines the difference between two microfluidic devices: polydimethylsiloxane (PDMS) and silicon. The PDMS microfluidic device could potentially replace silicon devices in labs to study biomolecules. PDMS devices are less expensive and easier to manufacture.

The performance of these two devices was examined during an association reaction (approximately 60ms) by mixing two biomolecules (30S and 50S ribosome subunits) which form the biomolecule (70S ribosome). The results showed that the PDMS device produced consistent and repeatable results. However, the PDMS microfluidic device was slower in producing the 70S ribosome. In addition, the silicon device produced more of 70S ribosome than the PDMS device. The study concluded that the time frames of the PDMS device must be increased to match the performance efficiency of the silicon device.

THE USE OFA CELL CULTURE-BASED MODULE IN A BIOLOGY COURSE

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Undergraduate biology students are required to learn, understand and apply a variety of cellular and molecular biology concepts and techniques in preparation for biomedical, graduate and professional programs and careers in science. In 2015, our lab developed and published a simple lab module to teach the concepts of cell division, cellular communication and cancer, through the application of animal cell culture techniques, to sophomore level biology majors. This lab module exploits the mouse mammary tumor cell line (MMT) as a model for breast cancer. Students learn to grow and characterize animal cells in culture and test the effects of traditional and non-traditional chemotherapy agents on cell proliferation. Specifically, students determine the optimal cell concentration for growing cells, learn how to prepare and dilute drug solutions, identify the best dosage and treatment time course of the antiproliferative agents, and ascertain the rate of cell death in response to various treatments. The module employs both a standard cell counting technique using a hemocytometer and a novel cell counting method using microscopy software. The experimental procedure lends to open-ended inquiry as students can modify critical steps of the protocol, including testing homeopathic agents and over-the-counter drugs. Here we report the results of the initial implementation of this teaching module into a gateway cellular and molecular biology course at a liberal arts college in NYC. The application of the module was modified to fit into the last two weeks of the fall academic term, when students were learning about the core concepts of cell signaling, cell cycle control and cancer. This restricted time frame allowed for the study and application of core biology concepts and principles of lab methods but necessitated the elimination of hands-on lab work. The students first read the published article describing the lab module and expanded their knowledge by selecting additional primary literature articles. Student learning was assessed through oral discussion, written instruments and a performance activity. Assessments posed questions about the lab module, specifically addressing core concepts, principles behind the methodology and data analysis. Students also expanded the experimental strategy and proposed additional experiments and predicted the results. Student knowledge base was initially tested by a pre-survey at the start of this project, followed by a post-survey at the end of the semester. Our results indicate that this teaching module helped students use the scientific process to understand the cell cycle, cellular signaling pathways, cancer and modes of treatment, while honing their ability to analyze experimental data in a way not routinely taught in the undergraduate classroom.

PROVING "PROOF" BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

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" Proof," as it applies to the distilled liquor industry, is a term that has been used for a very long time. Simply put, today, "proof" of an alcoholic beverage is calculated as twice the volume/volume (v/v) ethyl alcohol/water percentage. Thus, if a vodka is labeled as 80 proof, the percent of ethyl alcohol is 40% (v/v). Clearly, because this designation has been used for a very long time, today there are very strict guidelines regarding determining the proof of alcoholic beverages. Because the liquor industry is heavily taxed, the government is very demanding with respect to the accuracy of labeling such beverages.

It is not that simple to determine the volume/volume percentage of ethanol in an alcoholic mixture for a variety of reasons. One of these is the fact that combining, for example, 50 milliliters of ethyl alcohol with 50 milliliters of water does NOT yield 100 milliliters of total solution. The reason for this is that the strong hydrogen bonding interactions between ethyl alcohol and water result in a shrinkage of the total volume.

In the liquor industry, a hydrometer is used to determine proof. The value obtained is actually based upon using the density of the mixture to determine the percentage of ethyl alcohol in the beverage. This whole issue becomes even more complicated because density of a liquid, whether pure or a mixture, varies with temperature. We are exploring whether or not the simpler and easier-to-use nuclear magnetic resonance (NMR) spectrometer could be used to quickly perform the same determination of "proof." Preliminary results indicate that NMR spectroscopy can be used to determine "proof" of distilled alcoholic beverages with an accuracy of ~1-2%, providing one with a very quick and easy way of proving "proof" in specific cases.

HIGH-YIELD RECOMBINANT PRODUCTION OF HYPOXIA-INDUCIBLE FACTOR PROLYL-HYDROXYLASE DOMAIN PROTEIN 3: A KEY REGULATOR OF THE HYPOXIC RESPONSE SYSTEM

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Prolyl-hydroxylase domain (PHD)-containing proteins are the primary regulators of the hypoxia inducible factors (HIFs). HIFs are responsible for controlling the low-oxygen response within a cell. PHDs have been identified as an important potential protein target for treatment of ischemic events including heart attack and stroke. There are three known PHD isoforms that differ significantly in size and activity. To investigate the structure and function of these proteins, we will use solution nuclear magnetic resonance (NMR). Initial efforts for this project primarily focused on PHD-3 (27.3 kDa), the smallest of the HIF-prolyl hydroxylases. Prior to NMR studies, however, the protein must be purified in large amounts. Histidine-tagged and non-histidine-tagged versions of PHD3 were recombinantly expressed in inclusion bodies in *E. coli* and compared. Unfolded protein was extracted from the inclusion bodies and refolded. After refolding the protein in a standard buffer containing arginine and glutathione additives, it appeared to be pure. Optimization and characterization of the purification procedure is presented, and the catalytic activity is being measured by fluorescence assay.

DETERMINATION OF CRITICAL MICELLE CONCENTRATION OF AEROSOL-OT USING FLUORESCENCE SPECTROSCOPY

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The project aimed to develop an analytical method for measuring the critical micelle concentration (CMC) of sodium dioctyl sulfosuccinate (AOT). Reverse AOT micelles were prepared in a nonpolar environment, using hexane as a solvent. The formation of micelles was monitored using the fluorimetric probe Coumarin-120 (C-120). A matrix study of varied C-120 and AOT concentrations was conducted to optimize multiple experimental parameters simultaneously. Once the C-120 concentration was optimized, studies with varied AOT concentration were performed to encompass a wide range of AOT concentrations, which included the known CMC.

OPTIMIZATION OF A FLUORESCENCE ASSAY TO TEST INHIBITION OF PROLYL-HYDROXYLASE DOMAIN PROTEINS

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Hypoxia-inducible factor prolyl-hydroxylase domain proteins (PHDs) are transcription factors that regulate the cellular response to hypoxic conditions. There are three isoforms of PHD proteins which have the potential to be targeted for treatment of heart attack, stroke, and other ischemic events. We have developed a method for high-yield recombinant production of the truncated version of PHD2 (trPHD2) from inclusion bodies in *E. coli*. The function and inhibition of this protein may be assessed using a fluorescence assay. Data from the standardization of this assay suggested fluorescence quenching due to a high concentration of molecules and the presence of oxygen atoms in solution. Optimizations to reduce fluorescence quenching within this assay have been tested and implemented. Data of trPHD2 function measured by our optimized assay will be presented. Future directions for this project include testing the function of PHD proteins in the presence of known and unknown inhibitors for selective drug design.

ADSORPTION OF ACETAMINOPHEN ON ACTIVATED CARBONS FROM CASHEW NUT SHELLS

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Activated carbons were prepared from cashew nut shells by chemical activation of shells with phosphoric acid and heat treatment at elevated temperatures. Prepared activated carbons were studied for the adsorption of acetaminophen. Acetaminophen and other pharmaceuticals are found in ~ 80% of wastewaters in the U.S. Acetaminophen is considered to be the most common cause of acute hepatic failure and the second most common cause of liver failure in humans.

The effect of phosphoric acid impregnation ratio and heat treatment temperature on the adsorption of acetaminophen were studied. Equilibrium adsorption data had the best fit to Langmuir model for all the carbons. It was found that the impregnation ratio has little effect on the adsorption of acetaminophen, which is likely related to the insignificant differences in porosity and the amount and nature of surface functional groups present on the surface of the carbons as a result of impregnation. Carbons impregnated at higher ratios had slightly lower adsorption capacities due to a high amount of surface groups possibly blocking the pore entrances. These groups are mostly oxygen- and phosphorous-containing. The nature of surface functional groups was studied using Fourier transform infrared spectroscopy (FT-IR). The heat treatment of the shells impregnated at 1.7:1 (H_3PO_4:shells) ratio, in the temperature range 400-700 °C, showed the increase in the aromatization of carbons upon increase in temperature, which is related to the removal of surface functional groups and increase in porosity. The latter one was studied using nitrogen sorption. The adsorption capacity of acetaminophen was found to increase with the increase in surface area and pore volume, with the exception of the sample carbonized at 400 °C, whose capacity was lower than expected in the trend. The latter fact could be related to the rich surface functionality of this carbon, and the blockage of some pores by the surface functional groups.

The relationship between the adsorption capacity of acetaminophen and the surface pH was also studied. It was found that the capacity increased with the increase in pH, indicating the importance of basic functional groups in the adsorption process.

The carbon heat treated at 600 °C showed the highest adsorption capacity for acetaminophen (150 mg/g). It is likely that the right combination of porosity and surface chemistry of this carbon resulted in its best performance for acetaminophen adsorption.

IN SEARCH OF TRANS FATS IN HYDROGENATED VEGETABLE OILS

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Recently, there were issues with respect to olive oils and their place of origin. GC-MS analysis of fatty acid methyl esters (FAMEs) derived from oils provides a fingerprint with regards to the region of the world from which the olive oil was obtained. It was shown that there was a lot of fraud involved in the labeling of (especially) European oils. In other words, pricey oils labeled with a specific place of origin often ended up being blended from a mixture of oils from all over Europe.

Much less effort has been spent on analyzing the fats that are available on the market. Fats can be natural (as in butter) or synthetic (as in hydrogenated vegetable oils). The latter have been reported to contain trans fats, which are formed during the hydrogenation reaction that converts oils to spreadable materials. Trans fats are undesirable because, in the body, they behave much like saturated fats when it comes to cardiovascular diseases. The FDA allows a product to be labeled as containing "0 trans fats" even if it contains up to 3.6% trans fat. That by itself is problematic. Will our results be even more problematic?

We have obtained a variety of synthetic fats, from various sources, as well as butter. We prepared methyl esters from these fats. Fats are too large and non-volatile to be directly analyzed by gas chromatography. They have to be converted to fatty acid methyl esters (FAMEs) for GC-MS analysis.

There are a number of methods available for this reaction, which can be done either under acidic or basic conditions. We have optimized this reaction and have preliminary results. Much to our surprise, the less expensive the hydrogenated vegetable oil, the higher the percentage of trans fats. In fact, a number of the commercially available hydrogenated vegetable oils were found to contain significantly higher amounts of trans fats (as much as 20%) than allowed by the government.

AN INFRARED SPECTROSCOPIC ANALYSIS OF SHRINK-WRAPPED PLASTICS TO FACILITATE SORTING IN RECYCLING PLANTS

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The manufacturing of plastics has increased dramatically over the last few decades since the development of synthetic polymers, and plastics have become ubiquitous in our everyday life. Most plastics end up in landfills, accumulate over time, and result in environmental damage due to the inability to be decomposed. In waste treatment plants, plastics are the most common material that can be recycled and sorted by resin type using automated vision-based sensors, including those applying infrared (IR), near-infrared (NIR), Fourier transform near-infrared (FT-NIR), Fourier transform infrared (FT-IR), and RAMAN laser spectroscopy. Since the penetration depth of IR radiation is very low, these technologies have difficulty distinguishing containers from their label materials, particularly shrink wraps that obscure the majority of the underlying container. This confounds the automated recycling process at modern recycling facilities that use IR cameras for sorting, including the Sims Municipal Recycling Plant in New York City. Only a small fraction of such materials is being recycled, primarily because of the difficulties in identifying and separating the various types of plastics.

We analyzed 15 different plastic containers, encompassing resin types 1-2 and 4-7, by attenuated total reflectance– Fourier transform infrared (ATR- FTIR) spectroscopy, with a particular focus on containers with enshrouding labels. We find that some plastic containers have very different IR spectra than their enshrouding labels, indicating differing composition between the label and the underlying container. In addition, the underlying container cannot be analyzed through the label because the IR beam will not penetrate beyond a few microns (penetration depth at 1000 cm^{-1} with a ZnSe crystal on the ATR device is ~2 μm). For example, we find that in a white high-density polyethylene (HDPE) bottle, the major characteristic absorption peaks in the spectrum appear at 2918 cm^{-1}, 2848 cm^{-1}, 1472 cm^{-1}, 1462 cm^{-1}, 730 cm^{-1}, and 719 cm^{-1}, typical of alkane C-H and C-C resonances. By contrast, its shrink-wrapped label displays major peaks at 2924 cm^{-1}, 2853 cm^{-1}, 1715 cm^{-1}, 1261 cm^{-1}, 1099 $cm^{-1}$and 726 cm^{-1}, characteristic of the absorption spectrum of polyethylene terephthalate (PETE), with C=O appearing at 1715 cm^{-1} and C-O at 1099 cm^{-1}. These results suggest that the difference in spectral patterns between the bottle and the label would confuse sorting cameras in waste treatment plants, potentially placing these plastics with enshrouding labels into incorrect resin bins. In other cases, we found that the label had the same resin composition as the plastic, offering a better alternative for recycling-friendly package design.

CHROMATOGRAPHIC ANALYSIS OF AMPHETAMINES IN BIOLOGICAL SAMPLES

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Analysis of amphetamines and its derivatives found in biological samples such as urine is usually done by chromatographic methods like gas chromatography (GC) and liquid chromatography (LC). The complex nature of biological samples results to the needs of using sample pretreatment methods such as solid phase extraction (SPE). In this study, chromatographic analysis (HPLC) of amphetamines was performed using sample pretreatment method utilizing two solid phase extraction sorbents namely: a HLB Oasis SPE product and a molecularly imprinted polymers (MIP). Results showed better results (higher recovery of amphetamine in complex samples) with the use of the MIP as sorbents. The HPLC results will then be compare to a GC-MS method that we are trying to develop.

GREEN SYNTHESIS OF POLYRHODANINE MICROSPHERES AND ITS APPLICATION FOR THE ADSORPTION OF ORGANIC DYE

[1] Yousif Saleh, [1]Anjali Gaba**,** [2]Qiaxian Johnson , [1]Dr. Moni Chauhan, and [2]Dr. Bhanu Chauhan

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Rhodanine (Rh) and its derivatives have immense antibacterial, antiviral, antihistaminic, and anticorrosion properties. High-quality polyrhodanine (pRh) films prepared electrochemically and silver/pRh nanotubes and nanofibers composite materials synthesized via chemical oxidative polymerization exhibits immense antimicrobial efficacy against Gram-negative, Gram-positive bacteria and yeast. pRh similar to polypyrrole, polyaniline, and polythiophene are very useful materials for micro sensors, high environmental stability, and catalysis attributed to pi-electron delocalization. Recently, hollow polymeric composite materials have triggered great interest in the area of material science due to their large surface area, alterable particle diameter, shell thickness, low permeability, and density. To our knowledge, there is no report for the direct one-pot green synthesis of pRh nano spheres either with or without using a template. Since pRh has coordination sites N, O and S with lone pair of electrons, it is known to complex with heavy metals and remove them from aqueous solutions. These nanospheres have a positive charge localized over its backbone and hence make it an ideal candidate for the removal of anionic dye (Methyl Orange) from the wastewater. This presentation will cover microwave synthesis of metal catalyzed pRh micro spheres and its characterization via SEM, TEM, FT-IR, UV-vis, and Raman Spectroscopy. Kinetic study of Methyl Orange adsorption by Polyrhodanine nanosheres will also be discussed.

SHAPE AND SIZE CONTROL OF SILVER NANOPARTICLES AND THEIR COATING OF WITH 2,7 DICHLOROFLUORESCEIN

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The major goal of this research is to control and predetermine the shape and size of silver nanoparticles. The shape of the nanoparticle is important for transfection efficiency, being able to reliably control the shape is of useful interest for drug delivery and other applications.[1, 2] The reaction parameters such as temperature, concentration and mode of addition were varied for each reaction to confirm what conditions consistently produce specific outcomes in terms of morphology. In addition, we also have investigated for first time what physical and chemical change is the cause of a specific outcome.

The reaction temperature is varied to identify the role heat plays as a catalyst for specific results in the shape and the size, and to identify the activation energy for the corresponding outcomes. The intensity of mixing is varied to identify the role increasing the collisions between reactants plays in varying and improving the lattice of the nanoparticles. The reaction time is also varied to identify the rate of nanoparticle growth under the varying conditions, as well as to identify how stable the product is. Reactant amounts were varied to identify yield limits. The reaction mixture was initially analyzed using UV-vis to identify peaks of interest. When the reactant amounts are the same, changes in the UV-vis peaks are used to identify how the parameters that were varied affect the morphology or the yield of desired materials. In most circumstances, the reaction mixture was dropped onto a TEM grid and allowed to dry overnight and then analyzed using TEM for confirmation of morphological evaluation.

The second objective of this research is to investigate the reactivity of 2,7-dichlorofluorescein (2,7-DCF) to determine whether the nanoparticles would be coated by 2,7-DCF, via undergoing ligand exchange reactions. In this paper, we will present the result of these studies and products analysis using fluorescence, IR, UV-vis, and TEM. The product and data from this experiment will be used to further imaging research in Biological and Non-Biological systems.

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[2.] Chauhan, Bhanu P. S.; Latif, Umar |Macromolecules, 2005, 38 (15), pp 6231–6235 | Inorganic/Organic Hybrid Nanoreactors Based on Cyclic and Cubic Siloxane Scaffolds

SINGLE NANOPARTICLE INVESTIGATION FOR HYDROGEN EVOLUTION REACTION

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To combat the harmful effects of the current global energy consumption, the development of more efficient and affordable forms of energy are required. One potential solution is to produce renewable molecular hydrogen (H_2), which can be used as a carbon-free replacement for energy storage and transportation. Renewable hydrogen is produced from water electrochemically by the hydrogen evolution reaction (HER). HER electrocatalysts are typically Pt group metals, which are often employed as nanoparticles (NPs) to decrease cost. Here, we present a study of HER at the single nanoparticle level by monitoring stochastic collisions between Pt NPs and a substrate electrode. The experimental setup uses a small diameter microcapillary (≈3-6 μm) that is filled with a solution containing 1 mM H_2SO_4 and Pt NPs and placed in contact with a semiconducting electrode, creating an electrochemical cell. We observe individual nanoparticle collisions display several current "blips" or "steps" which is an indication of the particle hitting the semiconductor or sticking to its surface when -1.0 to -1.3 V are applied to the system. The size/shape of the current spikes correlate with nanoparticle size and the frequency of the impacts depends on their concentration. The results of this study highlight the inherent variability in populations of nanoparticle electrocatalysts and enable a better understanding to the nanoscale electrocatalytic properties which are most effective for HER.

FORMATION OF GELS USING DIFFERENT AMINO GROUPS INCORPORATED WITH NANOPARTICLES AND MULTI-WALLED CARBON NANOTUBES

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Nanoparticles display a high surface area to volume ratio, making them excellent for chemical **application.** Furthermore, carbon nanotubes have high rigidity, tensile strength and Young's Modulus, making them ideal agents for scaffolding with other nanostructures and making nanocomposites. In addition, we have been investigating the gelification of amino functionalized gels synthesized from various different silanes. By using different silanes, we can impart some of the desirable properties to our materials such as hydrophobicity, reactivity and any self-assembly they may impart to our generate materials.

In this presentation, we will be describing the gelification of amino functionalized silanes. These composites were made using multi-walled carbon nanotubes, noble metal nanoparticles and functional silanes. These materials were made under ambient temperature, and water. This is unusual because silanes readily hydrolyze in the presence of water, however 2-AST is stable in water. With the addition of another silane, 2-AST can copolymerize and form a gel matrix. The spectroscopic analysis was done using UV-Vis, FT-IR, Raman, SEM and TEM.

CATALASE ENCAPSULATED IN NANOSIZED MATRICES CAN BE USED IN SKIN CARE

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Numerous pathologies and skin conditions are due to increased levels of reactive oxygen species (ROS) or decreased antioxidant defense systems. Oxidative stress leads to aging of the skin, to skin disorders, and skin disease. Besides the intrinsic factors, in the case of skin there is influence from environmental factors such as sun exposure and UV radiation (responsible for photoaging – the superimposition of damage produced by light on the aging process), whose action can be prevented/limited. Catalase *(CAT)* metabolizes hydrogen peroxide (H_2O_2), a product of many oxidases reactions and an important ROS, to water and oxygen. Besides the beneficial role as antibacterial agent, high concentrations of H_2O_2 inhibit amine oxidases, and promote oxidative damage to tissues, making the use of CAT in the treatment of burns and in skin care a good option. The cosmetic industry uses it in formulations for the skin as an antioxidant or in facial masks, together with hydrogen peroxide, targeting increased cellular oxygenation in the epidermis. The problem with using CAT, a protein, in skin care is its bioavailability. The *stratum corneum* allows only small, lipophilic molecules to be absorbed through the skin and this excludes amphoteric molecules like proteins.

The present study focuses on using nanoparticulate chitosan (polymeric 2-amino-2-deoxy-□-D-glucan formed through 1→4 glycosidic bonds) as delivery vehicle for CAT to the skin. It was chosen because it is inexpensive (prepared from chitin obtained from crab/shrimp), biocompatible, biodegradable, mucoadhesive, and it can be easily converted into nanoparticles using green reagents and procedures. The high surface to volume ratio and its own biological activity (antibacterial and antifungal agent) make it a good ingredient in formulations for the skin.

Nanoparticulate chitosan encapsulating CAT from beef liver was prepared by ionic gelation and crosslinking (using sodium tripolyphosphate). Taking into consideration the common seafood allergies present in the general population, in parallel procedures chitosan from fungi was used to prepare the nanosized matrices encapsulating CAT. All nanoparticles were characterized by: encapsulation efficiency, loading capacity, ratio of residual amino groups (obtained by colloidal titration), FTIR spectroscopy, and scanning electron microscopy (SEM). Nanochitosan obtained from fermentation showed a lower loading capacity but higher encapsulation efficiency. The activity of the encapsulated CAT was assayed and compared to that of the starting enzyme. Chitosan from marine species (obtained by a chemical process) is compared with chitosan obtained from fungal sources (by fermentation) as starting materials for nanosized matrices encapsulating a protein.

A water-based formulation for skin care was prepared and nanoparticles encapsulating CAT were included in the recipe. Kinetic studies for the protein release from nanoparticles were conducted over one week period. The percent release of CAT from the chitosan from marine sources was higher by an order of magnitude. The kinetics of the release was studied also on the composites included in the formulation for the skin. All samples collected for the release studies were assayed for CAT activity and the encapsulation stress and the influence of the diffusion are discussed.

VARIOUS APPLICATIONS OF RHODANINE AND METAL COMPLEXEX

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Rhodanine is known for playing a major role in biological reactions such as therapeutics. It is currently being examined for its antimicrobial, antiviral, antihistaminic, and anticorrosion properties that it gains in conjunction with nanoparticles[1]. However, due to its poor selectivity the compound is not ideal. The use of silver derivatives such as silver salts, colloidal silver, and nanoparticles have been well documented for the antimicrobial and therapeutic properties. When coupled with rhodanine in a facile one-pot reaction, a powerful antimicrobial agent is generated. This procedure can be altered in order to explore the fabrication of poly rhodanine nanospheres. The spectroscopic characterization was accomplished by UV-Vis, FT-IR, Raman, SEM, and TEM.

(1) Rhodanine 118192 https://www.sigmaaldrich.com/catalog/product/aldrich/118192 (accessed Mar 27, 2018).

ELECTROCHEMICAL EXPLORATION OF GRAPHENE OXIDE

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Graphene oxide is a versatile compound, and has many unique features despite its tiny size. Graphene oxide's full potential is yet to be fully known but a great deal of research has gone into discovering more of this compound. Graphene oxide is also known for having electrochemical sensing properties. Silicon is found to be unstable, and decays in aqueous solutions, reduction of graphene is a potential way of allowing electrochemical measurements to be made in solutions where a metal is unstable. If graphene oxide is successfully able to be reduced on silicon, and is stable then it would bring us to closer to making a light addressable microelectrode array, that would minimize the amount of sample needed. In a lower amount of time one would be able to retrieve more information of the sample of interest. Through Electrochemical measurements we explore the properties of graphene oxide in both aqueous and non aqueous environments to investigate the origin of the redox species. Eventually we would like be able to efficiently reduce graphene on silicon.

PROBING THE PROPERTIES OF IONIC LIQUID MIXTURES WITH SINGLE-WALLED CARBON NANOTUBES

Rawlric Sumner,[1] Katelyn Urena,[1] Fei Li,[1] Sharon Lall-Ramnarine,[1] James Wishart,[2]
And Dr. Tirandai Hemraj-Benny[1]
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The use of dye-sensitized solar cells (DSSCs) to replace silicon-based solar cells is attracting increased attention. However, it is necessary for more efficient electrolytes to be developed in order to facilitate their increased commercialization. It has been reported that ionic liquids (ILs) with intrinsic high conductivities are ideal media for dispersing single-walled carbon nanotubes (SWNTs) improving their ion diffusion properties. In this study, the transport properties of mixtures containing SWNTs in 1-(alkyl or ether)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ILs were determined to assess their potential as electrolytes in DSSCs. The ionic liquids were prepared by reaction of 1-methylimidazole with the alkyl halide or alkoxyalkyl halide to yield imidazolium halide salts. The halide salts were then converted to bis(trifluoromethylsulfonyl)amide (NTf_2) ILs. H-1 and C-13 Nuclear Magnetic Resonance (NMR) spectroscopy was used to confirm the structures of the ILs. SWNT-IL mixtures were prepared by grinding using a mortar and pestle followed by sonication. The temperature dependent conductivity, viscosity and the thermal profile of the pure ILs and SWNT-IL mixtures were measured and compared. Preliminarily, conductivity values greater than 5.0 mS/cm at 25 °C were obtained for SWNT-IL mixtures, showing that SWNTs have the ability to raise conductivity therefore making them promising electrolytes for use in electrochemical devices.

NON-PRECIOUS METAL CATALYZED OXIDATIVE ESTERIFICATION OF ALLYLIC SP^3-CARBON FOLLOWED BY *IN-SITU* REDUCTION

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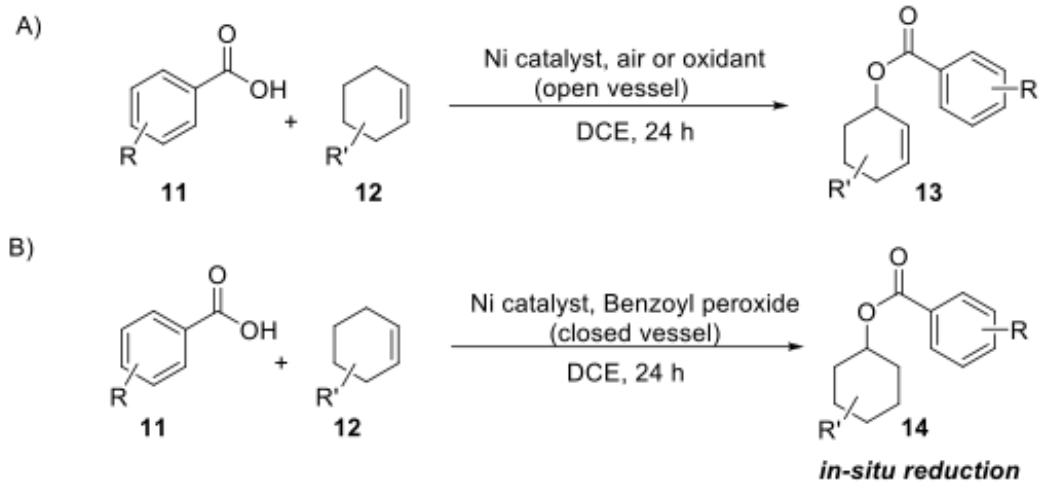
The oxidative and dehydrogenative couplings have been an area of great interest in the past few years. They have emerged as one of the most important strategies for the development of new and greener synthetic methodologies in organic synthesis in recent years. To carry out these reactions, several transition-metal based catalyst were used in literature such as palladium, and copper, for the esterification of allylic sp^3 C–H bonds. However, non-precious metals such as nickel has never been employed as a catalyst for oxidative esterification of allylic sp^3 C–H. In this current study, we would like to report the successful use of nickel metal as catalysts for oxidative esterification of cyclohexene and its derivative with various carboxylic acids. In our attempts to carry out the reaction by reacting benzoic acid with cyclohexene in presence of $NiBr_2$ (5 mol%) and benzoyl peroxide (as oxidant) in open vessel, moderate yield of the product was obtained. Interestingly, when we carried out the same reaction in the closed vessel, the in-situ reduction of the allylic ester (**13**) was observed and good yields of product (**14**, Scheme 2 (B)) was obtained.



A RECYCLABLE SOL-GEL CATALYZED APPROACH: EFFICIENT ONE POT SYNTHESIS OF α,α Di-HALOGENATED KETONES

Justin Domena, [a] Carlos Chong, [a] Qiaxian Johnson [a],* Dr.Yalan Xing,[a,]
*Dr. Bhanu P.S. Chauhan[a]
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Bis (3- (trimethoxysilyl) propyl) amine: "P1" is an organofunctional silane polymer post hydrolysis that has been found to catalyze the one-pot reaction of alkynes producing high yields of α, α, dibromoketones alongside high regioselectivity within our lab. A unique feature of organosilanes is that the silanol groups can readily condense with each other to form polymeric structures that contain very stable siloxane bonds, in this case being very stable within aqueous solutions due to internal hydrogen bonding. The organosilane P1 has also been found to exhibit properties as a green-catalyst that is both reusable meanwhile maintaining favorable conversion rates of desired product. It has also been proposed that the sol-gel P1 acts a reaction vessel that contains a mode of directly initiating halogenation. To our satisfaction, our method of di-halogenation has extended to both terminal and internal alkynes, as well as aliphatic compounds and compounds that vary in both steric and inductive effects with much success. Currently our manuscript is pending for journal acceptance. Our ambitions are now focused on the expansion of catalyst scope implemented as well as the further optimization of regioselectivity.

COPPER CATALYZED HOMOCOUPLING AND HETEROCOUPLING OF TERMINAL ALKYNES

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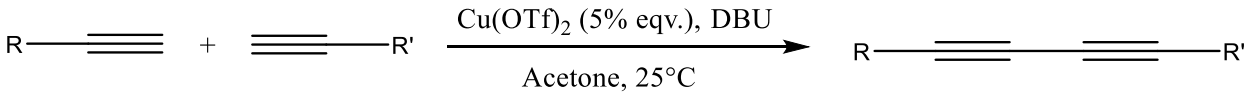
There have been numerous reports of bioactive compounds containing the 1, 3-diyne motif, as well as applications in organic synthesis. A compound containing this motif, known as Deblisone C, was discovered to have antimicrobial properties (Panthama et al. 2010). It was also found that this motif was used in the synthesis of 3, 5-disubstituted isoxazoles (Wang et al. 2012). Recently, our lab has developed a copper catalyzed reaction that synthesizes unsymmetrical and symmetrical 1, 3-diynes. We conducted experiments, in room temperature, with various copper compounds, as well as solvents, to determine the best reaction conditions for terminal alkyne homocoupling. We found that copper (II) triflate and acetone, were the optimal catalyst and solvent, respectively,ss for the homocoupling reaction of phenylacetylene. We then expanded our substrate scope, using copper (II) triflate and acetone, to other terminal alkynes, conducting several homocoupling and hetercoupling reactions.



Mn-TERPYRIDINE CATALYZED DEHYDROGENATIVE ACCEPTORLESS COUPLING OF AMINES AND ALCOHOLS TO GIVE ALDIMINE

Laura Lopez, Brenda Calalpa, Giovanni Berrera, and Dr. Parminder Kaur*
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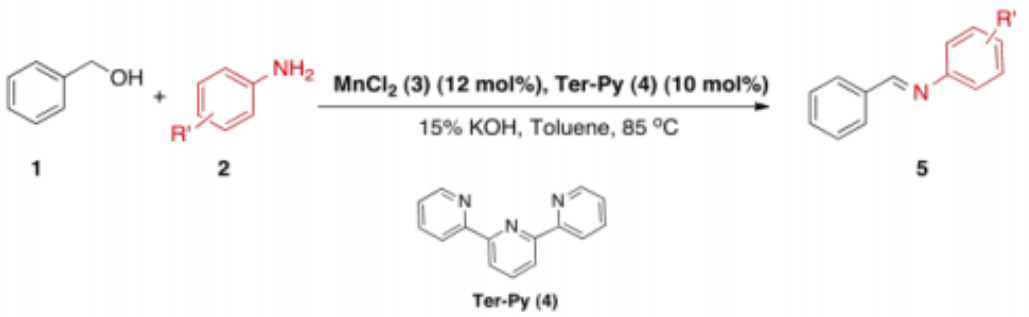
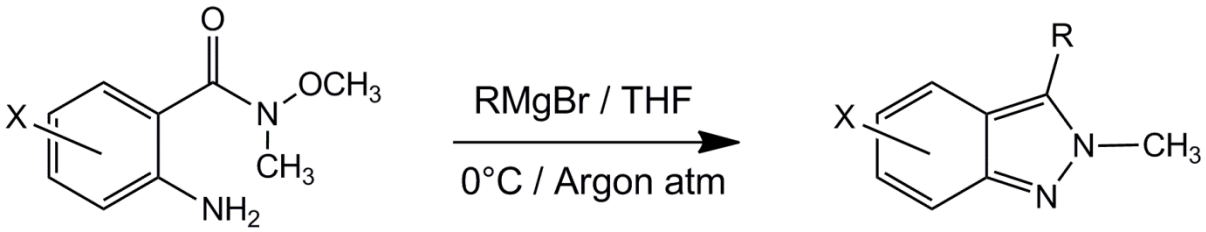


Despite the fact that manganese is one of the most earth abundant transition metals, only next to Fe and Ti, its use in cross-dehydrogenative coupling reactionsis still very limited. The transition metal complexes coordinated to terpy and terpy based ligands has been used in literature to carry out reactions such as water oxidation, and hydrosilylation of alkenes but they have never been used for the dehydrogenative coupling of amines and alcohols. In this work, we are reporting the use of Mn as metal center with ter-pyridine derivatives as coordinating ligand as an efficient catalytic system for the cross-dehydrogenative coupling of amine and alcohol to give the corresponding imines. The reaction was carried out in presence of 12 mol% of the Mn salt and 10 mol% of the Ter-py ligand in toluene for a day at 85 ^{o}C. Moderate to high yields of the products were obtained.

INDAZOLES SYNTHESIS: ACCELERATING CYCLIZATION VIA MANIPULATION OF ELECTRON DENSITY

Tran Nguyen, and Dr. Edward Salaski
Department of Chemistry
Fairleigh Dickinson University, Madison, NJ



In this synthesis reaction, 2H-Indazole is synthesized by reacting Weinreb amide with organometallic reagent called Grignard reagent which is one of most potent nucleophilic base. Traditionally, the product of this type of reaction is expected to be a derivative of ketone however, after difference experimental data, we came to conclusion that the product create by this reaction is actually a different compound and it was determined to be 2H-Indazole. After investigating on potential factor that could contribute to the formation of this valuable compound, one main factor that is taken into consideration is to influence the electron density on the aromatic ring of the Weinreb reagents by adding electron donating/withdrawing group at different position and observe the effect it has on favoring the formation of 2H-Indazole. According to reported literature, substitutes that are on the para position, position at the opposite end of the aromatic ring, have the strongest influence on each other therefore, having an electron donating group on the para position with the $–NH_2$ will accelerate the rate at which it attacks the methoxy and form N-N bond and vice versa. Based on this principle, several substitute groups were considered to be place on the aromatic ring with variation in location to test out its effect on forming indazole. This presentation will outline the details of the research that have been performed on this specific speculation about accelerating cyclization to synthesize indazole by manipulating electron density outside of the benzene ring.

A NOVEL SYNTHETIC METHOD FOR THE PREPARATION OF [2H]-INDAZOLES

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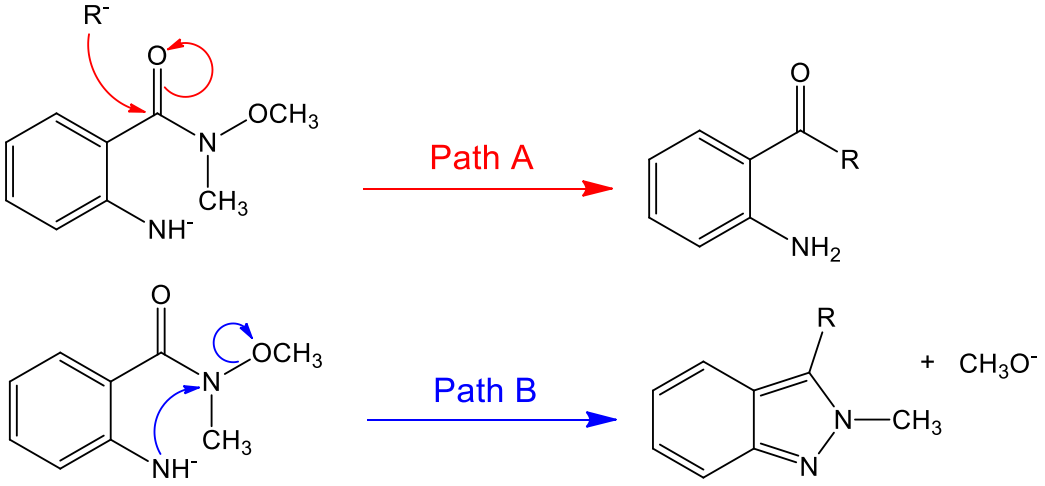
A well-developed method is currently used to convert carboxylic acid derivatives into ketones and aldehydes through the addition of organometallic reagents. N-methoxy-N-methyl amides are key intermediates for this conversion. Our lab has developed a synthetic method that is regioselective to producing [2H]-indazoles. Investigations into the collected data showed that intramolecular substitution was slow and yields of desired product were low. It became apparent that there were two competing pathways leading to the type of product formed. Strong organometallic addition led to ketone synthesis (Pathway A) while not so strong organometallic addition increased nitrogen-nitrogen bond formation and methoxy group elimination (Pathway B). Modifications were required to improve the efficiency of the intramolecular substitution reaction. Several leaving groups were considered and investigated to replace the N-methoxy group. Literature investigations suggested that N-sulfonyl derivatives would be optimal. This presentation will report on the details of our efforts to accelerate the indazole pathway and inhibit the ketone pathway through the incorporation of better leaving groups into our amide reagents.



SYNTHESIS OF DAUMONE ANALOGS AND ANTI-AGING ACTIVITY STUDY

Chiara St. Amant,[a] Mansi Patel,[a] Claudia Kim,[a] Maria K. Holganza,[b] Dr. James Arnone,[b,] * Dr. Yalan Xing,[a,] * Dr. Xiaofan Liu,[c] and Dr. George O'Doherty[c]

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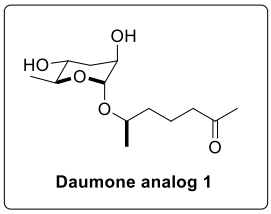

Daumone analog 1

The daumone is in the family of pheromones, and is found in the nematodes *Caenorhabditis elegans* and *Heterodera glycines.* When this pheromone is released, it allows the species to adapt calmly to a stressful environment as well as increase lifespan. This "anti-aging activity" of the Daumone is important in understanding lifespan and aging.

Obtaining the synthetic samples of the Daumone and analogs is critical for the study of biological activity. We proposed the synthesis of Daumone analog 1 which contain a ketone functional group. The Daumone 1 can be synthesized from the intermediate pyranone provided by Northeastern University. After four-step transformations including epoxidation, opening of the epoxide, diol-protection, and hydration of alkyne followed by deprotection, Daumone 1 is expected to be prepared in good yields. Currently, the key step alkyne-hydration is under investigation. Preliminary anti-aging study of the synthetic intermediate diol was carried out.

VISIBLE LIGHT INDUCED ALKYNE FUNCTIONALIZATION

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William Paterson University, Wayne, NJ

A photocatalytic approach for the conversion of aromatic terminal alkynes to carboxylic acids was developed. Eosin-Y was employed as the photocatalyst coupled with visible light (blue and green LED) to induce the oxidative transformation from an alkyne to form a carboxylic acid. The implementation of photo chemistry to functionalize alkynes is a novel and sustainable method. This approach offers mild reaction conditions by eliminating the use of a potentially toxic transition metal catalyst and replacing it with an organic dye (eosin-Y). This reaction supports the idea of green chemistry as it utilizes sustainable visible light as an energy source. This becomes especially significant in the field of organic synthesis where the rich abundance and availability of alkynes from natural resources make them strong precursors for the development of more complex compounds. One pot synthesis of esters was also observed. Future research ventures include the establishment of the reaction conditions which optimize the formation of a carboxylic acid and those which lead to the formation of an ester.

THE COORDINATION OF GENE EXPRESSION VIA GENOMIC CLUSTERING

Maria Katrina Holganza, Alanna Nolan, Irvin Gamarra, Exequiel M. Sisso, Dr. Jay Foley, and Dr. James T. Arnone
Department of Biology and Department of Chemistry
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Proper transcriptional regulation is essential for cellular survival. Large sets of functionally related genes that the cell needs in roughly stoichiometric amounts pose an interesting challenge – and many mechanisms are in place to ensure coordinated transcription. One such mechanism is that of adjacent gene co-regulation – which is the co-expression of functionally related genes that are found clustered on the chromosome. Surprisingly, the role that the spatial positioning of functionally related genes plays is still under-characterized and is ripe for functional dissection. Using the budding yeast, *Saccharomyces cerevisiae*, our project focused on understanding the role of spatial positioning to coordinate the expression of functionally related gene families. The purpose of this research is to explore the following hypothesis: functionally related genes cluster in genomic regions that allow greater transcriptional coordination. We initially focused on the genes in the heat-shock protein and toxin response gene families, comparing the clustered gene family members to the unpaired members. Microarray gene expression data was pulled from five stress response time-courses (heat-shock, MMS, H_2O_2, nitrogen starvation, and glucose to glycerol transition) for every member of each regulon and their ten closest genetic neighbors. The Spearman correlation coefficient for the genomic neighborhood was calculated, plotted as a function of distance, and the decay function was fit to the data. Based on the data from these regulons, we have found that we do see functionally related gene pairs clustered in more transcriptionally permissive areas in the genome in the toxin response gene family, but not for the heat shock gene family. We are currently expanding this analysis to the nitrogen metabolism regulon and the ribosomal protein regulons. Work is currently on going, however our preliminary analysis has found that the nitrogen metabolism gene are clustered in the genome. This work suggests that one level of transcriptional control for functionally related gene families is by clustering genes into more transcriptionally permissive areas of the genome.

THE EFFECT OF CD44 ON REDD1 IN BREAST CANCER

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Breast cancer is the most common type of cancer in the United States. In 2016, breast cancer made up 14.6%, or 246,660 of all new cancer cases, and resulted in around 40,450 deaths. A key contributor to cancer progression is the control of cellular metabolism. mTOR (mammalian target of Rapamycin) signaling is a known and well studied, dysregulated pathway in diseases. This pathway is known to regulate cell growth, apoptosis, cell survival, protein synthesis, cell proliferation, transcription, and translation. mTOR signaling is inhibited by REDD1, a gene that is response to hypoxia and stress. Our research has shown that over expression of CD44 in breast cancer cells results in a down regulation of REDD1 expression and REDD1 protein level in a hypoxia-induced dependent fashion. This regulation may result in altered mTOR signaling resulting increased cancer cells metabolism.

SYNTHESIS OF A MINI-REPORTER CONSTRUCT TO TEST GENE TRANSFER OF RNA THERAPEUTICS

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Glioblastoma multiforme (GBM), a grade IV tumor of the central nervous system, is the most common malignant primary brain tumor, and has a median survival of only 14 months. Poor survival is due to a lack of efficacy in current therapies, including radiation and chemotherapy, which is limited by the blood-brain barrier (BBB). GBM requires new blood vessels, which is essential for tumor growth and survival. Endothelial cells connect with each other and form the walls of new blood vessels, bridging the gap between the growing tumor mass and the established vasculature of the circulatory system. The membrane receptor that activates tumors to recruit endothelial cells to create new blood vessels is vascular endothelial growth factor receptor 2 (VEGFR2). In our lab, we are developing a novel therapy to alter the expression of the VEGFR2 receptor. Changes in VEGFR2 expression to block its activation would inhibit the development of new blood vessels. We are designing therapies to bypass the BBB and deliver the genetic sequences of anti-sense RNA molecules to alter the splicing pattern and expression of the VEGFR2 transcript, creating a soluble VEGFR2 decoy. 9 different antisense sequences were designed to target and block critical elements of the VEGFR2 pre-mRNA transcript, and were cloned into two different therapeutic platform vectors, pAAV-U7-smOPT and pAAV-PTM (contains a pre-trans splicing molecule). We have designed and are cloning a mini-reporter-system that contains the regulatory elements of VEGFR2 splicing. This system measures the efficacy of RNA anti-sense therapeutics to alter the splicing of the VEGFR2 transcript. The visual marker, eukaryotic green fluorescent protein is used to mimic the natural splicing product, whereas the red fluorescent protein, mCherry detects changes in the efficacy of our RNA anti-sense therapy.

EFFECT OF A6 PEPTIDE ON CD44 IN OVARIAN CANCER

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Ovarian cancer is the fifth leading cause of cancer related deaths in women. This year, over 22,000 women will be diagnosed with this devastating disease and over half of them will die due to the disease. More effective therapies targeting biomarkers found on ovarian cancer cells will help lead to better treatment outcomes. The focus of this research is to elucidate the mechanism behind the effects of a peptide, A6, that targets CD44 and increases the effectiveness of various treatments. The transmembrane protein CD44 is known to colocalize with P-gP and lead to multidrug resistant phenotype in ovarian cancer. In this experiment, TOV112D cells stably expressing CD44 and empty vector cells will be treated with A6 peptide. MTT assays will be performed to observe drug resistance via viability in cell culture. In addition, western blotting will be used to determine the level of ubiquitination on PGP. An increase in ubiquitination with A6 treatment leads to destruction of PGP pumps, which would explain the decreased drug resistant phenotype caused by A6 and possibly indicate the mechanism by which A6 functions.

EXOSOMES FROM HPV NEGATIVE CERVICAL CANCER CELLS NEGATIVELY AFFECT NORMAL CELL GROWTH

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Most cervical cancer is caused by a human papillomavirus (HPV) infection in the cervix of a woman[1]. Approximately 12,990 women in the United States will be diagnosed with cervical cancer this year. Out of those women, an estimated 4,120 will die from this disease[2].The HPV vaccine can prevent HPV related cervical cancer, but there are some cases where women are getting cervical cancer tumors that are HPV negative. This has caused an increase in research to determine the molecular mechanism that is causing this HPV negative cervical cancer.

Scientific research has been taking a new approach lately by examining and studying exosomes. Exosomes are small extracellular vesicles that are released from one cell and taken up by a different cell. Exosomes are released at high concentrations from cancer cells[3]. They have the ability to induce micro-environmental changes. For example, exosomes have the ability to turn off anti-tumor responses or promote invasion and metastatis[3]. There is evidence that demonstrates exosomes play a role as mediators of extracellular signaling[3]. This is important because the cell cycle depends on both intracellular and extracellular responses in order to successfully proliferate.

To fully determine the molecular mechanism that is causing HPV negative cervical cancer (HNCC), it is important to understand if and how the exosomes are having an effect on the normal epithelial cell growth. The hypothesis for this experiment is that HPV negative cervical cancer cells release factors in the exosomes that help promote cell growth. Exosomes were successfully isolated from DOTC cervical cancer cells and an uptake of HPV negative cervical cancer (HNCC) exosomes were observed by the normal human fibroblast cells, WI-38. However, we found the opposite of what was expected. Normal epithelial cells treated with HNCC derived exosomes showed a decreased rate of proliferation. Interestingly, however, the cells did seem to have an increase in cell size. A cell cycle analysis was performed by using Flow Cytometry. WI-38 cells treated with HNCC exosomes appeared to be blocked in the G2 phase of the cell cycle. Further studies will be completed to try to determine which cell cycle pathways are being affected in the WI-38 cells and why they are being blocked at this check point.

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DELIVERY OF THERAPEUTIC RNA MOLECULES TO ALTER EPIDERMAL GROWTH FACTOR RECEPTOR EXPRESSION IN GLIOBLASTOMA MULTIFORME

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Glioblastoma multiforme (GBM), the most common central nervous system (CNS) malignancy, is characterized by overexpression of the transmembrane tyrosine kinase epidermal growth factor receptor (EGFR). Activated EGFR promotes GBM tumor proliferation and growth. Current prognosis for patients receiving standard care is approximately fourteen months due to the aggressive nature of this cancer and the isolating abilities of the blood brain barrier. Our novel approach to deliver DNA encoding anti-sense RNA molecules to alter pre-mRNA splicing of the EGFR mRNA transcript in GBM cells has the potential to bypass this barrier. In the strategy presented, we have designed a pre-trans-splicing RNA molecule (PTRM) to deliver a polyadenylation signal (PAS) into the EGFR pre-mRNA transcript upstream of the exon corresponding to the transmembrane domain, altering the mature EGFR transcript. In our design, optimization of the EGFR antisense binding domain and a U7 snRNA-SmOpt localization signal will enable the PTRM to compete against the downstream 3' splice sites of the EGFR transcript, generating a shortened mRNA transcript. Additionally, antisense oligonucleotides (AOs) were designed to target critical splicing motifs along the EGFR pre-mRNA transcript to induce alternative splice variants. These shortened transcripts could translate into non-membrane bound soluble peptide decoys and inhibit activation of the EGFR pathway. The PTRM therapy construct and AOs were cloned into an adeno-associated viral plasmid vector and delivered to GBM cell lines. Total RNA was isolated from cells and reverse transcribed using a random primer mix and target-specific primers to generate cDNA. PCR with specifically pre-designed primer sets were used to detect therapy expression and alternative splicing of EGFR transcripts. Our novel approach to harness the cellular pre-mRNA splicing machinery and gene therapy to generate targeted therapeutics may be an effective strategy in the treatment of GBM.

THE ROLE OF BRaf IN AhR SIGNALING AND MELANOMA PROGRESSION

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Melanoma is responsible for over 80% of all skin cancer deaths. Outside of the plethora of environmental factors that influence melanoma's incidence, a crucial part of its tumorigenicity is due to its ability to upregulate matrix metalloproteinases (MMPs.) MMPs breakdown the skin's basement membrane and allow for vertical expansion of the tumor. Once the vertical growth phase occurs, melanoma becomes one of the most aggressive and deadly types of cancers. It has been shown that a critical enzyme collagenase, MMP-1, is induced through the activation of the Aryl Hydrocarbon Receptor (AhR) pathway (Villano et. al 2005). It is also known that a mutation (V600E) in the BRaf molecule of the MAPK signaling pathway exists in over 70% of all advanced melanoma, and affects levels of MMP-1 (Whipple and Brinkerhoff 2015.) We seek to elucidate how AhR and BRaf signaling affect MMP-1. We know both AhR and BRaf affect MMP-1 expression in melanoma cells individually; our previous system had an endogenously mutated BRaf (V600E) and high levels of AhR, which made it difficult to study them exclusively. Now we have a system that allows for the isolation and manipulation of BRaf and AhR. Preliminary results indicate that the levels of MMP-1 and AhR are both higher in the BRaf V600E than in wild type BRaf Bowes melanoma cells. Further testing may provide clues and knowledge necessary to further understand the mechanism of synergy between these two molecules. This understanding would help develop treatment options to those suffering from melanoma, potentially lessening the progression, resilience and overall tumorigenicity of the cancer.

IDENTIFYING PATHWAYS WITH SIGNALS OF GLOBAL REGULATION LINKED TO ENVIRONMENTAL ADAPTATION IN HOUSE MICE

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House mice from different climates in the Americas show strong evidence of environmental adaptation, including differences in gene expression. Here, the goal was to determine if there was evidence for differences in global regulation of pathways in mice from different environments. To do this, we used existing data on gene expression for lab-raised mice derived from different climates and gene pathway data. We identified all the genes in all annotated pathways for mice and determined whether expression was greater in cold climates vs warm climates or vice versa for each gene. We repeated this for different tissues. Then, we used a binomial test to determine whether, in each pathway, more genes than expected were responding in the same direction. In each tissue, we identified a number of pathways that show concerted changes between the populations, including some related to traits known to differ between the populations. In particular, we found overwhelming evidence of pathway level differences in expression in fat tissue and body weight is a trait that stands out as a major difference in morphology between these populations. Future analyses will include applying this method to classes of genes known to affect phenotypes in mice and to genes associated with ontology categories.

SURVEY OF SPIDER FAUNA AND DNA BARCODE IDENTIFICATION ON WILLIAM PATERSON UNIVERSITY CAMPUS

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DNA barcoding is a technique by which organisms are identified by sequencing a small region of DNA that is common across eukaryotes to match unidentified individuals to identified specimens' homologous DNA in widely-accessible databases. I set out to test whether this method was practical for identification of spiders from our local area. Multiple lab techniques are implemented in this process, primarily Polymerase Chain Reaction (PCR) and Sanger sequencing. Our project consisted sequencing the "barcode" region of the cytochrome oxidase I (COI) gene, using the well-characterized primers Lco1490 and Hco 2198 to amplify a segment approximately 680 base pairs long, from 10 spiders collected near the William Paterson campus. We successfully identified 4 individuals: *Pseudoeuophris lanigera*, *Agelenopsis pennsylvanica*, *Frontinella communalis*, and another *Agelenopsis pennsylvanica.* We discovered that *Pseudoeuophris lanigera* is a non-native species from Central/Eastern Europe, and has not been recorded in this area of the world. Although it is not a native species to New Jersey, it does not appear to be an invasive species. Additionally, were able to achieve identification percentages above 99% for all specimen in the public genetic databases. The benefit of barcoding showed us that we have a non-native, unrecorded species in our local fauna, and demonstrated that DNA barcoding is an inexpensive and fast way to identify small or hard-to-distinguish species. Furthermore, our research provided new barcode data to add to the genetic public databases for future workers to use for comparisons.

NAUTILOID CEPHALOPODS FROM GLACIAL ERRATICS: EVIDENCE FOR LAG DEPOSIT FORMATION IN THE RICKARD HILL FACIES OF THE SAUGERTIES MEMBER OF THE SCHOHARIE FORMATION (LOWER DEVONIAN-LATE EMSIAN), HELDERBERG MOUNTAIN REGION, NEW YORK STATE, U.S.A.

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Glacial erratics belonging to the Rickard Hill facies (RHf) of the Saugerties Member of the Schoharie Formation occur scattered throughout the Lower Hudson Valley of New York and northern New Jersey Piedmont. These glacial erratics are most similar to lithologies exposed ~200km north in the Helderberg Mountain Region of New York. The RHf glacial erratics contain a concentrated assemblage of well-preserved nautiloid cephalopods dominated by large orthoconic and coiled taxa. These taxa are exposed along bedding planes by a complex sequence of physical and chemical weathering during transport within the Hudson-Champlain Lobe of the Laurentide Ice Sheet and deposition within acidic soils of regional ground moraines. Weathering also reveals taphonomic details within body chambers and phragmocones of these nautiloids that are not readily observable in outcrop exposures of the RHf. Some nautiloids display similar orientations on bedding surfaces that contain casts and molds of numerous invertebrates including trilobites, brachiopods and corals. Original taphonomic conditions indicate that the RHf nautiloids represent a post-mortem, localized lag assemblage transported by wave and current activity prior to final burial and fossilization. This lag deposit occurs at the boundary between third order eustatic sea level cycles Emsian 5 and Eifelian 1 and accumulated as part of a shallowing upward cycle bounded below and above by the sub-Aquetuck and sub-Edgecliff unconformities. Nautiloids and other invertebrate fauna were concentrated during multiple exhumation and reburial events where localized wave base was capable of eroding into the shallow shelf platform in this area of eastern New York.

VARIATION IN REPRODUCTIVE TRAITS AMONG HOUSE MICE ADAPTED TO DIFFERENT CLIMATES IN THE AMERICAS

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Although house mice, *Mus musculus domesticus*, are not native to the Americas, they have quickly adapted to diverse climates. For example, body size and nesting behavior are two traits linked to fitness that vary among populations from different latitudes, and those variances contain a genetic basis. However, little is known about differences in female reproductive traits among populations. Reproductive traits have a direct impact on fitness and there are clear predictions from life history theory regarding strategies in environments experiencing seasonal variation versus little seasonal variation. In this study, we analyzed breeding data from colonies of mice derived from populations in Canada, New York, Brazil, Florida, and Arizona. To best address the effects of inbreeding and of potential maternal effects, we focused on first and second generations of wild-derived mice. Female reproductive traits like age at first litter, average litter size, etc. were compared among the five colonies. We found that litter size varied significantly among climates; mice from the cooler regions (Canada and New York) produced larger litters than mice from the warmer regions (Brazil, Florida, and Arizona). This pattern suggests that mice from climates with limited breeding seasons may invest more effort in a given litter. However, more data on pup size is needed to evaluate overall reproductive effort.

THE EXTINCTION OF THE MEGATOOTHED SHARK *OTODUS MEGALODON*: EVIDENCE FROM CLUMPED ISOTOPE THERMOMETRY (CIT)

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The largest and most iconic shark to have ever lived is *Otodus megalodon*. Fossil teeth and vertebra indicate this highly successful apex predator achieved lengths up to 20 meters, weights exceeding 20,000 kg, and global distribution throughout the Miocene and Pliocene (23-2.5 MYA). A general consensus indicates that the ability to thermoregulate in *O. megalodon* acted as a key driver for the evolution of gigantism, which impacted its ecological role and success in surviving environmental changes. However, little agreement exists as to the primary cause for the disappearance of *O. megalodon* where models suggest predator-prey dynamics or environmental change resulted in extinction.

To address these alternative extinction hypotheses, 'clumped' isotope thermometry (CIT) was performed on modern shark teeth with known thermoregulatory physiologies to validate a previously reported calibration equation. Application of this calibration equation to fossils from *O. megalodon* reveal a much higher body temperature (~50 °C) compared with its smaller and modern equivalent, *Carcharodon carcharias* (~30 °C). We hypothesize *O. megalodon* would have had to consume large quantities of prey in order to maintain such a high body temperature. However, cooling of ocean temperatures during the Pliocene would have constrained the species to lower latitudes where ocean temperatures were warmer, whilst its preferred prey (i.e. whales) evolved traits to adapt to cooler temperatures of the higher latitudes (e.g. 'blubber'). Therefore, substantial climatic shifts combined with evolutionary limitations may provide the "smoking gun" for the extinction of the largest shark to ever roam our planet.

A PRELIMINARY STUDY OF MICROPLASTICS AND MICROFIBERS AT THE MOLLY ANN BROOK, NJ

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Anthropogenic microplastic pollution in freshwater bodies continues to be a growing health concern to aquatic and human health. The aim of this study is to investigate the presence and distribution of microplastic pollution at eight sample locations along the 7.8 mile stretch of Molly Ann Brook in Wayne, New Jersey. A variety of tributaries, lakes, and ponds were sampled during the fall 2017, with a total of 40 one liter water samples that were stored in glass containers. These grab samples taken from a depth of 0-18 cm were filtered through 0.45µm filter paper after which the filtrate was allowed to oxidize in the presence of 30% hydrogen peroxide for one week. Oxidized filtrate was filtered through a 0.45µm filter paper and observed at 100X with a binocular microscope. All samples contained pellets, fragments, and fibers; the three types of particles defined for this study. Flow rate, stream depth, and particle count were found to be positively correlated, especially after precipitation events. Raman spectroscopy was used to determine polymer structure of pellets large enough to be scanned. The results from this preliminary study will add to the growing understanding on how precipitation and flow rate affect microplastic distribution in a watershed. The data obtained from this study suggests that there is a relationship between pollution pathways and hydrodynamics is affected by precipitation events.

INSECT BIODIVERSITY AT HIGH MOUNTAIN PRESERVE

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For this project, we surveyed the insect diversity of High Mountain Preserve, a natural area bordering the William Paterson University campus, during the summer of 2017. We used sweep-nets, aerial nets, and ground collecting to catch a broad range of insect taxa. The work was performed over five collection dates, totaling 10 person-hours of collection effort. Our final sample totaled 121 individual insects, representing 42 morphospecies. These insects were then identified using appropriate taxonomic keys and grouped by order, family, and the collection date sorted into 6 orders and 42 families. The most diverse insect orders were Hemiptera and Hymenoptera. An accumulation curve plotting total collected taxa over time suggests that for the patch of forest studied, and techniques used, we sampled a reasonably complete representation of the insect biodiversity.

DNA EXTRACTION FROM ATLANTIC STURGEON SPINE AND FIN TISSUE

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The Atlantic Sturgeon, *Acipenser oxyrhinchus oxyrhinchus*, is an anadromous fish listed under the US Endangered Species Act. Along the East Coast, it spawns predominately in the Hudson, Delaware, and James rivers. It is estimated that there been a 99.5% loss of population in the Hudson River area since 1890. This population crash has been primarily attributed to anthropogenic activities that endanger both the fresh-water juveniles and the salt-water adults. Smaller populations are vulnerable to the effects of inbreeding and genetic drift that can lead to decreased genetic diversity impacting future generations. The goal of this project was to determine if standard methods for the extraction of DNA from tissues could be easily amended with a liquid nitrogen grinding step to extract DNA from archaic bony spine samples. We found that while high quality, high concentration DNA could easily be extracted from fin clips stored in ethanol, only low quality, low concentration DNA could be extracted from spines. While this DNA may be adequate for some genetic screens, future work will focus on testing more sophisticated methods for extracting DNA from archaic bone samples. The ongoing goal of this project is to assess genetic change in Atlantic Sturgeon populations and aid the conservation efforts.

CREATING AN AXENIC CULTURE OF THE TOXIC DINOFLAGELLATE *KARENIA BREVIS*, AND COMPARING ITS GROWTH RATE AND BREVETOXIN PRODUCTION TO XENIC CULTURES OF *K. BREVIS*

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Accumulation of algae in the sea can cause harmful algal blooms also known as red tides, resulting in the visible coloration of water (Blanquart et al., 2016). *Karenia brevis* is a toxic red ride dinoflagellate that is responsible for harmful algal blooms being common around Florida and in the Gulf of Mexico. *K. brevis* produces brevetoxins, which are potent neurotoxins that harm marine life along with causing toxic shellfish poisoning in humans if contaminated fish is consumed (Templeton et al., 1989). Bacteria coexist alongside these algae and phytoplankton communities in the marine ecosystem. Numerous bacteria surrounding *K. brevis* were captured along with the dinoflagellate when isolates were taken from the ocean, and have continued to be propagated in laboratory cultures of *K. brevis*, making these cultures a model system for studying interactions between *K. brevis* and members of the bacterial community. The overarching goal of the lab is to understand the potential role bacteria might play in the growth, survival, and brevetoxin production of *K. brevis*. This study outlines how *K. brevis* growth rate and brevetoxin production will be affected by the removal of bacteria from the cultures. Cultures were treated with antibiotics to make them axenic (bacteria-free). Treatment with nalidixic acid, streptomycin, spectinomycin, and gentamycin led to the elimination of many but not all members of the bacterial community. Treatment with ampicillin, tetracycline, erythromycin, and neomycin led to *K. brevis* death, indicating either a direct inhibitory effect on the dinoflagellate or elimination of a bacterial community member necessary for *K. brevis* survival. Growth rate analysis of the *K. brevis* cultures showed a slight increase in the growth rate of the antibiotic-treated compared to untreated cultures of both a wild type strain of *K. brevis* and a strain with reduced toxicity. We will perform an immunoassay ELISA to characterize brevetoxin production and results of treated and untreated cultures will be compared.

RECOVERY OF DNA AND RNA FROM MICROORGANISMS IN WATER SAMPLES

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Natural water sources are essential for the growth and fitness of some of the most abundant microorganisms in the biosphere, including bacteria, bacteriophage, and water-borne viruses. Multiple studies on the diversity of waterborne organisms in natural sources have revealed a myriad of microorganisms, however work remains to be done to better understand how this diversity varies across different water sources or over time. Since every organism or virus has a unique sequence of DNA or RNA carrying the genetic instructions used in growth, development, and reproduction, these sequences can be used to identify organisms within a sample. The objective of this research is to develop techniques to filter water samples from around New Jersey, isolate DNA and RNA from microorganisms in the samples, and then use polymerase chain reaction (PCR) to specifically amplify segments of the genetic material. The amplified DNA or RNA can then identify the microorganisms present in the water samples. Reliably obtaining a sufficient amount of quality DNA or RNA from water samples is vital to reflect on the diversity in multiple local populations as well as changes in diversity based on season, weather events, or extended periods of time. As such, preliminary research has focused on studying and comparing methodologies for nucleic-acid extraction and purification. Common procedures include phenol-chloroform extraction and enzymatic lysis for genomic DNA and RNA extraction, but the most popular and efficient techniques utilize commercial extraction kits. Given this information, the next step was to determine which kit would yield the best results with consideration of cost, ease, and ability to extract both DNA and RNA from water samples. Many commonly used kits such as the RNeasy and DNeasy PowerSoil Kits and the QIAamp DNA Kit were eliminated as options as they are designed to analyze soil or tissue samples. Other kits in the running, such as the DNeasy and RNeasy PowerWater Kits specialized in water samples, but only extracted one nucleic acid. Because the objective of this research is to isolate both DNA and RNA, more kits were investigated to better meet these requirements. The MagAttract PowerWater DNA/RNA Kit and AllPrep DNA/RNA Kit allow for the simultaneous extraction of both DNA and RNA from water samples, however, the former requires a PowerMag magnet, a powerful separator designed to work with automated liquid handling systems. This piece of equipment, combined with the physical kit, proved very costly, thus it was not selected as the ideal option. Ultimately, because the AllPrep Kit is easy to use, simultaneously extracts both DNA and RNA, and is cost-effective, it was found to best fit the needs of this research. After modifying the AllPrep Kit protocol to obtain the greatest amount of quality DNA and RNA from samples, it will be used to recover nucleic acids collected from bodies of water across the state. Quantitative PCR will be used to determine microbial populations, and map out fluctuations in diversity due to environmental factors such as change in season or anthropogenic effects.

QUANTIFICATION OF FECAL *AKKERMANSIA MUCINIPHILA* AS AN INDICATOR FOR A HEALTHY GUT-MUCIN COMMUNITY

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The bacteria at the gut-lining constitute the bulk of the core gut-microbiome most closely linked to host health. The presence of specific bacteria that are nourished by the mucus barrier reportedly protects the epithelium and result in lower levels of inflammation. Our longer-term hypothesis is that *Akkermansia muciniphila,* could serve an indicator species for this community: present at high levels in feces when the gut is healthy and depleted when stress is affecting the gut, particularly oxidative stress. In this part of the study, we developed a quantitative, high-sensitivity, nested-PCR assay to determine levels of *A. muciniphila* in the feces of mice. The assay was tested with feces collected from diverse mouse strains in our facility (C57-6J, BTBR, DAT CNR2, and CX3CR1CN2). The first two are well known as wild-type and autism mouse models. The last two are custom strains developed for investigating the role of Cannabinoid type 2 receptors on immune cells. The nested-PCR protocol first-round amplification used 27F/1492R universal bacterial ribosomal primers. The second-round primers (S-St-Muc-1129-a-a-20/S-St-Muc-1437-a-A-20) were specific to *A. muciniphila* and re-amplified these 16S sequences from the first-round mix. Dilutions of *A. muciniphila* DNA from ATCC served as reference concentrations. The limit of detection is approximately one genome. The levels of *A. muciniphila* were variable, both within strains and between strains.

QUANTIFICATION OF PATHOGENIC FECAL BACTERIA ON NEW YORK CITY SIDEWALKS

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Evolution has given the genome of pathogenic bacteria in the genus *Enterococcus* the ability to survive and proliferate in extreme conditions. The essential organelle that aids this gram-positive bacterium in resisting environmental pressures is the durable and strong peptidoglycan cell wall. *Enterococcus* is found in the intestines of mammals including humans and domestic animals such as dogs. When humans are infected with these bacteria, acute symptoms include stomach cramping, nausea, blood poisoning, and urinary tract infections. *Enterococcus* is also associated with endocarditis, which is an infection caused by the linking of the heart and enterococcal meningitis.

In the urban environment, poorly maintained sidewalk sanitation in public areas can expose individuals to *Enterococci* via direct or indirect contact. We hypothesized that due to its ability to survive in extreme environments, *Enterococci* originating from dog feces could proliferate on New York City streets. To test this hypothesis, we investigated puddles that had accumulated after wet weather on the NYC sidewalk, in a 15-block radius of Marymount Manhattan College at 221 E 71st St. The Enterolert Quanti-tray system was used to quantify the most probable number (MPN) of Enterococci bacteria in diluted puddle water. All materials were carefully sterilized using the autoclave, and aseptic technique was practiced. Once the puddle water was mixed with the Enterolert reagent, it was incubated at 41°C for 24 hours.

We observed a high degree of variability in our results, with the MPN of *Enterococci* ranging from 1.3 cells·mL^{-1} to 1,400 cells·mL^{-1}. On rainy days, the MPN values were substantially higher, due to accumulation of bacteria in natural puddles. We also performed controlled studies with artificial puddles created from sterile water on the sidewalk, and we found that the bacteria proliferate on very short timescales, reaching 4.4 cells·mL^{-1} after transfer times of only 10 minutes. All of this evidence indicates an abundance of this single genus of pathogenic fecal bacteria on NYC sidewalks, giving ample reason for caution to prevent exposure and infection.

DISCOVERY OF A MARINE BACTERIA WITH A WIDE SPECTRUM ANTI-BACTERIAL ACTIVITY

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Biofilms forming and antibiotic resistant bacteria are responsible for most infectious diseases and hospital related bacterial infections. The need for new antimicrobial and antibiofilm compounds is becoming vital as the incidence of these types of infection is dramatically increasing. The focus of our research is the identification and characterization of new anti-biofilm and anti-microbial substances. An unknown marine bacterium found in the Newark Bay coastal water was isolated and tested for possible anti-biofilm and anti-microbial activity. Cell free extracts of the unknown marine bacteria were made and tested against various strains of *Staphylococcus aureus*, *Staphylococcus epidermidis*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, *Erwinia carotovora*, and *Escherichia coli*. The unknown extract consistently exhibited strong antimicrobial activity against a wide range of gram negative and gram-positive bacteria. The active compound appears to be greater than 100 kDa in size, and heat sensitive. Proteinase K, DNAse and RNAse treatment had no effect on the activity of the extract. Further studies will be conducted to characterize and identify the unknown bacteria and the active fraction of the extract.

DESIGNING NEW INHIBITORS FOR MYCOBACTERIUM TUBERCULOSIS USING BIOINFORMATIC SOFTWARES

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Traditional protocols like 2D approaches for drug discovery, it does not consider the 3D the active site of the protein, thus requiring more resources and time. With the use of bioinformatic software to study the 3D structure, specific amino acid interactions can now be identified. Also by following this approach, we reduce the amount of time and resources during the discovery process. With the use of bioinformatic tools, users can make more accurate design choices compared to 2D Structure Based Drug Design, and reduced the resources needed to synthesize the ligands using other methods.

Tuberculosis is currently the ninth deadliest disease in the world, killing 1.4 million people yearly. The mycolic acid coating the outside of the bacteria is what makes the tuberculosis difficult to treat. With the addition of mutations in the genes of the bacteria, traditional first line drugs, such as Rifampicin and Isoniazid, are rendered useless. The goal of my research was to build a new inhibitor for an enzyme found in Mycobacterium tuberculosis called fatty acid degradation D32, better known as FadD32. This enzyme contributes to the condensation of mycolic acid, which gives its antibiotic resistance property. With the use of bioinformatic tools in our disposal, we were able to replicate the known crystallized structure of FadD32; and docked with other ligands that were designed. This allowed us to analyze the binding sites and conformational change. This information will help us to provide a foundation of new molecules that have never been tested to our knowledge before. If this research is successful, then the inhibitor could potentially be further synthesized into a drug to treat patients with *M. tuberculosis*.

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KIRBY-BAUER DIFFUSION SUSCEPTIBILITY TEST RESULTS FROM BSL1 BACTERIA IN THE MICROBIOLOGY TEACHING LABORATORY

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Safety is paramount in all microbiology labs. The Centers of Disease Control and Prevention (CDC) have designated biosafety levels (BSL) that range from 1 to 4 with 4 being the most dangerous level of microorganisms to work with. The most common BSL used in university microbiology labs is BSL-2, defined by the CDC as "microbes that pose moderate hazards to the person [working with] them," unlike BSL-1 organisms that "are not known to consistently cause disease in healthy adults and present minimal potential hazard". For this reason, more Microbiology teaching labs are seeking ways to work with safer BSL-1 bacteria. The goal of this research project was to determine if we could use BSL-1 bacteria in common laboratory exercises in the microbiology teaching lab without compromising the student's experience. The Kirby-Bauer Diffusion Susceptibility Test consists of using Muller-Hinton agar for confluent growth and antibiotic disks impregnated with known concentrations of antibiotics. After 48 hr of incubation, zones of inhibition surround the disks for organisms killed by the drug. These zones are used to classify if the microorganism is resistant, intermediate, or sensitive to the antibiotic. Antibiotic resistance profiles are well documented for clinically important BSL-2 bacteria, however data for related BSL-1 species are less widely available. We collected antibiotic sensitivity data from a wide range of bacteria including gram-positive and gram-negative bacteria from nine different genera, as well as multiple species from within some of those genera. Data was analyzed to determine the consistency between experiments in both zone size and antibiotic sensitivity classification. In preliminary experiments using *Escherichia coli*, *Micrococcus luteus*, and *Staphylococcus epidermidis* the results demonstrated that *S. epidermidis* was the most extensively resistant and *M. luteus* was the most sensitive to the antibiotic drugs, despite being more closely related to each other than *E. coli*. One challenge of data collection has been interpretation of zone sizes for BSL-1 organisms that do not grow well as BSL-2 species in common laboratory conditions. Additional data will help to determine which BSL-1 species are best suited for Kirby-Bauer laboratory exercises, but can also help microbiology students identify unknown bacteria in the standard "unknown" lab exercises.

SYNTHESIS OF UNIQUE LUBRICANTS MADE OF EXOTIC BUTTERS INFUSED WITH INDIGENOUS OILS TO PROMOTE INHIBITION OF BACTERIA AND PROTECTION AGAINST UV RADIATION

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Throughout the world people are coming to the realization that naturopathic methods are effective alternative to allopathic methods, as they show favorable results with minimal and less harmful side effects. Though the effects of allopathic remedies are potent, side effects of antibiotics such as metronizole and tinidazole can cause severe nausea, vomiting, skin flushing, dizziness, and drowsiness; naturopathic remedies for skin infections can eliminate discomforting side effects. *Staphylococcus* is a bacterium found commonly on skin which causes boils, impetigo, and cellulitis and *Trichophyton* is a genus of fungi that is associated with the parasites that cause tinea, athlete's foot, and jock itch; through our research we have been able to analyze the growth of these species and formulate surfaces that will prevent the development of these uncomfortable skin infections while demonstrating UV protection on skin. To generate these antimicrobial/antifungal surfaces Ucuuba butter, Tamanu butter, and Aloe Vera butter are infused with various concentrations of natural oils, which include chaulmoogra oil, Jamaican black castor oil, dragon's blood, coconut oil, vetiver oil, black cumin oil, and hemp oil. The surfaces generate were then tested against the bacteria strains *E. coli* and *S. aureus* as well as for UV penetrability. We herein report the preparation of these novel surfaces and the antimicrobial and UV efficacy.

STRONG ANTIMICROBIAL ACTIVITY DISPLAYED BY NEWLY SYNTHESIZED HYDROXAMIC ACIDS AND THEIR ANALOGS

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Antibiotic resistant pathogenic bacteria are a growing worldwide health concern according to the Centers for Disease Control and Prevention. These bacteria are responsible for most infectious diseases and healthcare-associated infections in hospitals (HAIs). The need for new therapeutic approaches using novel antimicrobial compounds is becoming vital as the number of infections caused by antibiotic resistant strains of bacteria such as *Staphylococcus aureus* and *Staphylococcus epidermis* has drastically increased. The focus of our study is to test newly designed and synthesized therapeutic agents for antimicrobial properties. Several hydroxamic acids and their analogs were newly synthesized by the chemistry department and tested in our laboratory for antibacterial activity against five different ATCC strains of pathogenic bacteria. The antimicrobial activity of each compound was evaluated using the disk-diffusion assay and the liquid broth assay. All compounds displayed a various spectrum of antibacterial activity that will enable us to narrow down the potential active site or functional group in the molecules responsible for the activity. Future work will focus on designing and testing new derivatives with a broader spectrum of activity that will be further tested for cytotoxicity against human cell lines.

EVALUATION OF *IN VIVO* TOXICITY OF NB1207, A NOVEL SYNTHETIC ANALOG OF miR-1207-3p

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Prostate cancer is the most common solid organ cancer in men in the Western world. And the metastatic castration-resistant prostate cancer (mCRPC) subtype is highly lethal. Our laboratory has discovered that increased expression of tumor suppressor microRNA-1207-3p significantly inhibits proliferation, migration, and induces apoptosis in prostate cancer cells. We have created a synthetic analog of microRNA 1207-3p, NB1207, and evaluated its therapeutic activity *in vivo* by administering NB1207 to male NOD scid gamma (NSG) mice bearing 22RV1 and C4-2B mCRPC xenografts. We observed that NB1207 significantly inhibited mCRPC growth and metastasis. We, then, sought to assess the toxicity of NB1207 *in vivo* in comparison to no treatment of NB1207 using NSG mice that were not implanted with tumor cells to determine the effects of the analog on normal tissue. This is important because determining the effects of the analog on normal tissue is essential in not only checking how safe the analog is, but also to characterize the possible toxic effects it can produce. The mice were treated with a dosage of 1.5 uM in 100uL so that the diluted concentration of the drug is 100nM in 1.5 mL of blood volume for male mice weighing 25 grams. Mice were observed for 11 days after treatment and subsequent complete blood count (CBC) and differentials analysis was performed. We observed that there are no differences between red blood cells, hemoglobin, white blood cells and platelets between the NB1207 treated NSG mice and the no treatment NSG mice. Consequently, the anti-cancer and anti-metastatic candidate therapeutic, NB1207, is not hematotox

INVOLVEMENT OF HYPOTHALAMIC NEURONS IN CONTROLLING MIDBRAIN NOCICEPTIVE NEURONS: A NEUROANATOMICAL EXAMINATION

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Glutamate is a major neurotransmitter involved in sensory signaling including nociception. Glutamate and its receptors are found both in the spinal cord and in medullary/midbrain regions well known for processing the spinal and supraspinal nociceptive information. The circuitry of nociceptive system has been well characterized by others where the medullary adrenergic/serotoninergic nuclei receive input from the midbrain glutamatergic centers. In this study, we used neuronal tracer to determine the axonal projections between the midbrain and the forebrain. An orthograde tracer was microinjected into the mibrain of C57BL/6J mice. Three to 4 days later, animals were perfused and brains were removed for immunohistochemical analysis. Our data showed several forebrain nuclei send direct axonal projections to mid and hindbrain nuclei known to be involved in controlling nociceptive information.

CREATINE MONOHYDRATE INCREASES RESISTANCE TO REACTIVE OXYGEN SPECIES (ROS) IN *CAENORHABDITIS ELEGANS*

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The free radical theory of aging suggests that one of the leading causes of aging is the accumulation of reactive oxygen species (ROS) which create molecular damage and reduce lifespan. Previous studies showed a reduced lifespan in *Caenorhabditis elegans* (*C. elegans*) in response to environmental stress from ROS. These studies have shown that anti-oxidant amino acid derivatives, selenocysteine and N-acetyl-L-cysteine, can mitigate the effects of these stresses. In the present study, we examined the effects of an amino acid derivative, creatine monohydrate, in preventing damage from oxidative stress.

The lifespan of *C. elegans* was compared between untreated control and creatine monohydrate-treated groups after treatment with oxidative stress induced either by hydrogen peroxide or ultraviolet (UV) irradiation. Three-day, age synchronized *C. elegans* were transferred to nematode growth agar (NGA) treated with 0, 5, 10, and 15 mM of creatine monohydrate prior to exposure of oxidative stress. The *C. elegans* were then treated either with 1-2 mM of hydrogen peroxide for 6 hours or 1-2 min of UV irradiation to induce oxidative stress. The numbers of worms alive were analyzed on a 24 hour basis until all worms were dead. When exposed to six hours of 1 mM hydrogen peroxide, the untreated control group completely died after 48h compared to 29% of worms survived when treated with 10 mM of creatine monohydrate. In addition, 37% of worms treated with 15 mM of creatine monohydrate survived after 48hr post 1 min exposure to (UV) irradiation when compared to the untreated control group which completely died. These findings demonstrate that 15 mM of creatine monohydrate increased the lifespan of *C. elegans* when exposed to oxidative stress induced by (UV) irradiation. Thus, supplementation with creatine monohydrate increased resistance to oxidative stress in *C. elegans* supporting the free radical theory of aging.

HORMONAL CONTROL OF CUTANEOUS DRINKING IN THE CHACOAN HORNED FROG (*CERATOPHRYS CRANWELLI*)

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The Renin-Angiotensin-Aldosterone system is the major regulator of water and electrolyte balance in vertebrates. Dysfunction of the hormonal cascade leads to negative systemic effects, most commonly hypertension, which affects one in three adults (AHA, 2016). The goal of this study was to identify the role of the hormone angiotensin II in regulating water balance in the Chacoan Horned Frog (*Ceratophrys cranwelli*). Previous studies have identified angiotensin II as increasing the rate of cutaneous water absorption in certain anurans (frogs and toads), with proposed direct mechanisms including changes in water absorption behavior and cutaneous blood flow. In addition, angiotensin II may indirectly cause changes in skin permeability to water by stimulating secretion of the hormone arginine vasotocin (the antidiuretic hormone found in non-mammalian vertebrates). A first experimental series (behavioral arena assay) was unsuccessful in identifying a significant effect of angiotensin II on water absorption rate ($P = 0.2914$; $n = 8$) or time spent in the water absorption posture ($P = 0.9705$; $n = 8$), relative to a Ringer's solution control. In a second experimental series (forced hydration assay), the effects of intraperitoneal injections of the following on water absorption rate were compared: (1) angiotensin II; (2) angiotensin II + saralasin (an angiotensin II receptor antagonist); and (3) Ringer's solution (control). There was a significant overall effect of treatment ($P = 0.0074$) and time interval since injection ($P < 0.0001$; $n = 8$) on water absorption rate once the behavioral component was excluded. The results suggest that angiotensin II has a strong physiological effect on water absorption rate in *C. cranwelli*, while the behavioral effect may be minimized in association with the cryptic burrowing habitats of this species.

PLASMA EXPOSURE AND TAIL REGENERATION: THE INTERPLAY OF CALCIUM WITH MITOCHONDRIA AND PEROXISOMES

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Atmospheric pressure plasma treatment has emerged as a new form of regenerative medicine, with therapeutic applications in wound healing, tissue regeneration, and cancer therapy. Reactive oxygen species (ROS) signaling is required for wound healing and tail regeneration of tadpoles, *Xenopus laevis*, and plasma-treated tadpoles have a in higher concentration of ROS compared to the unexposed control (Rivie et al., 2017). Calcium is essential for all living organisms, where Ca^{2+} sequestration and release into and out of the cytoplasm functions as a signal for many cellular processes such as growth and cell death. Calcium signaling pathways also interact with other cellular signaling systems including ROS signaling. Peroxisomes are also known to play a role in Ca^{2+} homeostasis and antioxidant defense. Mitochondrial permeability transition pores (mPTPs) are voltage and Ca^{2+}-dependent channels and prolonged opening of these mitochondrial pores can lead to massive release of matrix Ca^{2+} and swelling of the mitochondria.

In the present study, we have focused on the role of Calcium (Ca^{2+}), mitochondrial permeability transition pore (mPTP), and peroxisomes during wound healing and blastemal formation following tail amputation. Tail amputation was carried out by removing 40% of the tail and the amputated region was immediately exposed to helium plasma (generated inside a quartz tube with a single electrode powered by an AC voltage (15kHz) having peak-to-peak voltages of 18kV) for 40 seconds. *In situ* staining for calcium, mPTP, and peroxisomes was carried out in amputated tail tissue at 24 hours and 5 days after plasma exposure.

Our results on *in situ* staining, for calcium, mPTP and peroxisomes 24 h and 5d post amputation indicate that all these parameters were increased in plasma exposed tadpoles compared to control. In conclusion,

a. there is an increase in calcium resulting from exocytosis of calcium from its stores (mitochondria and peroxisomes) that leads to cell death of damaged cells, cell repair and regeneration.
b. *increased mitochondrial and mPTP staining* indicates that there is a fission of mitochondria which also induces mPTP formation leading to mitophagy and removal of these damaged organelles.

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THE EFFECTS OF TRICLOSAN ON *CAENORHABDITIS ELEGANS* SURVIVAL, REPRODUCTION, AND MOVEMENT

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Triclosan is an antibacterial agent that has been used in common everyday products such as soaps, toothpastes, body washes and some cosmetic products. Its benefits as an antibacterial additive may be outweighed by the growing evidence of its toxicity in eukaryotic organisms. Others have shown that triclosan affects the muscle function of mice. Very recently, several groups have show that triclosan also affects the reproduction and lifespan of the nematode, *C. elegans*. We have seen that triclosan treatment decreases *C. elegans* survival. In addition, we have evidence to suggest that triclosan decreases egg production. To test whether triclosan effects egg production, we conducted a brood size assay. The worms were exposed to triclosan (0 ug/ml, 1 ug/ml, 2.5 ug/ml, 5.0 ug/ml and 10 ug/ml) for 24 hours, and the number of eggs and larvae present on the plate were counted. A decrease in brood size was seen with increasing concentrations of triclosan. This suggests that exposure to triclosan may reduce egg production. These data are consistent with recently published reports.

We have seen that triclosan also affects *C. elegans* movement. We are interested in the mechanism through which triclosan acts to effect movement in *C.elegans*. Others have shown that triclosan acts through the ryanodine receptor, specifically type I, in mice. Ryanodine receptors play an important role in excitation-contraction coupling, a process that results in the contraction of muscles. Ryanodine receptor I is expressed by the gene *unc-68* in the body wall muscle of *C.elegans*. We conducted a movement assay in which we counted the number of body bends over time in worms exposed to triclosan (0 ug/ml, 2.5 ug/ml and 5.0 ug/ml). There was an increase in the number of body bends between 0ug/ml and 2.5 ug/ml triclosan. No increase was seen in worms without functional UNC-68. These data suggest *unc-68* is required for the effect of triclosan on *C. elegans* movement.

SEASONAL VARIATION IN LOCOMOTOR PERFORMANCE OF THE RUBBER BOA (*CHARINA BOTTAE*)

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In this experiment, we examined seasonal changes in locomotor performance of Rubber Boas (*Charina bottae*). We measured metabolic rate during physical activity of six individuals during the late active season and during artificial hibernation using a paired design. Specifically, we quantified rates of O_2 consumption and CO_2 production during forced activity using an open-flow respirometry system. After adjustment for variation in snake body mass, we found that both mean O_2 consumption and mean CO_2 production rates during activity were significantly lower during artificial hibernation. Mean respiratory exchange ratio did not differ between seasons, suggesting similar patterns of substrate use to fuel physical activity in each season. To determine if seasonal differences in aerobic capacity result in seasonal differences in locomotor performance, we also compared the thermal sensitivity of crawling speed and righting time between seasons for seven *C. bottae* at each of three test temperatures (7, 16, and 25°C) using a full repeated-measures design. Crawling speed was measured along a one-meter racetrack, and righting time was determined as the time required for subjects to right themselves after being rotated 180º onto their dorsal sides. We found that mean crawling speed was significantly slower during artificial hibernation at 16 and 25°C, but did not differ between seasons at 7°C. Mean righting time was significantly longer in duration during artificial hibernation across all test temperatures. Taken together, these results are consistent with the hypothesis that decreased aerobic capacity is associated with decreased locomotor performance during hibernation when snakes are generally inactive.

TESTING OF INNATE IMMUNITY STIMULATION AS A METHOD TO AMELIORATE AD PATHOLOGY IN NON-HUMAN PRIMATES

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Alzheimer's Disease (AD) is the most common cause of dementia characterized by the presence of parenchymal amyloid-β (Aβ) plaques, cerebral amyloid angiopathy (CAA) and neurofibrillary tangles. Genome-wide association studies have demonstrated the importance of macrophage and microglia—the primary innate immune cells of the brain—in AD pathogenesis (Karch et al., 2014). Prior work has showed that stimulation of innate immunity with CpG ODN can reduce plaque pathologies without causing toxicity in mouse models based on cytokines, the molecules inciting an immune response (Scholtzova et al., 2009). Long-term safety of a well-characterized immunotherapeutic drug, TLR9 agonist CpG ODN 2006 (cytosine-phosphate-guanine oligodeoxynucleotides) is assessed in aged squirrel monkeys (SQMs) using peripheral cytokine concentrations. SQMs are small New World primates with cerebrovascular and immune systems similar to those in humans. An important feature is that cerebral amyloid deposition in SQMs has a predilection for abundant CAA and low levels of parenchymal Aβ deposition, supporting SQM as a translational model for Alzheimer's Disease. Hence, these exciting non-human primate data indicate that long-term treatment with TLR9 agonist CpG ODN results in amelioration of CAA and cognitive improvements in aged SQMs without inducing adverse events. Overall, these extensive preclinical research findings suggest that this innovative immunomodulation is effective at reducing all cardinal AD related pathologies without toxicity in multiple experimental models of AD. This study supports the viability of CpG ODN 2006 as a cure for Alzheimer's Disease and would have a significant chance of achieving clinical efficacy.

THE ROLE OF CANNABINOID 2 RECEPTOR IN MODULATING MICROGLIA ACTIVATION AFTER A TRAUMATIC BRAIN INJURY

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Traumatic brain injury (TBI) occurs when a sudden trauma is applied to the head and causes damage to the brain. TBI can result from a multitude of events including most commonly from sports injuries, vehicle collisions, violence, falls, and war. It is estimated that there are 1.4 million cases of TBIs in the USA every year. Injury can result in permanent disabilities and in severe cases it can be fatal. Symptoms after a TBI can be mild, moderate and severe depending on the extent of brain damage as well as location. Long-term behavioral effects can be characterized including depression, anti-social behavior, and fear/anxiety. Additionally, TBI injuries have shown symptoms that are closely related to Parkinson's and Alzheimer's like-symptoms. Currently, there are no specific treatments for a TBI injury. TBI occurs in two phases, the primary injury (physical aspect of the injury) and the secondary injury which consists of cellular process activated hours, days, and months after the initial injury. Neuroinflammation arising during the secondary injury can lead to neuronal death and involves the activation of microglia. The Endocannabinoid system (ECS) consist of two major receptors CB1 and CB2, including the endocannabinoids that activate these receptors and the enzymes involved in their synthesis and degradation. Previously published *in vitro* data indicates that activation of CB2 receptors in microglia decreased the production of pro-inflammatory factors; thus expression of CB2 receptor in microglia may play a role in the modulation of the immune response. This research evaluated the role of microglia activation after TBI by using CB2 receptor knockout mice (Cx3-Cnr2) which would not express the characteristic neuroprotective effects on local neural circuits. The mechanism of action in which this occurs is not fully understood. We found that Cx3-Cnr2 mice show little to no difference compared to control mice.

SUSTAINED RELEASE OF HISTAMINASE ENCAPSULATED IN NANOCOMPOSITES MAY BE BENEFICIAL IN TREATMENT OF SKIN ALLERGIES

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Histaminase (diamine oxidase, DAO) is a copper oxidase, which catalyzes the oxidative deamination of histamine and other biogenic amines to corresponding aldehydes, ammonia and hydrogen peroxide. Besides its protective effect in cardiac patients and in intestinal ischemia, histaminase is important in reducing tissue inflammation due to an increase in allergenic species, and even as an antineoplastic agent (in tumors associated with high histamine levels). Low levels (sometimes associated with low activity) of DAO may exacerbate pain and inflammation due to histamine accumulation. Dry skin, eczema and pruritus which affect a large segment of the general population may be favored by local but also by systemic immune response to biogenic amines and would benefit from topical applications of histaminase as would benefit psoriasis patients for whom there is no known cure. The problem is that the *stratum corneum* allows only small, lipophilic molecules to be absorbed through the skin and DAO, a protein, is a big amphoteric molecule.

We used a biopolymer (polymeric 2-amino-2-deoxy-β-D-glucan formed through 1→4 glycosidic bonds) as delivery vehicle for DAO to the skin. It was chosen because it is inexpensive (prepared from chitin obtained from crab/shrimp), biocompatible, biodegradable, mucoadhesive, and it can be easily converted into nanoparticles using green reagents and procedures. The high surface to volume ratio and its own biological activity (antibacterial and antifungal agent) make it a good ingredient in formulations for the skin. Due to the high number of people suffering from seafood allergies we used another type of chitosan as well, prepared using chitin from a fungal source.

Chitosan nanoparticles encapsulating DAO from porcine kidney were prepared by ionotropic gelation (using sodium tripolyphosphate as crosslinker). All nanoparticles were characterized by: encapsulation efficiency, loading capacity, ratio of residual amino groups (obtained by colloidal titration), FTIR spectroscopy, and scanning electron microscopy (SEM). Nanochitosan obtained from fermentation showed a lower loading capacity but higher encapsulation efficiency. The two types of chitosans were evaluated as starting materials for nanosized matrices encapsulating a protein (in terms of residual enzyme activity).

A water-based formulation to be used in topical applications for skin conditions was prepared and nanoparticles encapsulating DAO were included in the recipe. Kinetic studies for the protein release from nanoparticles were conducted over one week period together with DAO activity assays. The percent release of histaminase from the nanochitosan prepared from marine sources was higher by an order of magnitude. The kinetics of the release was studied also on the composites included in the formulation for skin treatment. The stress due to the encapsulation on DAO activity and the influence of the diffusion on enzyme activity are discussed.

CANNABINOID INTERACTION WITH THE CB1-RECEPTOR

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Cannabinoids have shown the capacity and ability to treat numerous diseases and ailments such as pain, grand mal epileptic seizures, anxiety, and migraines. These small molecules interact with known cannabinoid receptor sites, labeled cannabinoid 1 (CB1) receptor and cannabinoid 2 (CB2 receptor). These cannabinoids can function as either an agonist, inverse agonist, or antagonist. Although their function is known the reason why cannabinoids bind as either an agonist, antagonist, or inverse agonist is not. Using a series of bioinformatic tools our researchers began to investigate this question for the CB1-Receptor. We have done this by obtaining the recently crystallized CB1-Receptor, replicating the docking, and comparing it to the known crystal structure[1][2]. This allowed researchers to analyze how agonist binding cannabinoids and inverse agonist/antagonist binding cannabinoids interact with the CB1-Receptor site. This information will help us determine why cannabinoids induce different effects on their consumer based on the examination of key amino acid residue interaction. The results have began to provide us with a guide as how to construct better cannabinoids and determine how an unknown cannabinoid will function.

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CONVENTIONAL FMOC SOLID-PHASE SYNTHESIS, BIOCONJUGATION AND CHARACTERIZATION OF CANCER-TARGETING PEPTIDES

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Anti-cancer peptides and their bioconjugates have played pivotal roles in the progression of cancer detection and treatment methods. In spite of their potential, their lack of specificity to cancer cells leads to the many undesirable side effects. In an effort to overcome this limitation, cancer-targeting peptides (CTPs) have been developed and applied to the treatment of a wide range of cancers. They have not only served to improve detection and treatment of a wide range of cancers but have also served to address the issues related to specificity. In our research program, we have developed a wide range of CTP combinations in an effort to improve their anti-cancer and drug-like properties. For example, a cell-penetrating nucleolipid-peptide bioconjugate was found to exhibit cell apoptosis in a selected panel of non small cell lung carcinoma [1]. In our current study, we have explored conjugating the pro-apoptotic peptide with a cancer-targeting sequence for potential anti-cancer applications in tumors that overexpress the Glucose Regulated Protein of 78 kilodaltons on the cells surface [2]. The Glucose Regulated Protein of 78 kilodaltons (GRP78) is a chaperone protein which exists within all mammalian cells, however, it is uniquely presented on the surface of cancer cells where it signals tumor activity. In a related application, a small series of peptides were derived from the binding site epitope of B7-H6 [3]. B7-H6 is a tumor antigen for NKp30-dependent immunostimulatory activity of NK cells, which ultimately leads to the eradication of B7-H6 presenting tumor cells. In a related strategy, we've developed a series of peptides designed to target B7-H6 presenting tumors, leading to potential cancer-targeting applications. Lastly, the development of a new class of synthetically modified Peptide Nucleic Acids (PNAs) will provide entry points into cancer-targeting, gene delivery and gene silencing activities [4]. In sum, this presentation will highlight our most current research progress towards the solid-phase synthesis, characterization and anti-cancer applications of a selected panel of cancer-targeting peptides.

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INVESTIGATING IONIC LIQUID EFFECTS ON TRP-CAGE STABILITY

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Room temperature ionic liquids (ILs) are known to have a variety of applications in biological systems due to their highly tunable physical and chemical properties. However, the number of possible cations and anions that can be used in ILs also presents a challenge in that the selection of a specific IL for a desired application typically involves a guess-and-check approach. Here we present the results of microseconds of all-atom molecular dynamics simulations of the small, fast-folding miniprotein Trp-cage in 13 different ILs, in order to develop an atomistic understanding of how the molecular characteristics of a cation/anion pair can influence protein structural stability. Trp-cage was chosen because it has been extensively studied computationally, and is quite stable under standard conditions in aqueous solution.

For this work we chose four cations ([BMIM], [EMIM], [CHO] and [TMA]) and three anions ($[Cl^-]$, [DCA] and $[Tf_2N]$) from which we constructed all possible IL combinations and simulated all twelve permutations. We also studied the IL $[C_4mpy][Tf_2N]$ because our group has simulated Trp-cage in this ionic liquid in the past. Thirteen 1 μs simulations of the folded Trp-cage protein in low concentration IL were conducted, in addition to a control simulation of Trp-cage in water. The stability of Trp-cage was assessed by analyzing various structural qualities of Trp-Cage, including the root mean squared deviation of the Trp-cage backbone atoms, secondary structure, the radius of gyration and distances between key residues in the protein. We used the Principal Components Analysis (PCA) method to discern the major types of motion exhibited in the molecular dynamics simulation. Our initial results indicate that the ILs $[BMIM][Tf_2N]$, $[EMIM][Cl^-]$, [TMA][DCA] and $[C_4mpy][Tf_2N]$, have larger destabilizing effects on Trp-cage structure than the other ILs, where the behavior of Trp-cage resembles that observed in water. Finally, we calculated the radial distribution functions for cations and anions to each residue in Trp-cage to investigate how IL components associate with the protein. From this analysis, we found that ILs containing the anions $[Tf_2N]$ and [DCA] more closely approached Trp-cage residues than the cations.

EXPLORING THE ROLE OF DISULFIDE BONDS IN A COMP/DNA COMPLEX

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Type IV pili (T4P) are long protein filaments that protrude from the surface of bacterial cells and are assembled from monomers called "pilins." T4P serve many functions for bacteria, including the uptake of DNA from their environment. This is enabled by a "minor" type IV pilin known as ComP. ComP aids in the recognition of double stranded helical DNA by binding to a specific DNA uptake sequence (DUS). A recent computational model of the ComP/DNA complex from *Neisseria subflava* has provided insights into which amino acids of ComP are most important for stabilizing the protein/DNA interface. However, the static docked model does not provide any information into the dynamic motions of the ComP/DNA complex.

In this work, all-atom molecular dynamics simulations using the AMBER16 software on GPUs is used to study the ComP/DNA complex. These simulations aid in determining which interactions between ComP and DNA are most critical for overall stability. In particular, the ComP protein includes two disulfide bonds which help to hold together the "DD" region of the protein. This region's importance for DNA recognition and binding has been previously reported, indicating that both disulfide bonds are essential for ComP to remain stably bound to DNA. This notion is evaluated by carrying out molecular simulations of the wild-type ComP/DNA complex and comparing them to simulations in which the disulfide bonds have been removed. Analysis of the stability of the complex after simulation includes quantifying properties such as backbone root mean square deviations, amino acid and nucleotide root mean square fluctuations, and distances between DNA and critical amino acids in the DD region of ComP. Interaction energies and hydrogen bonding interactions between ComP and DNA are also calculated. The MM-PBSA method with alanine scanning is specifically used to investigate how individual amino acids in ComP mutated to alanine impact the binding free energy between the components of the complex. From these analyses, it was determined that removing the disulfide bonds has a dramatic effect on the stability of the ComP/DNA complex compared to the wild-type system.

ETHYLENEDIAMINETETRAACETIC ACID AS AN INHIBITOR OF ALKALINE PHOSPHOTASE

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Ethylenediaminetetraacetic Acid (EDTA) is a versatile molecule with many uses both in medicine, and in industry. EDTA is used in the body as a chelating agent that binds to substances to remove them from our body. The primary targets for EDTA removal through urine are metals ions of calcium and iron. EDTA can be administered via an oral form or be injected into the body via IV. (1)

Alkaline Phosphatase (ALP) is an enzyme most often found in the liver and its function is to help break down proteins in the body, along with being able to check the body for liver or bone disease. Levels ALP are kept at a stable level by the flow of bile in the body. If the body experiences a sudden change in the normal levels of ALP, this could be an indication of liver disease or bone disorder. (2)

EDTA is a known inhibitor of ALP. The purpose of this research was to determine if EDTA exhibits competitive, non-competitive, or uncompetitive behavior using the Michaelis-Menten model to enzyme kinetics. Using APL from bovine intestinal mucosa, results indicate that EDTA is a non-competitive inhibitor of APL. (3)

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EXAMINATION OF BORIC ACID DERIVATIVES AS ANGIOTENSIN CONVERTING ENZYME INHIBITORS

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The angiotensin-converting enzyme (ACE) is of the upmost importance to maintain homeostasis in the human body as it primarily functions to maintain the body's blood pressure. However, ACE doesn't always work ideally, and hyperactivity of ACE may lead to hypertension—a condition that is becoming more common amongst developing nations. Due to the prevalence, researchers have created and found many ACE inhibitors (ACEi's); current ACEi's work less than optimally and cause many side effects, which is why there is an ongoing need to find a more proficient ACEi. Typically, presumed ACEi's are tested in assays with ACE and a substrate. In this study, 10 boric acid derivatives were tested in an enzymatic detergent based assay to evaluate how well they inhibit ACE. The ACE was extracted from rabbit lung acetone powder and hippuryl-histidyl-leucine (HHL) acted as the substrate. Five boric acid derivatives tested showed potential inhibition towards ACE.

BINDING INTERACTION OF NANOCERAMICS (METAL OXIDES) WITH HUMAN SERUM ALBUMIN

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Nanomaterials are defined as materials with at least one external dimension in size range of approximately 1-100 nanometers. The extremely fascinating and useful properties of nanomaterials make them versatile materials in various fields of science, ranging from material science, energy, to medicine. Knowledge on the interactions of nanomaterials with different biomolecules is limited hence this study was conducted. The interaction of nanoceramics (aluminum oxide, silicon oxide, titanium oxide and zinc oxide) with human serum albumin (HSA), the most abundant protein constituent of blood plasma, was investigated by various spectroscopic methods (absorbance, fluorescence, and circular dichroism). Results showed aluminum oxide significant changes in terms of reduced absorbance and emission and change in the CD profile in comparison to the other nanoceramics. Absorbance reduction in samples with silicon oxide was also observed. In addition to the reduction of emission intensity in all samples with metal oxides, a peak was observed to arise around 420 nm for zinc oxide and 410 nm for aluminum oxide and silicon oxide when more amount of nanomaterials were added.

ENZYME CATALYST FOR POLYSTYRENE

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Plastics such as polystyrene resist degradation, making them environmentally deleterious. A wide variety of peroxidases, such as those produced by the gut bacteria of meal worms, bind to and degrade polystyrene and thus show promise in remediation of this persistent pollutant. Due to the chemical similarity between lignin and polystyrene, lignin binding peroxidases are particularly likely to degrade polystyrene. Proteins capable of binding lignin are known to have large hydrophobic patches on their surfaces. We report our progress in using homology modeling to systematically identify peroxidases with large, surface hydrophobic patches. We anticipate that lignin binding peroxidases thus identified will be promising starting points for engineering readily expressed, stable and active enzymes catalyzing polystyrene degradation.

3D PRINTING OF NANOMATERIALS FOR APPLICATIONS IN MEDICINE AND CATALYSIS

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In this work, we have been able to show that the silane n-(2-aminoethyl)-3 aminosilanetriol (2-AST) is capable of stabilizing noble metallic nanoparticles without using other external reducing agents. [1] Our goal is to create hybrid polymer systems, which also have varied amounts of nanoparticles nucleated in them. With these systems, we are investigating such these materials for real life applications in the field of 3D printing. Our working hypothesis is that we are exploiting the properties of hybrid polymers on a nanoscale to create devices with tiny features that is impossible to synthesize through a more macro scale. We plan to create inexpensive methods to prepare catalysts, support strong fibers, and synthesize medical devices. [2] In our approach, the methodology focuses on the simplicity and inexpensive starting materials with results of high-end utility of the products.

Sonochemistry has been used extensively in industry for various applications from emulsifying biphasic systems, catalysis to quality control for assembly lines in part to its high throughput and quick reaction rate. In this presentation, our research into the sonication chemistry of gold and silver nanoparticles (AuNP's/ AgNP's), which serve as a nucleating agent with the presence of these Si-H containing polymers such as polymethylhydrosiloxane (PMHS). This polymer can enhance the production of unique nanocomposites under mild conditions. We will present our investigation of this new idea where we have been able to create and establish heterogeneous fibers containing metallic nanoparticles that form at the top of the reaction, which is easily separated from the rest of the solution. We will present our results of these studies and the detailed characterization of obtained products using NMR, TEM, SEM, FT-IR, Raman, TGA and UV-Vis techniques.

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$NiO-Al_2O_3$ OXIDES FROM SOL-GEL SYNTHESIZED TAKOVITES

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Layered double hydroxides (LDHs) are very interesting for their industrial applications in the field of heterogeneous catalysis and the purification of water containing organic and inorganic waste anions. Catalytic applications of the LDHs, used mainly as calcined forms, have been reported for several reactions, such as basic catalysis (polymerisation of alkene oxides, aldol condensation), reforming of hydrocarbons, hydrogenation reactions, oxidation reactions and support for Ziegler-Natta catalysts. Owing in part to their anion exchange properties, certain LDHs are useful materials for pollution prevention, waste cleanup and have properties suitable for the in situ remediation of contaminated soils.

A series of Ni-Al LDHs $[Ni_{1-x}Al_x(OH)_2](CO_3)_2 \bullet mH_2O$ have been synthesised by the sol-gel method. The oxidic forms obtained by calcination of LDHs at 450ºC and 900ºC, respectively were structurally investigated using X-Ray diffraction, IR and UV-VIS spectroscopy. In addition, temperature programmed reduction (TPR) led to a good identification of the oxidic forms. By performing TPR experiments combined with isothermal reduction, it was concluded that the oxides obtained at the two calcination temperatures contained the same type of oxidic phases identified for oxides derived from coprecipitated LDHs, although the difference consists in the different reducibility of the Ni(II) ions. The reactivity of the systems obtained by heat treatment of the sol-gel Ni-Al LDHs was greater than the reactivity of the oxides obtained in case of coprecipitated samples.

These different structural and textural properties of the sol-gel prepared LDHs and their derived oxides can encourage the development of the sol-gel process in synthesis of LDHs, for their application purposes, in catalysis and maybe, in the environmental processes.

TAILORABLE MESOPOROUS SOLGELS CATALYZED BY HALOSUCCINAMIDES

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Tailor-made mesoporous solgels are materials that have important applications as catalysts in organic transformations. By controlling the synthetic route, we are able to control some of the characteristics such as surface features and roughness. We are interested in creating functional silicon based platforms, which not only act as catalysts but also provide recyclability properties

In this presentation a synthetic approach for a multifunctional silicon molecule catalyzed with a halosuccinamide (NXS) is being described. Bis(trimethoxysilylpropyl)amine (2-TMESP) is polymerized and halogenated in a one step process in presence of a halosuccinamide (NXS). Halosuccinamides were added to the reaction mixtures as catalyst to provide materials of various texture and morphologies. The variation in the catalyst amount lead to gels of varying morphologies and amount of halogenated silicon centers with predictable stability. Structural and spectroscopic analysis of these samples was carried out by 29Si NMR, 13C NMR, 1H NMR, TEM, SEM/EDX, TGA, FT-IR and Raman techniques.

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STRUCTURE-BASED DESIGN OF MOLECULARLY IMPRINTED POLYMERS FOR G-QUADRUPLEX NUCLEIC ACIDS

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Nucleic acids containing guanine-rich sequences have the potential to form G-quadruplexes (G4). These higher-order structures have emerged as attractive targets primarily due to their overrepresentation in genomic regions directly participating in regulatory roles. G4 structures are composed of stacked G-quartets, each consisting of four guanines arranged in a cyclic planar Hoogsteen hydrogen-bonded array stabilized by monovalent cations, held together through negatively charged loops. G4 structures vary greatly in topology. Traditionally, the design of G4 binding ligands focused primarily on nucleic acid sequence specificity, our strategy shifts towards structure specificity, which we look to achieve by generating water-soluble molecularly imprinted polymer (MIP) biomimetic structures. Unlike conventional methods used for MIP preparation, we propose the introduction of G4 binding domains within synthetic polymers by use of G4-binding ligands as cross-linkers for nucleic acid binding polymers. Polyethyleneimine (PEI) is a cationic polymer, known for its high affinity towards nucleic acids, it forms polyplexes via electrostatic interactions, is cross-linkable, water-soluble and as a result has been selected as the imprinting polymer. Our previous investigations demonstrate that the high charge density of PEI induces conformational change to G4 structures upon binding. To maintain template topology, the charge density of PEI has been reduced. PEI (10 kDa) was acetylated with increasing amounts of acetic anhydride. The degree of acetylation of 1° and 2° amines was determined by a copper (II) UV-Vis assay and NMR spectroscopy. Native PEI and PEI partially acetylated at 25, 50, 75 and 100% was subsequently cross-linked using H_2mTCHePyP via EDC/sulfo-NHS carbodiimide coupling. Cationic porphyrins are well-known, non-specific, G4 binding ligands that contain large planar aromatic surfaces capable of π-stacking with G-quartets and cationic charges that interact electrostatically with polyanionic nucleic acids. H_2mTPyP was synthesized using a combination of Lindsey and Adler-Longo methods. Cationic porphyrins were prepared via *N*-alkylation yielding the quaternized pyridinium porphyrin cross-linker.

DEVELOPMENT OF NANOPOROUS THIN FILM SEMICONDUCTORS FOR SUN-DRIVEN WATER SPLITTING APPLICATIONS

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Hydrogen is an ideal renewable energy source that can be stored, transported, and can be converted into electricity using fuel cells as a clean energy source without producing CO_2.[1] Recently, sun-driven water splitting semiconductor materials have drawn considerable attention because they require only sunlight and water as their medium to produce hydrogen. Particularly, nanoporous semiconductor materials have been widely studied to improve performance in the field of energy conversion and storage applications because of their exceptional properties, including high surface areas, tunable pore sizes, and shape.[2] However, the preparation of nanoporous semiconductor materials involves multiple fabrication steps, such as template preparation, synthesis of target materials, and template removal. To tackle this, we have developed a simple one-pot fabrication of nanoporous MoS_2 and WS_2 thin films by incorporating polystyrene microspheres (500nm in size) as a template in molecular precursor solutions via self-assembly. Nanoporous semiconductor thin films were created after removing polystyrene microspheres by annealing process. Consequently, this one-pot solution synthesis not only provides a new synthetic route to create nanoporous materials, but also allows control of pore size by changing the size of the polystyrene spheres so that we can engineer the functionality of the semiconductor materials. Structural and optical properties of the synthesized thin film semiconductors were characterized by Power X-ray diffraction and UV-Vis spectroscopy, respectively. The surface morphologies of the synthesized thin films were investigated by Atomic Force Microscopy.

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SYNTHESIS OF BORANE-FUNCTIONALIZED POLYMERS FOR CATALYSIS APPLICATIONS

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The goal of our project is to develop new polymers that can serve as recyclable Lewis acid catalysts by incorporating highly Lewis acidic yet air-stable functional groups into their side chains. These borane-functionalized polymers will be explored in the metal-free hydrogenation of unsaturated organic substrates. The steric hindrance of the bulky Lewis-acid functional group is critical key for effective heterolytic cleavage of hydrogen. The unique and novel aspect of our design is that the polymeric catalyst can be recovered and reused through simple filtration, after completion of the catalytic process. Suitable monomers have been prepared and characterized by ^{1}H-NMR, ^{13}C-NMR, UV-Vis and GC/MS. They have then been subjected to ring-opening metathesis polymerization (ROMP).

PREPARATION AND PROPERTIES OF PROPYL MODIFIED ORGANIC–INORGANIC HYBRID GLASSES

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Melting gels (MGs) are silica-based hybrid gels. Unlike other gels, MGs are rigid at room temperature, but they can soften at 110°C. MGs are transformed into hybrid glasses (HGs) by thermal treatment at their consolidation temperatures. Once their consolidation temperatures are reached, the gels will no longer soften. Propyl-substituted MGs were prepared by the sol-gel method using propyltrimethoxysilane (PrTMS) and di-isopropyldimethoxysilane (DiPrDMS). Four different MG compositions were prepared between 80%PrTMS-20%DiPrDMS and 65%PrTMS -35%DiPrDMS. The consolidation temperatures increase from 135^{o}C for 80%PrTMS -20%DiPrDMS to 142^{o}C for 65%PrTMS-35%DiPrDMS. The thermogravimetric weight loss measurement coupled with differential thermal analysis indicated that the MGs decomposed in two steps with an exothermic effect at ~350^{o}C due to the combustion of the propyl groups. The glass transition temperatures (T_g) were determined using differential scanning calorimetry (DSC) and oscillatory rotational rheometry (ORR). The T_g determined by DSC decreases from -33.7 for 80%PrTMS-20%DiPrDMS to -56.5^{o}C for 65%PrTMS -35%DiPrDMS. According to ORR, at room temperature, the gels behave as viscous fluids, with a viscous modulus, $G''(t, \omega_0)$, that is larger than the elastic modulus, $G'(t, \omega_0)$. While decreasing the temperature, the moduli cross over, and this temperature is recorded as the T_g. The T_g values measured by DSC were confirmed by ORR. The structure of the HGs obtained by the consolidation of the MGs were studied using FT-IR, where the presence of C-Si bonds was evident in the spectra. The contact angle (θ) measurements show that the HGs have hydrophobic surfaces with $\theta \sim 90^{o}$.

COARSE-GRAINED MODELING AND SIMULATION OF TYPE IV PILI

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Type IV pili (T4P) are long biopolymers composed of many copies of the protein pilin. T4P are both strong and flexible and are found on a wide variety of microorganisms, including Gram-positive and Gram-negative bacteria, as well as archaea. It has been demonstrated experimentally that T4P can withstand extremely large tension forces (10,000 times the bacterial bodyweight), and under such force go through an extensive conformational change in which they become three times longer and 40% narrower. Interestingly, this transition is found to be fully reversible. However, a fundamental understanding of the great strength and flexibility of T4P is still not clear from the molecular perspective.

In this study, coarse-grained molecular dynamics simulation using the MARTINI force field are carried out for a T4P filament composed of 26 pilin subunits. The filament is extended at constant velocities ranging from 50 Å/ns to 0.1 Å/ns using steered molecular dynamics. These simulations allow the exploration of T4P extension under force at the molecular level of resolution. The overall extension of the filament, as well as the extension of highly conserved alpha-helical regions within each pilin subunit, are monitored. Specifically, the elongation of a disordered region within each pilin subunit alpha helix is measured in order to determine its contribution to T4P extension. Amino acid sequences which become exposed to the surrounding solvent as a result of T4P extension are also monitored. This analysis reveals the sequence EYYLN (residues 49-53 in a pilin subunit) becomes exposed, which is consistent with experimental observations. Identifying such sequences which become exposed in the elongated T4P conformation can inform the design of antibodies to specifically target these sites.

INHIBITION STUDIES OF NCI MOLECULES ON MMP-1 ENZYME BY FLUOROMETRIC ASSAY METHOD

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Matrix metalloproteinases (MMP) are class of zinc enzyme that are found abundantly throughout the body and play important role including degradation of Extracellular matrix components. MMP-1 inhibition has been associated with various diseases like cancer, ageing, etc. Our lab has previously reported MMP-1 inhibitors using computational screening and the inhibitors where examined against MMP-1 in the presence of detergent with colorimetric method. Here we report the same inhibitors but with a different method i.e Fluorometric method to confirm the observed inhibition with the colorimetric method.

ANALYSIS OF EXCITATION ENERGY TRANSFER IN PIGMENT-PROTEIN COMPLEXES WITH PyFREC SOFTWARE

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Discovery of fundamental mechanisms of photosynthesis and further advancements of solar cell technology requires the understanding of kinetics of electronic excitations and associated excitation energy transfer (EET) in pigment-protein complexes. Electronic couplings (EC) and rates of EET in pigment-protein complexes have been calculated and analyzed based on the Förster theory, analyzing the resulting spectral overlap of donor emission and acceptor absorption. The calculations have been carried out with the PyFREC (Python Fragment Electron Coupling) software which enables evaluation of EC and EET in a complex molecular system by splitting the system into individual coupled fragments (e.g., bacteriochlorophylls) based on their molecular geometry. UV-Vis spectral analysis was also carried out with TD-DFT methods on each fragment using Gaussian09 software to calculate the twenty lowest singlet excited states of each bacteriochlorophyll molecule of study. The information derived from each calculation is necessary in understanding the photosynthetic nature of each pigment-protein complex.

DYNAMICS OF TYPE IV PILI IN PERIODIC SIMULATIONS

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Type IV pili (T4P) are protein filaments that emanate from the surface of bacteria, and are comprised of many copies of a protein called pilin. T4P are implicated in bacterial adhesion to other surfaces and host cell infection. Recently, the highest resolution structures to date of several T4P were solved by a combination of cryo-EM and x-ray crystallography. In this study, we run molecular dynamics simulations of periodic T4P filaments to achieve the most accurate representation of a T4P in its biological environment, and to understand their great flexibility and strength. Molecular dynamics simulation provides insight into T4P structure and dynamics that cannot be obtained from simply investigating the static structures of these filaments. Specifically, we have performed a comparative analysis of T4P from the organisms *Neisseria meningitidis* and *Neisseria gonorrhoeae*. T4P from both of these organisms exhibit high structural similarity. Therefore, there is interest in exploring their dynamic differences in similar solvent environments. Approximately 1 microsecond of simulation is being carried out on each of these high resolution T4P models. The information obtained from these simulations can be applied towards understanding how T4P interact with one another and with their environment to successfully adhere to and infect other cells. The supercomputer ELSA at The College of New Jersey's High Performance Computing Center is being used to perform these simulations.

SIMULATING PILIN/DNA INTERACTIONS WITH MOLECULAR DYNAMICS

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One mechanism for the acquisition of DNA from the environment by bacteria is through the use of long, protein filaments called type IV pili (T4P) which emanate from the surface of bacterial cells. T4P are capable of binding DNA due to the presence of the minor pilin protein ComP within the filament. The ComP protein exhibits a number of basic amino acids that favorably interact with specific sequences of nucleotides called DNA uptake sequences (DUSs). In this work, the dynamics of the ComP/DNA complex are studied and the interactions important for strong binding between ComP and DNA are analyzed using all-atom molecular dynamics simulation. The analysis focuses on the ComP/DNA complex wild-type system, and several mutants, including K30A, K56A, K94A, and R107A. Mutation sites were determined using prior NMR results as well as calculations of interactions between ComP amino acids and DNA nucleotide bases. The effects of mutating the protein on the free energy of binding were calculated using the MM-PBSA alanine scanning method. Additionally, the stability of the protein/DNA interface was monitored by measuring the distances between protein amino acids and DNA nucleotide bases. Several structural properties of the protein and DNA were monitored, including the backbone root mean square deviations, DNA sugar puckering angles, and orientation changes of the DNA on the protein. The simulations provide support for the presence of multiple binding orientations for the DNA on ComP in the wild-type state, and demonstrate that ComP remains effectively bound to DNA in the case of single amino acid point mutations over the simulated time scales.

MOLECULAR DYNAMICS SIMULATION ON A MIXED SOLVENT SYSTEM

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A protein's cooperativity describes how the binding of a ligand at one site alters the affinity for ligands at other binding sites. This property is most well-known in the interaction of hemoglobin with oxygen, where affinity becomes stronger as the binding sites fill up. To gain insight into cooperative behavior, we have studied a simplified model, a synthetic crown ether1 that binds to a cation, in methanol-water solution using molecular dynamics (MD) simulation. Previous nuclear magnetic resonance experiments2,3 suggested that this solvent displays two types of water behavior even in the absence of the crown or cations. By conducting MD simulations on the methanol-water system, we aimed to understand the underlying reasons for this irregularity and its effect on binding by the crown. Using the freeware program GROMACS (GROningen MAchine for Chemical Simulations), we analyzed interactions between methanol and water molecules in a small virtual box for three formulations of the solvent with water concentrations of 20%, 5%, and 2.56%. The results of these simulations will be presented and discussed.

HOPPING-TYPE MODIFICATIONS OF QUANTUM INTERFERENCE CONDITIONS IN NANOSCALE THERMAL JUNCTIONS

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We examine quantum processes of heat (energy) transfer as carried by electrons transfered between two metallic heat reservoirs (thermal baths) via the system of coupled quantum dots in several interesting configurations, where quantum interference effects become essentially important. Our investigations are based on the hypothesis that quantum interference effects may be used to control nanoscale heat conduction. Our computational method is based on Landauer formula for heat flux expanded into Taylor series with respect to temperature difference in order to obtain expressions for thermal conductance and its nonlinear correction in terms of transmission probability function. The connections with heat reservoirs are treated within the Newns-Anderson model with semi-elliptical density of electronic states. Our results are discussed with respect to average temperature, resonant states, and specific hopping-like parameters characterizing connections between quantum dots and thermal baths.

Key Words: Quantum Transport, Quantum Interference, Nanoscale Thermal Devices, Landauer Formula, Non-Equilibrium Quantum Thermodynamics.

THE CAGE EFFECT: IONIC LIQUIDS MODIFY MEMBRANE PERMEABILITY

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Room temperature ionic liquids (ILs) have been proven to have a wide range of biological applications, from influencing protein folding and structural stability, to affecting enzyme activity, to modifying the permeability profile of lipid bilayers. In this work we use all-atom molecular dynamics simulations to study the effects of the ionic liquid choline geranate (CAGE) on lipid bilayers composed of POPE and POPC lipid types. CAGE was chosen based on previous experimental work that demonstrated this IL is effective at eradicating bacterial biofilms and at increasing the permeability of the biofilms to several antibiotics.

Our group previously carried out simulations of lipid bilayer assembly in the presence of CAGE, which demonstrated that the geranate and geranic acid components of the IL embed in the lipid bilayer, while choline predominantly remains in the aqueous phase. These assembly simulations are further supported by the results of enhanced sampling simulations, which demonstrate that geranate and geranic acid have smaller energetic barriers for entering the lipid bilayer environment compared to choline. Here we extend this previous work by employing enhanced sampling methods to analyze the transport of a sample drug across the model lipid membranes. Specifically, we run umbrella sampling (US) simulations to calculate the free energy profile of mannitol as it moves across the membrane. US simulations are carried out in both pure POPE and POPC bilayers, as well as POPE and POPC bilayers with CAGE present. Initial results indicate that the presence of CAGE decreases the free energy barrier for mannitol transport across the bilayer, supporting experimental evidence that shows that the presence CAGE increases membrane permeability to several small pharmaceuticals. The protocol developed for studying mannitol transport through lipid bilayers in the presence of CAGE can be applied to more complex pharmaceutical compounds relevant to the treatment of skin infections, such as trimethoprim and ceftazidime. The long term goal of the project is to screen a large number of possible combinations of small drugs and ILs to determine which is best suited for a given pharmaceutical need.

AUTHOR INDEX

AUTHOR	PAGE #	AUTHOR	PAGE#
Abboud, Alan	30	Domena, Justin	75
Adams, Faith	115	Dougherty, Catherine	98
Alb, Josh	116	Durda, Agata	48
Almouallem, Belal	30	Durosier, Louis	25
Ampomah, Natasha	124	Eita, Mohamed	34
Arias, Cristian	58	Eldabagh, Reem	35
Ashby, Christina	31	Embaby, Shayma	125
Bautista, Anthony	128	Eskow, Nicole	36
Bell, Eve	39	Espinosa, Aldrick	90
Biskup, Ksawery	40	Fairfield, Maria	119
Bogin, Bryan	131	Falotico, Sarah	37
Buendia, Dara	106	Farnan, Julia	133
Bustamante, Marjory	99	Fasano, Thomas	61
Calalpa, Brenda	74	Fatima, Syed	132
Chaimov, Diana	41	Finch, Jeffrey	32
Cheb Terrab, Dominique	42	Foster, Michelle	109
Cheng, Sandy	107	Furnari, Julia	53
Choudhary, Dinesh-Amaram	132	Geczo, Alexandra	62
Clarke, Chelesia	93	Gillan, Grant	133
Cole, Alicia	43	Gillot, Tamara	106
Cooley, Danielle	49	Golod, Arielle	127
Courtright, Trevor	44	Gomez, Fernando	120
Cowie, Christopher	32	Gomez, Sofia	99
Cruz Herrera, Yuliana	46	Goncalves, Rebecca	134
Currie, Michelle	59	Granda, Carla	25
Dager, Kevin	108	Gutierrez-Zuniga, Oscar	63
Dandash, Myar	41	Hacopian, Alexa	60
Darwich, Andrieh	117	Hammouda, Mariam	24
DeAlmeida, Rita	47	Hapatsha, Tatiana	74
Degen, Austin	40	Harty, Roshena	67
Deschaine, Megan	33	Holganza, Ma Veronica	110
DeSouza, Matteus	118	Hoganza, Maria Katrina	76 & 82
Djambozova, Katerina	60	Jacob, Amber	49

AUTHOR INDEX

AUTHOR	PAGE #	AUTHOR	PAGE#
Janusz, Jordyn	68	Neri, Kristina	121
Kamen, Emma	54	Neumann, Allison	93
Khamis, Noel	111	Nguyen, Tran	78
Khan, Marjan	100	Nieves, Samantha	55
Kline, Christi	91	Nissenbaum, Marialaina	45
Klinkerth, Jenique	101	Nolan, Tyler	122
Kuhlman, Laura	125	Noor, Mah	129
Lim, Eujin	102	Nowakowski, Aidan	52
Longia, Gurjeet	69	Nuno, Angela	103
Longia, Gurpreet	126	Patel, Keyur	135
Longo, Tiffany	92	Patel, Mansi	80
Lopez, Laura	77	Pavia, Ashley	64
Louis, Jennifer	99	Peppers, Jaquill	124
Macri, Christine	112	Persaud, Rudra	104
Magro-Machado, Katina	70	Plattel, Richard	94
Maldonado, Jessica	115	Quimby, Karisa	95
Mancuso, Molly	25	Ramani, Margish	113
Martelino, Leandro	26	Ramirez, Stephanie	105
Mautz, Clint	91	Reilly, Lauren	65
Mejia, Nelson	35	Reiss, Brian	96
Mizvesky, James	127	Reynolds, Elizabeth	85
Moallem, Elika	95	Rock, Melissa	79
Monsky, Richard	52	Rodriguez, Alexandra	72
Monzo, Christopher	50	Rohani, Tameh	28
Mora, Kevin	38	Rollanda, Bernadin	29
Morozova, Anastasia	128	Sahin, Medine	130
Mosley, Zachary	67	St. Amant, Chiara	80
Mowla, Shoron	83	Saleh, Yousif	66
Munoz, Jose	27	Schaffer, John	60
Muralidharan, Koushik	84	Schardien, Kayla	59
Murphy, Kyle	51	Silva, Andrea	86
Musli, Vivien	71	Sivetz, Nicole	87

AUTHOR INDEX

AUTHOR	PAGE #	AUTHOR	PAGE#
Soman, Eshaan	136	Uribe, Arladna	88
Soman, Manasi	56	Vaccaro, Kyle	51
Sumner, Rawlric	73	Vera, Sebastian	89
Tahir, Tehreem	97	Vidal, Lothar	39
Tonn, Hunter	137	Vogt, Kristen	138
Torres, Juan	81	Webber, Nakoa	61
Tran, Brandon	57	Yekanifard, Nazila	123
Tuladhar, Pragun	60	Zamora, Maria	114

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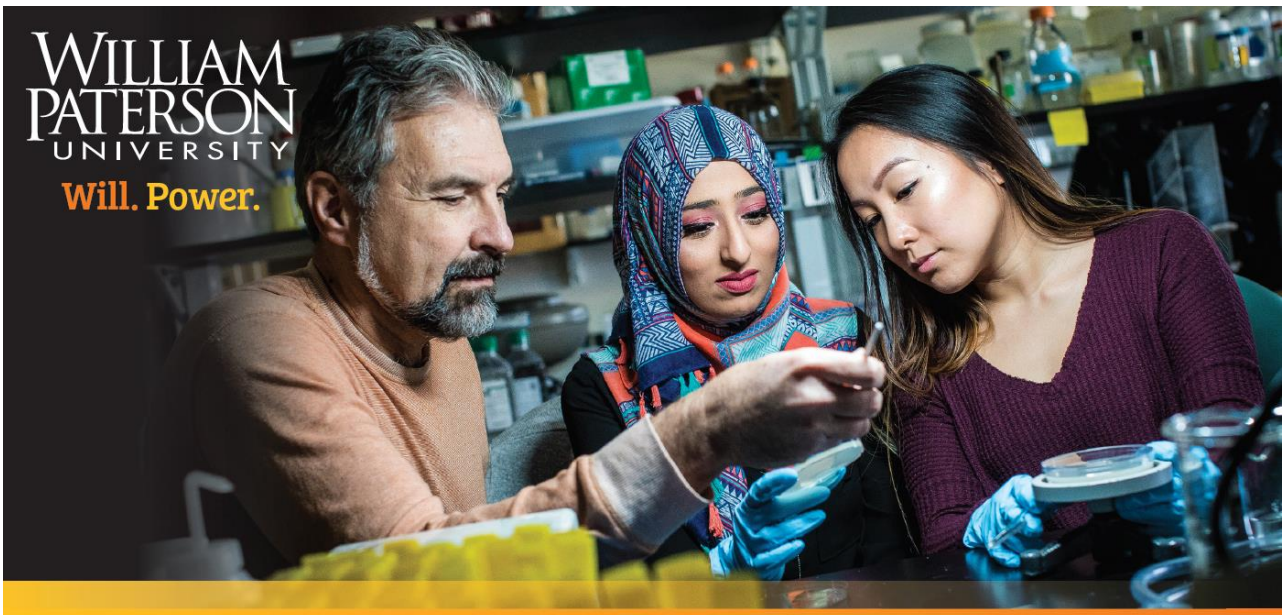

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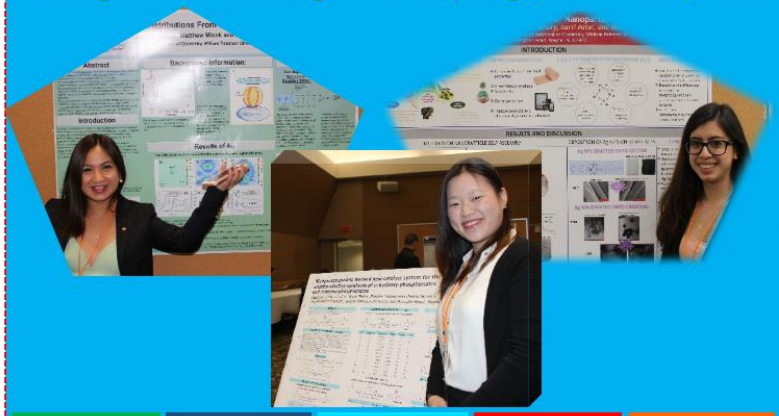

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