



William Paterson University

Biological and Chemical Sciences

SATURDAY, APRIL 11, 2015
300, POMPTON ROAD, WAYNE, NJ-07470

Program and Abstracts

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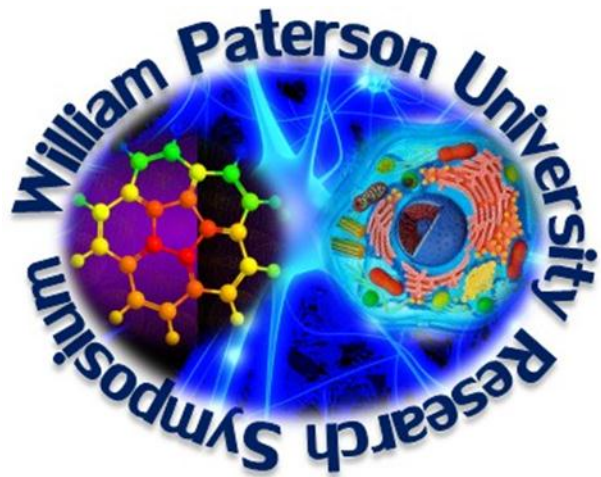


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HISTORY OF THE SYMPOSIUM

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 WPUNJ campus for students in biological and chemical sciences. In this event, undergraduate students present and display their research and creative work to the university and the scientific community from the Tri state area. This symposium provides an opportunity to the students to showcase their talents and share their research achievements with their peers from about twenty universities from Tri state area. The students and faculty from different universities as well as staff, and community members of WPU are invited to explore the latest in undergraduate research. Featured events include the poster presentation and Awards ceremony. The Symposium also features a keynote lecture by a distinguished researcher.





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. Mihaela Jitianu
Dr. Mukesh Sahni
Ms. Karyn Lapadura



SCHEDULE OF EVENTS

- 8:00 a.m. - 9:00 a.m.** **Registration & Breakfast**
Ballroom
- 9:00 a.m. - 9:15 am** **Welcome and Opening Remarks**
Dr. Warren Sandmann
Provost & Sr. VP for Academic Affairs
- 9:30 a.m. - 11:30 a.m.** **POSTER SESSION A**
Cell Biology I: CB 1 to CB 6
Ecology, Evolution & Environmental Science I:
E 1 to E5
Molecular Biology I: MB 1 to MB 6
Behavior & Genetics I: BG 1 to BG 7
Analytical & Theoretical Chemistry: A 1 to A 7
Materials Chemistry: MC 1 to MC 7
Biochemistry: BC 1 to BC 6
Inorganic Chemistry: IC 1 to IC 6
- 11:45 a.m. - 1:00 p.m.** **LUNCH**
Ballroom
- 1:00 p.m. - 2:00 p.m.** **PLENARY TALK**
Dr. Ilya Raskin
Distinguished Professor
Rutgers University



SCHEDULE OF EVENTS CONTINUED

- 2:00 p.m. - 4:00 p.m. POSTER SESSION B**
Cell Biology II: CB 7 to CB 11
Ecology, Evolution & Environmental Science II:
E 7 to E 14
Molecular Biology II: M B 7 to M B 12
Behavior & Genetics II: BG 8 to BG 13
Physiology: P 1 to P 9
Organic Chemistry: OC 1 to OC 6
Nanochemistry: N 1 to N 8
Computation Chemistry: CC 1 to CC 6
- 4:00 p.m. - 4:45 p.m. COFFEE & REFRESHMENTS**
- 4:45 p.m. AWARDS**

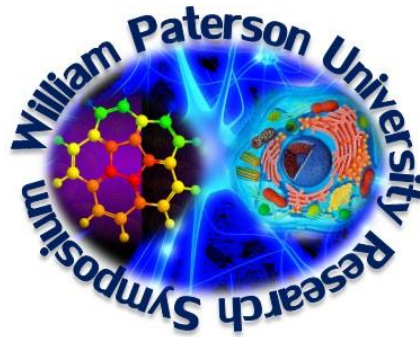


Cell Biology I

Judges: Dr. Joseph Spagna*
 Dr. Robert Benno
 Dr. Michelle Hersh

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*Coordinator



Ecology, Evolution & Environmental Science I

Judges: Dr. Michael Peek*
Dr. Karen Swanson

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Molecular Biology I

Judges: Dr. Carey Waldburger
Dr. Ted Brummel

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*Coordinator



Behavior & Genetics I

Judges: Dr. Kendall Martin*
 Dr. Harold Parzel
 Dr. Brian Olechnowski

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Judges: Dr. Mihaela Jitianu*
 Dr. Andrei Jitianu
 Dr. Natalyn Voloshchuk

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*Coordinator



Materials Chemistry

Judges: Dr. Suresh Sahni*
 Dr. Colin Abernethy
 Dr. Wei Yufeng

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***Coordinator**



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Judges: Dr. Parminder Kaur*
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Judges:

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Cell Biology II

Judges: **Alessandra Leri***
Dr. Olechnowski

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*Coordinator



Ecology, Evolution & Environmental Science II

Judges: Dr. Emmanuel Onaivi*
Dr. James Salierno

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*Coordinator



Molecular Biology II

Judges: Dr. Pradeep Patnaik*
Dr. Swayamjot Kaur

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*Coordinator



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Judges: Dr. Emily Monroe*
 Dr. Edith Myers
 Dr. Ish Kumar

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POSTER ABSTRACTS



PHYSIOLOGICAL PROPERTIES OF THE CAULOBACTER CRESCENTUS

Michael Bamimore and Dr. Eric Klein

Biology Department and Center for Computational and Integrative Biology,
Rutgers University, Camden, NJ

The variety of bacterial cell shapes and sizes found in nature are largely determined by the structure and composition of the peptidoglycan cell wall. The cell wall provides structure and shape to the cell and also protects it from osmotic forces. The general focus of our lab is the regulation of cell shape in *Caulobacter crescentus*. *Caulobacter crescentus* synthesizes a long thin stalk appendage at one pole that grows in response to phosphate limitation. The objective of this research is to characterize the differences in the stalk peptidoglycan versus the cell body peptidoglycan. The analyses will extend to identifying the proteins involved in the synthesis of the stalk peptidoglycan. In a preliminary study, we tested the lysozyme-sensitivity of cell body and stalk peptidoglycan. Interestingly, treatment with lysozyme resulted in the lysis of the cell body with the stalk unaffected. This experiment supports the hypothesis that the stalk produced by *Caulobacter crescentus* has a different peptidoglycan make-up than that of the cell body. Since the cytoskeletal protein MreB is known to regulate peptidoglycan synthesis in the cell body, we examined its role in stalk elongation. Using a novel MreB-GFP fusion protein, we determined that MreB localization to the cell pole is critical for stalk synthesis. Currently, we are using the MreB inhibitor A22 to disrupt MreB polymerization in order to determine whether MreB polymers have an effect on the stalk length of *Caulobacter crescentus*. Future studies will focus on the mechanism of MreB-dependent peptidoglycan synthesis in the stalk.

AN EMERGING ROLE FOR PIWIL1 IN NEOCORTICAL DEVELOPMENT

Ryan Kristopovich, Viljetic B, Dutra-Clarke M, Stillman A, Kraushar M, Arikala HM, Wijeratne HRS, Chen K, and Dr. Rokok Rasin
Department of Neuroscience and Cell Biology
Rutgers – Robert Wood Johnson Medical School
Piscataway, NJ

Neurons in the developing mammalian neocortex arise from multipotent progenitor cells called radial glia. Cells of this type first form lower neocortical layers before forming upper layers days later. This pattern appears to be critical for typical brain function, and disruption of glial mitosis or migration is associated with many neurological disorders. An important aspect of understanding neocortical development is to study its underlying molecular machinery. One of the cogs in the machine appears to be PIWI-like protein 1 (PIWIL1), a member of the Argonaute protein family. We show that, in mouse embryo brains, PIWIL1 is required for proper cell cycle dynamics and inside-out neuronal migration. We found that depleting PIWIL1 results in upper-layer neurons aberrantly located in deep layers at E18 and P7. In addition, in mice with the *Piwill* gene knocked out, we found neocortical circuitry to be disrupted, as evidenced by a thinner corpus callosum and aberrant dendrite formation. And bioinformatically analyzed microarray results found many genes regulated by PIWIL1 that are also associated with cell cycle, cell adhesion, transcription and migration in developing neocortices. All this suggests that PIWIL1, first found to be involved in germline functionality, also has a role in neocortical development and targets several other gene products.

ROLE OF GLUTAMATE RECEPTOR INTERACTING PROTEIN 1 (GRIP1) IN PSEUDOPHOSPHORYLATED CaMKII TARGETING INHIBITORY SYNAPSES

Giancarlo Perez*, Anthony Torres and Dr. Reed Carroll
The William J. Maxwell College of Arts and Sciences, Biology Department
New Jersey City University, Jersey City, NJ

The activity of neurons is controlled by a balance of signals from other neurons at excitatory and inhibitory synapses. This balance of excitatory and inhibitory signaling is highly important for information processing and in neuroplasticity. Ca(2+)/calmodulin dependent protein kinase II α (CaMKII α) can play a critical role in regulating the strength of both neuronal excitability and inhibition in response to different synaptic stimuli. Following strong glutamatergic stimulation, activated NMDA-type receptors strengthen excitatory synapses through CaMKII activation. With moderate NMDA activation, however, CaMKII strengthens inhibitory synapses. While the functions of CaMKII at excitatory synapses are well studied, it is not understood how CaMKII localizes to and regulates inhibitory synapses. This study first investigated whether Glutamate Receptor Interacting Protein (GRIP), found at inhibitory synapses strengthened by CaMKII, may act as a target to which activated CaMKII binds. HEK cell lines showed high levels of co-localization of transfected CaMKII/GRIP1 as did NMDA-treated neurons. Co-immunoprecipitation studies in HEK cells provide evidence for a direct interaction of active CaMKII and GRIP1. Additionally, knockdown of GRIP1 using si-RNA, reduced the ability of CaMKII to localize to inhibitory synapses. Further studies examined whether the phosphorylation of CaMKII could influence its localization at inhibitory synapses. Calcineurin reduces CaMKII phosphorylation. Cyclosporin A, an inhibitor of calcineurin, increased CaMKII co-localization at inhibitory synapses. A co-IP using wildtype and mutant forms of CaMKII suggests that a pseudophosphorylated mutant (T286D/T305D) interacted more strongly with GRIP. This indicates the phosphorylated state of CaMKII may have a critical role in the synaptic localization of CaMKII. This research was done under the support of the Closing the Gap – Title V Grant from the Department of Education and an LSAMP-NSF grant. Thank you to Summer High School Research interns Declan Wollard and Armando Jimenez.

REACTIVE OXYGEN SPECIES DURING TAIL REGRESSION IN TADPOLES: MITOCHONDRIA AND PEROXISOMES STRIKING A BALANCE

Sirai Ramirez, Adonis Rivie and Dr. Jaishri Menon
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

During anuran metamorphosis, the animal body changes dramatically to adapt from the aquatic to terrestrial habitat. Larval specific organ/tissue such as tail completely degenerates by several different mechanisms including reactive oxygen species (ROS). There are several sources of ROS such as mitochondria, endoplasmic reticulum and peroxisomes being the major sites. In the present study we have investigated the role of ROS derived from mitochondria and peroxisomes during tail regression in tadpoles, *Xenopus laevis*. Our results on *in situ* staining for ROS show that during early stages of metamorphosis, tail fin showed presence of ROS in moderate amount reaching its peak in climax period. Just before the tail starts regressing, large amount of ROS were noted especially in the epidermal cells of the fin. Further increase in ROS in fin epidermal cells occurs once the regression had begun. However, there was no double immunolocalization for ROS and mitochondria indicating that they are not the source of ROS production such as hydrogen peroxide and superoxide. *In situ* staining for mitochondrial derived NO in tail showed an increasing trend with metamorphic progress.

Tail epidermis shows significant increase in peroxisomal density as metamorphosis progressed. Progressive condensation of nuclei from the tip of the tail towards the body also corresponded with a reverse gradient for peroxisome localization. Ventral fin showed signs of cell death before the dorsal fin as wedges of cell death overlapped with ROS localization and peroxisomal staining. We conclude that ROS responsible for cell death in regressing tail is partly derived from peroxisomes and they seem to be ubiquitous organelles, which play a key role in both the production and scavenging of ROS during tail regression. There is a close relationship between peroxisomes and mitochondria, affecting each other's activity.

VERIFICATION OF GFP TAGGING AND ITS LOCALIZATION FOR *CDC20, TRX3 AND OKP1*

Devon Sneed, Alexi Palmer and Dr. Patricia Melloy
Department of Biological and Allied Sciences
Fairleigh Dickinson University, Madison, NJ

Saccharomyces cerevisiae is commonly known as budding yeast. It is a widely used model organism, since it is relatively quick and easy to grow in a laboratory setting, has a fairly short lifespan, can undergo DNA transformation and is inexpensive. Moreover, the cell cycle that budding yeast undergoes is similar to that of humans and other mammals. This cell cycle is even regulated by homologous proteins found in human biology. Some of these homologous proteins include cell cycle proteins, signaling proteins, and protein processing enzymes. Budding yeast's cell cycle has four main stages: G₁, S, G₂, and Mitosis.

The primary goal of this study was to take GFP tagged strains from our laboratory and confirm this tagging via DNA based techniques, such as genomic DNA preparation, polymerase chain reaction (PCR), and gel electrophoresis. Upon extensive analysis of the various techniques administered, our results obtained indicated successful GFP tagging of OKP1, TRX3 and CDC20, despite the fact that several primer sets and PCR conditions were tested for the CDC20 PCR analysis. Our TRX3 AND OKP1 strains were wild type, but the CDC20 strain tagged with GFP was a temperature-sensitive version of the gene, *cdc20-1*. Therefore, the GFP tagging can be used to study the stability of the temperature-sensitive protein. We then used fluorescence microscopy to observe the GFP signal. This signal was observed in several different examples of the *cdc20-1* mutant strain at room temperature and 37°C, however, some buds experienced a brighter signal than others, but it was clear that a GFP signal was tagged. In addition, most of the cells observed experienced a GFP signal in the nucleus.

Future studies will involve looking at GFP signal in the TRX3 and OKP1 tagged strains and our *cdc20-1* strain in more detail. Future students will use the same protocols developed for genomic DNA preparation and PCR analysis in order to confirm GFP tagging of other yeast strains.

HOMOLOGY MODELING AND FUNCTIONAL ANALYSIS OF THE MITOTIC CHECKPOINT COMPLEX IN BUDDING YEAST

Trevor Van Eeuwen[^], ***James Luginsland***^{*}, Dr. Patricia Melloy[^], and Dr. Gloria Anderle^{*}

[^] Department of Biological and Allied Health Sciences

^{*} Department of Chemistry and Pharmaceutical Science
Fairleigh Dickinson University, Madison, NJ

The interactions of Cdc20p/Mad3p/Mad2p, members of the mitotic checkpoint complex (MCC) in budding yeast, are important in regulating the cell cycle and ensuring the fidelity of chromosome segregation. These interactions were examined using computational chemistry and molecular biology to elucidate their nature. Computer analysis of target protein structure was compared with and used to inform observational data from *in vivo yeast* studies. The focus of computer modeling was to evaluate structure, conformation and functional domains; specifically the KEN box receptor and D box receptors, sites of Cdc20/Mad3/Mad2 interaction. Furthermore, the effects of known point mutations in CDC20 on the complex were also studied. To facilitate computational analysis, models of wild type Cdc20p, Mad3p, and Mad2p were constructed through homology modeling, using crystal structures (PDB ID: 4AEZ) of the *Schizosaccharomyces pombe* (fission yeast) homologs as the templates. Analysis was conducted to look at the effect of the *cdc20-1* mutation on functional domains in Cdc20, targeting KEN and D box receptors, and to evaluate potential interference with Mad3 binding. Homology models were studied at temperatures simulated to match the permissive and non-permissive temperature for the *cdc20-1* mutant. To complement the computational studies of interactions within the MCC complex, the *in vivo* localization of MCC proteins such as Cdc20p and Mad3p was examined using GFP tagging and fluorescence microscopy. The main objective of the *in vivo* studies was to understand the difference between the normal MCC protein interactions and the *cdc20-1* mutant protein when it is a part of the MCC. Our goal is to better understand interactions among members of the MCC complex; information that could lead to an enhanced understanding the machinery governing cellular replication, chromosomal segregation and the cell cycle.

POTENTIAL EFFECTS OF STREAM URBANIZATION ON PHYTOPLANKTON, ZOOPLANKTON AND MACROINVERTEBRATE COMMUNITIES

Katsiah Cadet and Dr. James Salierno
Department of Biological and Allied Health Sciences
Fairleigh Dickinson University, Madison, NJ

The goal of this study was to investigate the effects of anthropogenic factors, including waste water treatment plant (WWTP) effluent, on phytoplankton, zooplankton and macroinvertebrates in the Whippany River. The freshwater diatom, *Navicula pelliculosa*, and crustacean, *Daphnia magna*, were cultured separately in samples of Whippany River water collected from three sites: upstream and downstream of the WWTP, at the source of the effluent, and a laboratory control. At the same time, a long term field study was conducted to investigate macroinvertebrate diversity at similar sites. We predicted that the population size and growth rate of diatoms would be greatest at the WWTP effluent site. Further, we predicted that *Daphnia* growth (biomass and number of molts) and reproduction (number of eggs) would be lowest at the effluent site. Finally we predicted that overall macroinvertebrate diversity will be lowest at the WWTP effluent site. Diatom population growth was quantified (cells/mL) twice per week over a 5 week exposure. *Daphnia*, after confirming assay methods with a reference toxin (CuSO₄), was chronically exposed to the same Whippany River water as the diatoms for 96 hr. *Daphnia* growth (dry weight and number of molts) and reproduction (number of eggs) were quantified post exposure. Diversity (Shannon and Simpsons indices) was quantified through the collection and analysis of macroinvertebrates along with water quality (D.O., temp, pH, and nutrients) at the same three sites with the addition of a reference site for a total of 5 months. It was found that the growth rate of the *Navicula pelliculosa* cultured in the WWTP effluent was significantly greater than the upstream, downstream and control growth. In contrast, WWTP effluent had no significant effect on the biomass, average number of eggs, or number of molts of *Daphnia* when compared with the upstream and downstream sites. In terms of macroinvertebrate diversity, the reference site had the highest diversity and species richness compared with the other sites along the River. Nitrate (NO₃) was significantly higher at the effluent and downstream sites compared to upstream and reference sites. Similarly, dissolved phosphorus and phosphate concentrations (P and PO₄) were significantly higher at the effluent and downstream sites than the upstream site. The increased growth of *Navicula* can be attributed to the WWTP effluent and stream urbanization which increased the levels of nitrogen and phosphorus. Macroinvertebrates are also sensitive to polluted water and there is a decreased population of sensitive taxa. Overall, we believe that WWTP effluent will have a negative influence on the aquatic ecosystem of the Whippany River. Further attention needs to be focused on urban rivers, or we may see elimination of pollution sensitive organisms and diversity.

MOLECULAR PHYLOGENETICS OF NORTH AMERICAN AGELENIDAE

Derrick Dorph and Dr. Joseph Spagna
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

The family Agelenidae C.L. Koch 1837 is large (70 genera, 1157 species currently described, accounting for about 2.5% of all spider species) with a high level of endemism in the North America, and California in particular. Spiders from this family have recently been used as models for toxicological and behavioral research. In the Agelenidae, there have been eight genera (*Hololena*, *Rualena*, *Calilena*, *Novalena*, *Agelenopsis*, *Barronopsis*, *Tortolena*, and *Melpomene*) classified in the subfamily Ageleninae, tribe Agelenopsini, endemic to North and Central America. In the past year, an additional genus (*Rothilena*) has been described from Northwestern Mexico. We performed partitioned Bayesian likelihood analysis of molecular sequence data from mitochondrial (CO1 and 16S rDNA) and nuclear (28S rDNA) genes totaling 1100 base pairs from 25 representative species to develop a phylogenetic hypothesis for these genera. Results support monophyly of a group confined to Western North America extending south into Baja California (*Calilena* + *Hololena* + *Novalena* + *Rualena* + *Rothilena*). These are sister to a clade including the primarily Gulf Coast, Caribbean and Atlantic Coast genera *Agelenopsis*, *Barronopsis*, and *Tortolena*. Strong genitalic similarity within the latter group extends to the sole unsequenced genus *Melpomene* from Eastern Mexico and Central America, consistent with a clear biogeographic split between the Atlantic/Gulf Coast genera and those endemic to the Western US and Mexico. Tree morphology indicates an early period of rapid diversification, though large uncertainty in molecular clock estimates confounded our efforts to rigorously evaluate possible causes of this remarkable continent-wide radiation.

**SURVEY OF LARVAL DIGENETIC TREMATODE DIVERSITY IN
PHYSID AND PLANORBID SNAIL POPULATIONS FROM
NORTHWESTERN NEW JERSEY**

Kristen W. Harr and Dr. Joseph G. Bucci
Dept. of Mathematics and Natural Sciences
Centenary College, Hackettstown, NJ

Studies investigating digenetic trematode diversity in snail populations were performed in Northwestern New Jersey. These parasites are characterized by complex life cycles, requiring snails for development. Cercariae emerge from infected snails and swim in water to infect a definitive host, encyst on strata, or infect another intermediate host. The consequence of trematode infection has dramatic effects upon hosts including decreased reproduction in snails, as well as visceral pathologies and limb deformities in larval anurans. Previous studies have surveyed vertebrate species for parasite infection. The molluscan dependence for life cycle completion makes snails a convenient source for investigations of trematode diversity. *Physid* and *Planorbid* snails were collected from five freshwater sites and examined for production of cercariae production. Cercariae were used for snail infection studies. *Physid* and *Planorbid* snails collected at all sites produced cercariae, based upon morphology, representing the families *Plagiorchidae*, *Echinostomatidae*, *Diplostomatidae*, *Psilostomatidae*, *Strigeidae*, *Paramphistomatidae*, *Schistosomatidae*, and *Spirochidae*. Genera associated with amphibian pathologies including *Plagiorchis*, *Echinostoma*, *Echinoparyphium*, and *Ribeiroia* were observed at all sites sampled. These cercariae were used in tadpole infection studies and metacercariae were found in the dermis, nephric system, and livers. This work expands the knowledge required for the advancement of our research program by identifying parasite/host relationships in Northwestern New Jersey and how these impact amphibian communities that reside within

ENTEROCOCCUS LEVELS IN THE SAW MILL RIVER

Leslie Martinez, Shejla Pollozi, Sarah Fiordaliso, and Dr. Michelle Hersh*
Department of Biology
Sarah Lawrence College, Bronxville, NY

The Saw Mill River, a tributary of the Hudson River, has recently been daylighted at Van der Donck Park in Yonkers, NY, as part of an effort to expose a part of the river that had previously been covered. Considering exposure of bacteria to UV light has been shown to decrease their populations in contaminated water, our research set out to measure the effect of the river daylighting on levels of microbial fecal contamination found in that portion of river. To test for the level of fecal contamination, we used the Enterolert system to measure levels of the bacterial indicator species of fecal contamination, *Enterococcus faecalis*, at the end and beginning of the daylighted section. Over a four-week period, we collected water samples at both the end and the beginning of the daylighted portion and quantified levels of enterococci found in the water. Concluding our research, we found that there was a significant relationship between the amount of rainfall 72 hours prior to the sample collection and the percent change in enterococci levels from the beginning to the end of the daylighted portion. Interestingly, our research showed that when there was a large amount of rainfall 72 hours prior to the sample collection, there was a decrease in enterococci levels from the beginning to the end of the daylighted section. We speculate that this may be due to increased UV exposure in the daylighted section and flow rates, causing the levels of bacteria in that portion of the river to decrease as the water flows through the daylighted portion. A larger data set, consisting of more sampling points in location and time, is needed to fully understand the relationship between the amount of rainfall and the fluctuating levels of enterococci in the Saw Mill River.

HOST SPECIFICITY OF FUNGAL PATHOGENS IN FRAGMENTED HABITATS

Marienne Pinson, Cassidy Bernstein, and Dr. Michelle Hersh

Department of Ecology

Sarah Lawrence College, Bronxville, NY

Habitat fragmentation is an increasingly common phenomenon associated with decreased plant species richness, with smaller fragment size and greater isolation generally associated with decreasing levels of biodiversity. Mortality driven by host-specific pathogens is likewise a widely-discussed mechanism through which plant diversity is maintained via negative feedbacks ; but whereas this mechanism functions to promote biodiversity, in both macro- and micro-organisms fragmentation does the opposite. In this study, we aimed to examine patterns in the infection of annual plant seeds by fungal pathogens buried in an experimentally fragmented landscape in Lawrence, Kansas . Fungal pathogens cultured from surface-sterilized seeds were characterized using DNA sequencing. Given that decreased fragment size is correlated to both decreasing plant diversity and an increased rate of plant species turnover, we hypothesize that smaller fragments will be associated with lower species richness of host-specific fungal pathogens.

DESIGNING TAQMAN PROBES TO QUANTIFY SPECIES-SPECIFIC CONIFER DNA IN REAL-TIME PCR

Ammar Ali and Dr. Kendall Martin

Department of Biology

William Paterson University of New Jersey, Wayne, NJ

In an attempt to determine the distribution of roots under the ground of a coniferous forest site, a method has been developed which can amplify sequences from conifer roots and distinguish species within that mix of roots quantitatively. This method will prove to be very beneficial considering that visual separation is difficult, tiresome, and sometimes inaccurate when dealing with similar roots. From a multiple-sequence alignment, primer target sites were identified to distinguish the tree-species involved. The primer oligonucleotides were synthesized and optimized for PCR, producing 3 primer sets with good amplification rates. The primers amplify different regions of the gene for ribulose-1,5-bisphosphate carboxylase that include potential probe sites for fluorescence-based quantitative PCR. Sequences for the TaqMan probes were determined using standard criteria. The TaqMan probes, each specific to a conifer species, will be added to the PCR master mix along with the conifer-specific primers. This multiplex reaction in real-time PCR will allow us to determine the relative DNA concentrations of the different conifer species in the sample root mix. From this, root biomass and distribution below the ground can be determined.

CD44 INDUCES P-gp EXPRESSION THROUGH HA BINDING AND TRANSCRIPTIONAL ACTIVATION

Brittany Eason, Kyle Murphy, Dr. Swayamjot Kaur,
and Dr. Lorna Rodriguez-Rodriguez¹

Department of Biochemistry and Microbiology
Rutgers University, New Brunswick, NJ

¹Department of Gynecology and Oncology
Rutgers Cancer Institute of New Jersey, New Brunswick, NJ

The main causes of treatment failure and mortality in cancer are metastases and the development of drug resistance. CD44 and P-gp are two membrane proteins well-known determinants of metastases and drug resistance respectively. We and others have shown that CD44 induces P-gp expression in cancer cells. We also showed that there is a physical interaction between these two proteins as they immunoprecipitate and co-localize in the cell membrane. Hyaluronan (HA) is a well known ligand for CD44, involved in tumor cell signaling and the development of malignant properties. Others have shown that HA is necessary for the CD44 induction of P-gp expression and drug resistance. However, it is not known whether HA binding to CD44 is indeed necessary for this induction. To answer this question, we generated different mutants of the CD44 HA binding domains (CD44 HABD). We transfected CD44 HABD mutants as well as CD44 wt into ovarian cancer cells (TOV112D) and human embryonic kidney cell lines (HEK 293). Unexpectedly, we found that P-gp expression was induced both in CD44 wt and CD44 HABD mutants. However, the P-gp induction was significantly less in the CD44 HABD mutants. We tested whether the P-gp induced by the CD44-HABD mutants was functional by testing for drug sensitivity in an MTT assay. We observed that cells transfected with CD44 HABD mutants became drug sensitive as compared to CD44 wt transfected cells even when the whole HA binding domain was deleted. We then determined if deletion of the CD44 HABD domain had an effect on the physical interaction between CD44 and P-gp. By co-immunoprecipitation experiments we showed that CD44 and P-gp were physically interacting even in CD44 HABD mutants. These results indicate the existence of an additional mechanism for P-gp induction through CD44 that is independent of HA binding. Previously, we showed that the intracytoplasmic domain of CD44 (CD44-ICD) is transported into the nucleus where it binds to DNA promoters and is involved in the transcriptional regulation of various genes. Therefore, we investigated whether CD44 was involved in transcriptional regulation of P-gp as the additional mechanism of Pgp upregulation. Co-transfection of CD44 or CD44-HABD mutants with luciferase driven MDR1 promoter showed increased luciferase activity in both CD44wt and CD44-HABD mutants. However, this MDR1 promoter does not have the CD44 DNA binding consensus sequence. Therefore, CD44-ICD could be inducing other genes that in turn activate the MDR1 gene. We conclude that although HA binding to CD44 is important for the induction of P-gp, CD44 transcriptional activation of MDR1 promoter also plays a role. Furthermore, we show that CD44 transcriptional activation of MDR1 is independent of HA binding. These results further the understanding to the present knowledge of CD44 involvement in drug resistance and uncovers new mechanisms involved in this process that are HA-independent.

NO NOVEL ROLE FOR HISTONE HDKD6 METHYLATION IN Pre-mRNA SPLICING IN *SACCHAROMYCES CEREVISIAE*

Danielle Flood[#], Stefanie Ucles[#], Matthew Sorenson, Deepak Jha, Brain Strahl,
Scott W. Stevens*, and Dr. Tracy L. Kress*

Department of Biology
The College of New Jersey, Ewing, NJ

Proper gene expression involves multiple steps, including RNA splicing where non-protein coding regions of RNA are removed from the RNA transcript. RNA splicing is carried out by the large and dynamic spliceosome, which is comprised of small nucleoprotein complexes (snRNPs) that assemble on an RNA molecule in a precise order. Assembly of the spliceosome occurs co-transcriptionally and RNA splicing is tightly coordinated with transcription to ensure precise and efficient gene expression. However, the mechanisms that underlie this coordination are poorly understood. In order to identify proteins that function to coordinate RNA splicing with transcription we carried out a genetic interaction study using *Saccharomyces cerevisiae*. We identified negative genetic interactions between genes encoding RNA splicing factors and the *SET2* gene, a histone methyltransferase that methylates lysine36 on histone H3 (H3K36) to regulate transcription. Furthermore, we show that mutations that block H3K36 methylation also have negative genetic interactions with splicing factor genes, suggesting that H3K36 methylation is important for RNA splicing. Indeed, we have shown that deletion of *SET2* or point mutation of H3K36 inhibits RNA splicing and exacerbates splicing defects in yeast strains harboring deletions of splicing factor genes. Using chromatin immunoprecipitation, we demonstrate that deletion of *SET2* reduces the association of snRNPs with chromatin. Thus, we provide the first evidence that H3K36 methylation is required for appropriate RNA splicing in yeast and suggest a model in which Set2 or H3K36 methylation help to recruit splicing factors to RNA during transcription.

*co-corresponding authors

TCNJ undergraduate students

TESTING THE EFFICACY OF TWO RNAi STRATEGIES IN C. ELEGANS

John Fritsch, Matthew Von Bargan and Dr. Joost Monen

Department of Biology
Ramapo College, Mahwah, NJ

RNA-mediated interference (RNAi) is a process by which RNA molecules inhibit gene expression via specific degradation of mRNA transcripts. Since its discovery nearly 20 years ago, researchers have utilized this understanding to specifically knock-down genes of interest. In the nematode *C. elegans*, several RNAi techniques have been developed, including injection of double stranded RNA (dsRNA) and feeding of bacteria expressing dsRNA. In this study, we will test both approaches to knock-down an essential mitotic protein HCP-3, and assess the effectiveness of both strategies for use in future studies. Knock-down effectiveness will be measured by western blot analysis and immunofluorescence, and the phenotypic consequences will be assayed by live-imaging of cell division in mCherry:Histone-H2B & GFP: α -tubulin transgenic worms. Currently, we have synthesized the dsRNA and have begun to establish an effective injection and feeding protocol, which will be subsequently used to rigorously test the efficacy of both approaches.

DNA AND RNA ISOLATION FOR GENOTYPING AND CANNABINOID RECEPTOR GENE EXPRESSION IN RODENT MODELS OF BRAIN FUNCTION

Paola Velandia, Monika Chung, Steve Gross, Sue Sgro, Dr. Claire M. Leonard,
and Dr. Emmanuel S. Onaivi

Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Cannabinoids are the constituents of marijuana plant (*Cannabis sativa*) and endocannabinoids (eCBs) are the endogenous marijuana-like substances found in animals and humans. Advances in marijuana-cannabinoid research indicate the existence of naturally occurring endocannabinoid system (ECS) in mammalian physiology. The ECS consists of the cannabinoid receptors (CB1Rs and CB2Rs), endocannabinoids (eCBs), and the synthesizing and degradation enzymes of eCBs. Alterations of the endocannabinoid system (ECS) are involved in a number of neuropsychiatric disorders like depression, anxiety and drug addiction. Progress in cannabinoid research indicates that the cellular, biochemical and behavioral responses to marijuana are coded in our genes and cannabinoid receptors are coded in human chromosomes 1 and 6 respectively. CB1Rs and CB2Rs are activated by endocannabinoids, phytocannabinoid, and marijuana use (medical/recreational). These remarkable advances in understanding the biological actions of marijuana, cannabinoids and endocannabinoids, are unraveling the genetic basis of marijuana use with implication in human health and disease. In addition the advances in biotechnology and molecular biology, and availability of precise tools and protocols using *in-vitro* and various transgenic animals are being used to explore and identify the involvement of elements of the ECS in models of brain function and disorders. We are investigating the impact of mouse gene knockout (ko) models on cannabinoid induced behavioral changes and we have modified some of the generic protocols for DNA and RNA isolation for genotyping and cannabinoid receptor gene expression studies in rodent models of brain function. The standard genotyping protocols used are polymerase chain reaction (PCR) based gel electrophoresis. We have obtained some genotyping data from dopamine and serotonin transporter (DAT and SERT) and Mu opioid receptor ko, dopamine transporter – cocaine insensitive (DAT-CI) ko and the CB2 flox mice which we have recently developed. The genotyping protocols requires toe clipping of the animals and upon lysis, DNA is extracted, master mixes are prepared along with specific primers based on the gene ko for the PCR reaction. Then agarose gels are prepared and after electrophoresis, the gels are visualized using gel documentation system for the classification regarding the animal's genotype whether homozygous, heterozygous or wild type. The mutant mice (homozygous) allow for the investigation of the impact of different genes in cannabinoid induced behaviors. For the CB2R gene expression, three parts of the brain, pre-frontal cortex, and cerebellum and the rest of the brain are dissected for use. Briefly, RNA was isolated using Trizol reagent and cDNA synthesized using kit for first strand synthesis for the Real Time-PCR (RT-PCR). Custom-designed probes for the mouse CB2 gene and their GAPDH internal control with fluorescent markers VIC and FAM respectively were used for RT-PCR. We have successfully set up and genotyped transgenic mice and obtained RNA from male and female mu opioid gene ko mice. Further genotyping and cannabinoid receptor gene expression studies in mouse models of brain function are on-going.

ELAV RNA BINDING PROTEINS COORDINATELY REGULATE NEOCORTICAL NEUROGENESIS

Nicole Volk and Dr. Mladen-Roko Rasin
Neuroscience and Cell Biology
Rutgers University, Piscataway, NJ

The neocortex is the most complex brain region, and is crucial for complex motor functions, language, learning, and memory. Proper prenatal neocortical development is essential for these functions. Thus, a better understanding of the molecular mechanisms behind neocortical development is critical. Post-transcriptional events regulated by RNA binding proteins (RBP) have been shown to regulate neocortical neurogenesis. However, the roles of distinct RBPs during neocortical development are still poorly understood. One RBP of interest, CUG triple repeat binding protein 1 (Cugbp1), has been shown to promote growth during early neurogenesis. Cugbp1 is responsible for generating the lower layers neurons of the neocortex (layers V and VI) which project subcortically. Another RBP shown to participate in a critical role during neocortical development is Hu antigen D (HuD). HuD has been proven responsible for the formation of the upper layer neurons in the neocortex (layers II-IV) which project intracortically. We have successfully demonstrated that Cugbp1 regulates the translation of HuD. Based on our studies carried out both *in vitro* and *in vivo* using a mouse model, we hypothesize that the development of the neocortex is critically dependent on Cugbp1 and HuD.

ASSESSMENT OF ONE'S WILLINGNESS TO SEEK TESTING FOR DEMENTIA WITH LEWY BODIES

Sergio Almeida, Hiba Saleem, Dr. Laura Mackey Lorentzen, and Dr. Kristie Reilly
Biological Sciences Program
Kean University, Union NJ

Dementia with Lewy Bodies (DLB) is a debilitating neurodegenerative disease that affects the geriatric population. To find the right diagnosis for a patient with DLB, the patient must fulfill a combination of different core diagnostics, which include fluctuating cognition, visual hallucinations, and Parkinsonism. Additionally, there are many suggestive diagnostic features, which include neuroleptic sensitivity, rapid eye movement sleep behavior disorder, reduced striatal dopamine transporter uptake, and lastly, functional and psychological concerns of the quality of life that includes depression. Patients with DLB are said to have a shorter rate of survival time once diagnosed. Published studies have compared different symptoms used to diagnose DLB, but few research the psychology of whether or not an individual wishes to be aware of the presence of this neurodegenerative disease once they are informed of the process of diagnosis and functional consequences that follow. Using core and suggestive diagnostic criteria, along with relevant biomarkers, this study aims to explore whether or not knowledge of DLB and its diagnostic criteria will impact an individual's willingness to seek out biomarker testing. A survey was created and approved by Kean University's IRB prior to administration to college science majors. The results of the statistical analysis to compare the answers of underclassmen to upperclassmen will be presented.

GENETIC STRUCTURE OF NATIVE AND RESTORED POPULATIONS OF AMERICAN BEACHGRASS (*Ammophila breviligulata* Fern.) ALONG THE NEW JERSEY COAST

Alison Caceres, Dr. Carey Waldburger and Dr. David Slaymaker
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

New Jersey's coastal dunes provide both natural scenery and structural support for the shore's coastal communities. Therefore, millions of dollars have been spent on dune nourishment and upkeep. However, these dunes were subject to immense damage due to the tropical storm Sandy in October of 2012. *Ammophila breviligulata* is one of the most important species in New Jersey which had a huge role in the development and stabilization of the destroyed coastal dunes. Dune restoration projects currently involve this beachgrass species specifically and are becoming more and more focused on maintaining their genetic diversity and restoring ecological services and functions. In our study, we collected 150 samples of AB from two native populations along the shore. We then used a series of six unique ISSR primers optimized for this beachgrass species to compare their genetic diversity using PCR methods and manually scoring the band presence or absence of the polymorphic loci.

THE ROLE OF ADRENAL CORTICOSTERONE ON MEDIATING THE INFLAMMATORY PAIN RESPONSE OF BTBR T+ tf/J MICE: THE ANIMAL MODEL FOR AUTISM SPECTRUM DISORDER

Erin Connor, Rebecca Atencio, Alec Degraff, , Norman Schanz, Dr. Robert Benno
and Dr. J.W. Lee,

Department of Biology, William Paterson University of New Jersey, Wayne NJ

Previously, our lab reported BTBR T+tf/J (BTBR) mice display reduced response to inflammatory pain that may be mediated by the stress-induced analgesia. The adrenal hormones mediating the stress responses are well characterized: epinephrine/norepinephrine and corticosterone. The present study examined the effect of adrenalectomy (ADX) on inflammatory pain behavior in male BTBR mice.

Male BTBR and C57 BL6/J mice (n=42) were divided into five groups: a) BTBR+ADX, b) BTBR+sham, c) C57+ADX and d) C57BL/6J+sham. Seven days after surgery, all mice were injected with intraplantar formalin (30ul) and the number of paw flinches/licks was counter for 60 min. All BTBR and C57 mice displayed classic formalin phase I. The formalin phase II were not significantly different between BTBR-ADX and C57-ADX. Overall, adrenalectomy did not reverse the hypoalgesia observed in BTBR mice.

The hypoalgesic inflammatory response seen in BTBR may not be mediated by the adrenal stress hormones.

EFFECTS OF CRF₁-RECEPTOR ANTAGONIST ON STRESS INDUCED ETHANOL CONDITIONED PLACE PREFERENCE

*Eugene Dennis*¹, Dr. Zhichen Carl Lin² and Dr. Emmanuel S. Onaivi¹

¹Department of Biology, William Paterson University of New Jersey, Wayne, NJ

²Harvard Medical School, Boston, MA

The Hypothalamic-pituitary-adrenal (HPA) axis is primitive and one of the first if not the first pathways to develop in mammals because of how important it is for survival. Research has shown that stressful events that mother's go through during pregnancy can impact their children and alter the brain chemistry of the unborn child. By the time a child is born, the HPA axis is formed and fully functional. It plays a major role in how we deal with stress and its effects. Studies have shown that, exaggeration responses of the HPA axis is implicated in wide variety of disease conditions like Schizophrenia, anxiety, ADHD, depression, PTSD, alcoholism and autism. When the brain perceives stress, corticotrophin-releasing hormone (CRH or CRF in rodents) is released from the hypothalamus, this hormone stimulates the synthesis and release of adrenocorticotrophic hormone (ACTH) from the pituitary, and eventually cortisol is synthesized and released by the adrenal cortex. ACTH causes the release the glucocorticoids, cortisol in humans and corticosterone in rodents into the bloodstream leading to the well-known fight or flight response to stress. The frequency of a stressor whether chronic or acute can lead to hyper activation or the numbing of the HPA axis. So far it has been shown that the body's adaptations to acute and chronic stress are critical for physical and mental health. In rodents, two G protein coupled receptor subtypes have been found designated CRF₁ and CRF₂. Extensive research has shown the CRF-CRF₁ overactivity in the brain contributes to anxiety disorders and depression. In this experiment the conditioned place paradigm was used to assess how a CRF₁ receptor antagonist would affect the stress response. Previous studies both here at William Paterson and elsewhere have shown that alcohol enhances conditioned place preference (CPP). The CPP apparatus consists of a box with two sides, one easier to walk on and the other difficult for the mice. We investigated whether a combination of alcohol and the CRFR₁-antagonist will enhance or reduce the conditioned place preference of the mice? To answer this question the C57Bl/6N (Tac) mice were injected with the CRF₁-receptor antagonist following acute stress in a conical tube and then assessed for conditioning using CPP. The results show that the mice injected with the CRF₁-receptor antagonist prevented the effects alcohol CPP but subjects that had a combination of stress and alcohol were not conditioned.

AN INQUIRY-BASED LESSON PLAN ON THE MAMMALIAN DIVE REFLEX PROVIDES COMMON CORE COMPETENCIES FOR HIGH SCHOOL STUDENTS

Lauren Schmidt and Dr. Joost Monen
Department of Biology
Ramapo College of New Jersey, Mahwah, NJ

Inquiry-based lesson plans are essential for teaching students the critical thinking and science literacy skills needed to synthesize and analyze information effectively. Students are not sufficiently developing these skills and thinking processes from traditional procedural-based lab lesson plans. Inquiry-based lesson plans are better able to prepare students for the Common Core Standards and New Jersey Science Standards, which assess learning at the higher levels of Bloom's taxonomy. This study included the design and implementation of a 2 hour lesson plan for biology high school sophomores in the Upward Bound Program at Ramapo College. The purpose of the lesson was to expand students' understanding of the theory of evolution by analyzing molecular and anatomical evidence for the mammalian dive reflex between marine mammals and humans. Both cognitive and affective objectives were created for the students to emphasize major biological concepts including: the conservation of evolutionary adaptation, physiological responses to environmental stimuli, and how to use the scientific method to create an experiment that analyzes the possible conservation of the dive reflex in humans. Students rotated through stations where they received specialized information about the heart, ECGs, evolution, data analysis, and data collection. This inquiry-based teaching method enhanced students' understanding, comprehension, and retention of the material. From informal assessment and feedback from my advisor and volunteers, students were able to meet the objectives and explain why they were performing the lab in a larger scientific context. The three rotating stations provided students the opportunity to carry out their experiment as well as work on and develop the analysis skills needed to draw their own conclusions about the mammalian dive reflex's conservation in human evolution.

BEHAVIORAL ANALYSIS OF AGE DEPENDENT DECLINE IN FITNESS IN DROSOPHILA

Heather Weiland and Dr. Theodore Brummel
Department of Biology
Long Island University, Post Campus, Brookville, NY

Traditional aging studies rely on lifespan measurements as a tool to measure the rate of aging. This approach yields a quantitative measurement, which is intuitively related to the rate of aging, based on the understanding that increasing age leads to increased frailty and thus higher mortality. Numerous genetic, pharmacological, and environmental manipulations can enhance longevity, however, it is not always clear whether these manipulations also enhance the quality of life. Using the fruit fly, *Drosophila melanogaster*, I am performing behavioral assays to measure the age related decline in fitness in fruit flies of different genotypes and raised under different conditions. Currently, the focus is on how negative geotactic behavior declines with age. The results for wild type flies are being compared to those of flies with alterations in the Target of Rapamycin (TOR) pathway, which is one of the most important genetic components that affect aging in numerous organisms. Future work will focus on other more complex behavioral assays, such as flight and phototactic behavior. This work is important because it will allow for an independent and less labor-intensive method of measuring changes in aging. It is also beneficial since the goal of most aging research is to improve the nature of life in old age and not simply prolong life.

THE ROLE OF CANNABINOIDS IN ANXIOLYSIS IN AUTISTIC PHENOTYPIC MICE

Jasmine Wood, Norman Schanz, and Dr. Emmanuel S. Onaivi
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Autism spectrum disorders (ASDs) are heterogeneous neurodevelopmental disorders characterized by impairment in social and communication skills and stereotype behaviors. Diagnosis of autism has increased, affecting more boys than girls, and 1 in 68 children in the US have ASDs. Autism presents itself as a disability in a child between 18 and 24 months of age. The causes of ASDs are unknown and there is no cure, but some forms of treatment for symptoms are being applied. For example, Cognitive Behavior Therapy involves working with a child in speech therapy, lessening anxiety and increasing normal social interaction. Some medications are used, but mostly to keep the child manageable in terms of hyperactivity, psychosis, and affective disturbances. While autism may be uniquely human, there are behavioral characteristics in ASDs that can be mimicked using animal models. Alterations of the endocannabinoid system (ECS) are involved in the pathophysiology of neuropsychiatric disorders including ASDs. The ECS consists of the cannabinoid receptors (CB1Rs and CB2Rs), endocannabinoids (eCBs), and the synthesizing and degradation enzymes of eCBs. The ECS is involved in embryo neurodevelopment and growth and is a key regulator of the immune system via CB2Rs, which are expressed on macrophages, microglial cells, and neurons. The BTBR T+tf/J mice have been shown to exhibit autism-like behavioral phenotypes. Earlier work from our animal laboratory demonstrated exaggerated responses to stress in the BTBR mice that may involve the endocannabinoid system. The current study was designed to test the hypothesis that cannabinoid receptors (CBRs) are involved in ASDs and specifically in anxiety-like behavior pathways.

To test the hypothesis, BTBR T+tf/J and the C57BL/6J mice were used to study the effects of cannabinoid ligands in a two-compartment black and white box model of mouse aversive behavior as previously described. The cannabinoid ligands used were WIN55212-2, a mixed CB1 and CB2 receptor agonist; ACEA, a CB1R agonist; JWH133, a CB2R agonist; AM251, a CB1R antagonist; and AM630, a CB2R antagonist. The acute effects of the CBR ligands at selected doses of 1-2 mg/kg were evaluated after intra-peritoneal administration and a pre-treatment time of 30 minutes. Animals were placed in the two-compartment box, which has an interconnecting opening between the compartments. The time, activity, and entries into both chambers of the box were automatically recorded by a computer interface via photoelectric controls over the 10-minute test session for each mouse. In general comparison to the C57BL/6Js, the BTBR mice were more active, explored both compartments more, and spent more time in the white compartment. At the doses used of 1 mg/kg, JWH133, AM630 and AM251 did not have significant effects on the behavior of either strain, but WIN55212-2 at 1 and 2 mg/kg reduced activity of both strains, such that all entries were reduced. The number of entries into either chamber was reduced more in BTBR than the C57BL/6Js, with decreased activities in both chambers after ACEA administration. Furthermore, ACEA treatment significantly increased the time mice spent in the dark chamber and decreased the time spent in the white chamber when compared to vehicle-treated controls, suggesting an anxiogenic-like response. Further studies are required to determine the role of the different elements of the endocannabinoid system in ASDs.

EFFECT OF PH ON THE SPECTROSCOPIC PROPERTIES OF SEVERAL HYDROXYCINNAMIC ACID DERIVATIVES

Paris M. Hanson, Samantha J. Pace, Eric Nguyen and Dr. Elmer-Rico E. Mojica
Department of Chemistry and Physical Science
Pace University, New York, NY

Hydroxycinnamic acids are a class of aromatic acids and hydroxy derivatives of cinnamic acid. These compounds account for about one third of the phenolic compounds in our diet. They have gained a great interest because they are known to be potent antioxidants. In this study, the effect of pH on the spectroscopic properties (absorbance and fluorescence) of several hydroxycinnamic acids such as caffeic acid, coumaric acid, ferulic acid and sinapic acid were obtained. Computational calculations on absorbance were also carried out and compared with the experimental results.

FORMATION OF SUPEROXIDE [O₂⁻] ANION ADDUCTS FROM AMIDES UNDER ATMOSPHERIC PRESSURE HELIUM PLASMA IONIZATION (HEPI) CONDITIONS

Isra Hassan and Dr. Athula Attygalle

Center for Mass Spectrometry, Department of Chemistry, Chemical Biology, and Biomedical Engineering, Stevens Institute of Technology, Hoboken, NJ

Certain gaseous molecules are known to undergo anion attachment under negative-ion-generating atmospheric-pressure chemical ionization (APCI) or vacuum chemical ionization (CI) conditions. One of the gaseous anions found in the plasma of discharge ion sources under negative-ion generating conditions is the superoxide radical anion O₂⁻. Recently, Cody and Dane reported the formation of O₂⁻ adducts of linear aliphatic hydrocarbons (Cody and Dane, 2013) under direct analysis in real time (DART) conditions. Currently, the factors that determine O₂⁻ adduct formation and the mechanisms involved in their formation and fragmentation are poorly understood.

In our gas-phase studies of small molecules subjected to Helium Plasma Ionization (HePI) (Yang and Attygalle, 2011), we noted that under negative ion generating conditions, carboxamides undergo O₂⁻ adduct formation and/or deprotonation. We report on the significance of the NH function for the O₂⁻ attachment under negative-ion HePI conditions. For the generation of plasma, a stream of high purity helium was passed through a metal capillary held at a high voltage. Samples were deposited on a glass slide and placed in the source, about 1 cm from the capillary orifice.

Under helium-plasma ionization (HePI) mass spectrometric conditions, most amides synthesized from carboxylic acids undergo deprotonation. However, to our surprise, a peak at m/z [M + 32]⁻ was observed in the spectra of certain amides in addition to the typically observed m/z [M - 1]⁻ peak which corresponds to the deprotonated amide. Upon activation, the superoxide adducts generated from amides undergo fragmentation by two different pathways. Either a neutral loss of the precursor amide can occur or a hydroperoxyl radical can be lost. Apparently, the fragmentation channel that predominates depends upon the relative strength of the N—H bond in the amide. We also suggest two possible structures for the superoxide anion adduct. In the first structure, an oxygen atom in the superoxide anion is non-covalently bonded to the amide hydrogen. In the second structure the superoxide anion acts as a nucleophile and attacks the carbonyl carbon forming a tetrahedral adduct structure. Hydrogen-deuterium exchange experiments and computational calculations support the hypothesis that the hydrogen-bonded superoxide adduct exists in the gas phase. The intensity ratio of the m/z [M - 1]⁻ and m/z [M + 32]⁻ peaks can be manipulated by varying in-source fragmentation conditions such as the hexapole transfer lens voltage, cone voltage, and source temperature.

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INVESTIGATING THE STRUCTURAL DYNAMICS OF HUMAN GALECTIN-4 USING SMALL ANGLE X-RAY SCATTERING

*Kristina Malzbender*¹, Joane Rustiguel², Maria Cristina Nonato², and Dr. Nozomi Ando¹

¹Department of Chemistry, Princeton University, Princeton, NJ

²Faculty of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo

Human galectin-4 (hGal4), a member of the galectin protein family, has a variety of intracellular functions and is found in the human alimentary tract. Overexpression of hGal4 has also been implicated in inflammatory bowel disease and a variety of cancers. hGal4 has been proposed as a potential drug target or marker for cancer diagnoses. This protein is characterized by two distinct carbohydrate-binding domains connected by a flexible peptide linker. This flexibility has rendered hGal4 difficult to study by traditional structural methods due to challenges with crystallizing the full-length protein. To date, crystal structures of the individual carbohydrate binding domains have been solved but structural information of full-length hGal4 is lacking. In the current study, we investigate the structural dynamics of hGal4 using small-angle x-ray scattering (SAXS). SAXS can provide structural information from disordered systems without a crystalline structure and can thus be applied to macromolecules that are difficult to crystallize or contain disordered regions. Using both oscillating-flow cell SAXS and in-line size-exclusion chromatography, we have gained structural insight into the full-length hGal4 for the first time. Our results show that the predominant solution conformation of hGal4 is one in which the two carbohydrate-binding domains are closely associated. We further show that binding of lactose has a minimal effect on the conformation of hGal4. The compactness of the overall structure is consistent with the proposed involvement of hGal4 in cell adhesion, where the two carbohydrate-binding domains must bring together two surfaces.

ANALYSIS OF ELECTRONIC EXCITED STATES OF REICHARDT'S $E_T(30)$ DY IN SOLVENTS OF VARYING POLARITY

James Shaw, Amir Eldin, and Dr. Dmytro Kosenkov
Department of Chemistry and Physics
Monmouth University, West Long Branch, NJ

Pyridinium *N*-phenolate betadine dyes such as $E_T(30)$ (Figure 1) are highly sensitive molecular probes that are used for determining solvent polarity due to their solvatochromic behavior. This behavior is largely due to the intermolecular charge transfer from the phenolate to the pyridium component of $E_T(30)$. Experimentally, this behavior was examined by investigating UV-Vis spectra of $E_T(30)$ molecules in solvents of different polarity. Computationally, modeling the $E_T(30)$ solvent scale enables for in-depth examination of the charge transfer states, which give $E_T(30)$ its unique solvatochromic properties. The quantum chemical calculations using *Gaussian09* software have been carried out in order to optimize the $E_T(30)$ molecule in the gas-phase using the density functional theory. Then, *GAMESS* software has been used to examine the electronic excited states and orbitals contributing to the electronic transitions responsible for the experimentally observed absorption bands appearing in UV-vis spectra. Obtained results suggest increasing energy of the electronic excited state energies corresponding with increasing solvent polarity. Excited state energies have been verified by comparing them to the UV-Vis absorption spectra of solvated $E_T(30)$ obtained experimentally.

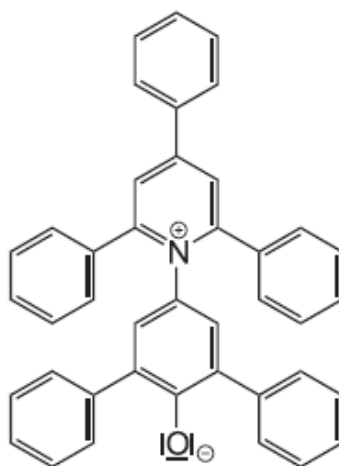


Figure 1. $E_T(30)$ 2,6-Diphenyl-4-(2,4,6-triphenyl-1-pyridinio)phenolate

CHROMATOGRAPHIC ANALYSIS OF BEE PROPOLIS

Kevin Symczak, **Samantha J. Pace** and Dr. Elmer-Rico E. Mojica

Department of Chemistry and Physical Sciences

Pace University, New York, NY

Propolis, a natural resinous substance collected by honeybees from buds and exudates of plants, is believed to be used in the beehive as a protective barrier against enemies. Also known to be a natural medicine, propolis contains beneficial activities such as antibacterial, antioxidative, antiviral, antimicrobial and many more. Depending on the season, bee species, vegetation, and the area of collection, the chemical composition of propolis are qualitatively and quantitatively variable. In this study, several propolis samples obtained from various parts of the world (Europe, Australia, USA and the Philippines) were analyzed using chromatographic techniques (MS and GC-MS). Based on the results, most samples have different composition with one another.

ORGANIC AND INORGANIC COMPOSITION OF DIFFERENT PHYTOPLANKTON SPECIES BY FT-IR ANALYSIS

Rosie Wenrich and Dr. Alessandra Leri
Department of Natural Sciences
Marymount Manhattan College, New York, NY

Phytoplankton are mostly autotrophic microorganisms that produce organic compounds through photosynthesis or chemosynthesis. Phytoplankton create more biomass than any terrestrial plant, therefore they are a great potential source of biofuels¹. The organic structures of different phytoplankton species differ dramatically in relation to their environment and function. We seek to analyze differences in the organic composition of different species of phytoplankton raised in aquaculture for biofuel production. Fourier Transform Infrared Spectroscopy (FT-IR) was used to analyze the isolated membranes of fourteen different phytoplankton species. The different species analyzed include a variety of microalgae, including diatoms with siliceous skeletons (*Thalassioria* sp., *Rhodomonas lens*, *Chaetoceros muelleri*, *Chaetoceros calcitrans*), dinoflagellates (*Prorocentrum minimum*), cyanobacteria (*Synechococcus* sp.), coccolithophores (*Emiliana huxleyi*, *Isochrysis* sp., *Pleurochrysis* sp.) and several others, many with calcareous skeletons (*Monodus subterraneus*, *Porphyridium cruentum*, *Porphyridium purpureum*, *Chlorella sorokiniana*, *Chlorella protothecoides*). Their membranes are composed of a variety of different molecules including proteins and lipids that can be observed in the FT-IR spectra and quantified in relation to each other.

The spectra reveal a wide variety of organic and inorganic functionalities throughout the different phytoplankton species. While almost every sample shows peaks at about 1645 cm⁻¹ and 1545 cm⁻¹ for amide I and amide II², respectively, and strong broad bands in the range of 3300-3500 cm⁻¹, representing the presence of organic alcohols³, some species present unusual peaks that may represent aromatic or alkenyl molecules such as 3013cm⁻¹ in *E. huxleyi*³. Many spectra contain a strong peak in the range of 1200-900 cm⁻¹, suggesting polysaccharides², silicate frustules⁴ or amorphous CaCO₃⁵. Comparison of functional group peak intensities reveals the relative quantities of lipids, proteins, and other biomolecules among the various phytoplankton.

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EXCHANGE SPECTROSCOPY IN REACTIONS GOING TO COMPLETION VIA COVARIANCE NMR

Chantel Woodard, Amaal Kalds, Brittany Murray and Dr. David Snyder

Department of Chemistry

William Paterson University of New Jersey, Wayne, NJ

Exchange Spectroscopy (EXCY) is a powerful Nuclear Magnetic Resonance (NMR) approach for understanding chemical kinetics and elucidating reaction mechanisms. By tracking exchanges of nuclei between multiple environments, EXCY establishes correspondences between protons on reactant molecules and protons on product molecules, thus establishing the pathway by which reactant molecules transform into products. NMR experiments typically require concentrations of at least 0.1 mM and hence the concentration of exchanged nuclei during a typical EXCY mixing time (0.5-1.0 seconds) must be at least 0.1 mM. Thus, EXCY applies to reactions with (forward) reaction rates of about 0.1 mM/second. Such (forward) reaction rates can only be maintained over the course of a 1-3 hour experiment (the typical acquisition time for 2D NMR data) for reactions at equilibrium. Covariance NMR has shown great promise in maximizing the NMR data obtainable within a given time constraint. Thus the application of covariance NMR potentially allows EXCY to apply to reactions reaching completion in less than the 1-3 hour acquisition time for a full resolution 2D NMR dataset. We report our progress in applying EXCY NMR to two mechanistically interesting reactions: Ruhemann's purple synthesis from an α -amino acid and ninhydrin and thiamine fragmentation. Our progress includes EXCY data for thiamine fragmentation, simulations of the application of Covariance NMR to EXCY data and resonance assignments (in D₂O) for Ruhemann's purple.

STUDY OF ACTIVATED CARBON – HYDROXYAPATITE COMPOSITE MATERIALS

Ebenezer Ewul^{1}, Emmanuel Calderon^{2*}*, Dr. Mihaela Jitianu², and Dr. Andrei Jitianu¹

¹Department of Chemistry, Lehman College, CUNY, West Bronx, NY

²Department of Chemistry, William Paterson University, Wayne, NJ

Hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$) is a common component of the human bones and teeth. Hydroxyapatite promotes the osteogenesis. Another interesting material is activated carbon cloth which has high mechanical strength, high porosity, flexibility and biocompatibility. Moreover, the carbon is partially “digested” by the human body through phagocytosis and partial oxidation. In this study we report the preparation of composite materials between the hydroxyapatite obtained by sol-gel method and the activated carbon cloth. This carbon based composite can replace metallic prosthetic bone replacements which are traditionally used in the bone surgery. The synthesis of the hydroxyapatite was carried out using the sol-gel method. For this, calcium nitrate hexahydrate ($\text{Ca}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$) along with phosphorous pentoxide (P_2O_5) in 200 proof ethanol were employed. The main advantages of the sol-gel method are that it led to homogeneous hydroxyapatite precursor solutions. Using these solutions we were able to obtain uniform coatings on activated carbon cloth by dip coating. The formation of the hydroxyapatite was identified by X-Ray diffraction. The composite materials obtained were characterized using thermogravimetric coupled with differential thermal analysis (TG-DTA), BET surface area. The uniformity of the coatings was visualized using SEM. The resistance to stress of the carbon cloth before and after coating with hydroxyapatite has been investigated by means of oscillatory rotational rheometry, by performing measurements in a wide stress range, along with time recovery investigations.

TITANIA AND HYDROTALCITE – A NOVEL COMPOSITE PHOTOCATALYS

Timothy Mc Clurg¹, Monika Baraniak¹, Naphtali O'Connor², Ravnit Kaur-Bhatia²,
Dr. Andrei Jitianu², Dr. Mihaela Jitianu¹

¹William Paterson University, Department of Chemistry, Wayne, NJ

²Lehman College – City University of New York, Department of Chemistry, West, Bronx, NY

Many organic compounds can be decomposed in aqueous solution in the presence of TiO₂ powders under irradiation with near ultraviolet light into carbon dioxide and water. The photocatalytic reaction takes place on the surface of the TiO₂ particles. When titanium dioxide (TiO₂) absorbs ultraviolet radiation from sunlight or is illuminated by a light source (fluorescent lamps), it will produce pairs of electrons and holes. Because oxygen is not strongly adsorbed on semiconductor surfaces in contact with aqueous electrolytes, it is nearly impossible for an electron not to recombine if it remains free on the particle. Consequently, to keep the photooxidation process going, it is necessary to avoid accumulation of the electrons on particles to ultimately avoid their recombination with the holes. Hydrotalcite has a particular structure that is hypothesized to eliminate the rapid recombination of excited electrons/holes during the photoreaction. Hydrotalcite is a lamellar mixed hydroxide, relatively easy and inexpensive to synthesize in the laboratory. Its structure is based on stacking of positively charged layers with anions and water that confers relatively high mobility to the anions. Hydrotalcites are represented by the general formula $[\text{Mg(II)}_{1-x}\text{Al(III)}_x(\text{OH})_2]^{x+}(\text{A}_{x/m})^{m-} \cdot n\text{H}_2\text{O}$, where A^{m-} is a compensating anion. Hydrotalcite-enhanced TiO₂ has been synthesized using Titanium (IV) isopropoxide, whilst the hydrotalcite constituent has been prepared starting from the corresponding Mg(II) and Al(III) nitrates. Composites have been tested for photocatalytic decomposition of vanillin, showing a high conversion rate into carbon dioxide and water.

STUDIES ON THE INTERACTIONS OF FOUR NANOCERAMICS (METAL OXIDES) WITH SERUM ALBUMIN AND HEMOGLOBIN PROTEINS BY SPECTROSCOPIC TECHNIQUES

Eric Nguyen, Paris Hanson, Tabitha Batte, and Dr. Elmer-Rico E. Mojica
Department of Chemistry and Physical Sciences
Pace University, New York, NY

Nanomaterials are materials with morphological features on the nanoscale, with special properties stemming from their dimensions. The extremely fascinating and useful properties of nanomaterials make them versatile materials in various fields of science ranging from material science, energy, to medicine. Due to this, knowledge on the interactions of nanomaterials with different biomolecules must be obtained. The interactions of four nanoceramics (aluminum oxide, silicon oxide, titanium oxide and zinc oxide) with bovine serum albumin, human serum albumin and hemoglobin proteins were investigated by various spectroscopic methods (absorbance, fluorescence, circular dichroism and line scattering). Results showed aluminum oxide significantly reduced absorbance and emission of all proteins in comparison to the other nanoceramics. Changes in the conformations of proteins were also observed upon mixing with the nanoceramics

SILANE BASED SYNTHESIS OF GELS AND NANOPARTICLES

Benjamin Onyechi, Qiaxian Johnson, and Dr. Bhanu P.S. Chauhan*

Engineered Nanomaterials Laboratory, Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

The utility of gels as ceramics, building materials, and protective coatings is quite widespread. In current times, these gels are also employed in catalysis, therapeutics, and as thickening agents [1]. In particular, gels made up of nanosized particles are important due to their unique physical and chemical properties, which allow one to control parameters such as hydrophobicity, solubility, and passivation. Based on drying method such as critical point drying or aging, nanogels can have applications in the fields of electronics, photonics, and thermal insulation [2]. It is well-established that transition metals, such as copper, cobalt, and palladium, are useful in organic reaction methodologies [3]. By incorporating these transition metals within the nanogel matrices, the organic transformations would be more effective and efficient. In addition, we would be able to control catalytic activity and selectivity by regulating the nanogel pore size, as well as recoverability and recyclability aspects of the catalyst.

In this work, we exploit the amine and silanol moieties of 2-aminoethyl-3-aminosilanetriol (2-AST). This silane is a polydentate ligand that can form complexes via the formation of multiple coordinate bonds with metals. In addition, the silanetriol can hydrolyze and crosslink to generate a silica matrix and eventually a gel [4]. In this study, we developed a one-pot *in-situ* synthetic route that generated nanogels with late transition metals. Due to the uniqueness of 2-AST, which allowed it to remain stable in hydrolytic environments, this synthesis was carried out under aqueous conditions. The formation of nanocomposites were monitored by using UV-Vis, and characterized by TEM, SEM, FT-IR, and NMR. The spectroscopic signatures provide unequivocal evidence that the metal complexes are stable in the silica gel matrix and no leaching was observed when the nanocomposites were subjected to multiple washings in presence of organic solvents. The integrity of the materials was further investigated via TEM and SEM. We are currently studying their catalytic activities and the progress will be reported in due course.

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CHIA GEL MIMICS: NANOSCALE 3D GEL NETWORK REGULATES FOOD INTAKE, A POTENTIAL CONTROLLED DELIVERY MODEL

Neetu Pottackal^a, Priyanka Das^b, Malik Samateh^c and Dr. George John^c

^aEdison High School, Edison, NJ

^bSouth Brunswick High School, Monmouth Junction, NJ

^cDepartment of Chemistry, The City College of New York, NY

Gels – from bacterial cell walls to the human eye – are ubiquitous in nature, and have expedient applications in food, cosmetics and drug-delivery. In particular, hydrogels are classified as either chemical or physical hydrogels. Interestingly, Chia (*Salvia hispanica*) seeds have the unique property to coagulate in water to form a hydrogel. In the past, Mayan warriors consumed chia seeds with their regular meal to slow down the digestion process and lengthen the fighting period. This study aims to explore the fundamental science at the nanoscale level on how Chia seeds form a network. We have found that the seeds are covered with a thin coat of fibers, and when exposed to water, their polar fibers extend outward and interlace with other proximate fibers to form a complex nanoscale 3D gel network. The natural gel creates a physical barrier between the carbohydrates (food) entrapped in the gel and the digestive enzymes. Since the enzymes need to cut through the network fibers to finally reach the entrapped food particles, the conversion of carbohydrates into sugar is decelerated. It is believed that the smart gelation process allows the body to save energy, thus, increasing its stamina. This discovery would improve our understanding of the gelation process of chia and moreover, facilitate the creation of future materials, such as controlled delivery devices. Even more, it could be possibly be used as a preventive medication for diabetes and obesity.

STUDY OF THERMAL STABILITY AND RHEOLOGICAL BEHAVIOR OF THE MELTING GELS

*Gabriela Rodriguez*¹, Timothy Mc Clurg², Monika Baraniak², Lisa C Klein³,
and Dr. Andrei Jitianu¹

¹Department of Chemistry, Lehman College, CUNY, West, Bronx, NY

²Department of Chemistry, William Paterson University, Wayne, NJ

³Department of Materials Science and Engineering, Rutgers University, Piscataway, NJ

Melting gels are silica-based hybrid gels with the curious behavior that they are rigid at room temperature, but soften around 110°C. They are prepared by a sol-gel process, starting with a mono-substituted siloxane, methyltrimethoxysilane (MTMS), and a di-substituted siloxane, dimethyldimethoxysilane (DMDMS). The melting gels were prepared by hydrolysis and polycondensation of the MTMS and DMDMS under acid and base catalysis. The hydrolytically stable methyl groups are retained in the gels, which become irreversible hybrid glasses when heated to higher temperatures. The temperature needed to convert the gels to hybrid glasses increases from 140 to 170°C with an increase in the amount of the di-substituted siloxane.

The thermal behavior of the gels before they transform to hybrid glasses was investigated using thermal gravimetry coupled with differential thermal analysis (TG/DTA) and differential scanning calorimetry (DSC).

To follow the evolution of the molecular structure, oscillatory rheometry studies were carried out on melting gels prior to their consolidation into hybrid glasses. It was found that at room temperature gels behave as viscous fluids, with a viscous modulus, $G''(t, \omega_0)$ that is larger than the elastic modulus, $G'(t, \omega_0)$. As the temperature is decreased, gels continue to behave as viscous fluids, with both moduli increasing with decreasing temperature. The temperature where the moduli cross over is recorded as the glass transition temperature (T_g). In this way the T_g was determined for the studied melting gels.

EXPLORING THE SYNTHESIS OF SOL-GEL BASED HYBRID NANOPARTICLES

Abbas Soloki, Suiying Huang and Dr. Uri Samuni
Department of Chemistry and Biochemistry, Queens College
City University of New York, Flushing, NY

Nanogels are crosslinked polymeric sol-gel based nanoparticles that offer an interior network for incorporation and protection of biomolecules, exhibiting unique advantages for polymer based delivery systems. We have successfully synthesized sol-gel hybrid nanogels by means of silicification reactions including the use of polycationic peptides, like polylysine, as capping agents. Transmission Electron Microscopy, dynamic light scattering and Zeta potential were utilized to characterize the nanogels size, shape, size distribution and aggregation. Macromolecules like Hemoglobin and Myoglobin were encapsulated inside the nanogels. Our initial studies have indicated that the nanogel encapsulated proteins are intact, stable and functional. We are exploring how changes in the conditions of the synthesis and primarily of the capping agents used may allow better control on the properties of the resultant nanogels.

SURFACE IMMOBILIZATION OF AMPs USING CLICK CHEMISTRY

*Maximillian Baria*¹ and Dr. Zhan Chen

¹Chemical & Physical Sciences, Pace University, New York, NY

¹University of Michigan. Ann Arbor, MI

Antimicrobial peptides (AMPs) are a rising topic within research. Compared to antibiotics, AMPs are less likely to develop bacterial resistance. Surface immobilization has been widely used in biochips and biosensors. In this study, AMPs with an azide mutation at different terminus were applied using “click chemistry” for immobilization with alkyne terminated abiotic surfaces. Click chemistry forms a triazole linker, when an alkyne and an azide interact with each other to induce immobilization. Surface immobilization of AMPs was monitored via contact angle to determine the surface characteristics of the alkyne functionalized surface and circular dichroism (CD) determined the abundance of the α -helix and secondary structures of immobilized AMPs. Contact angle results indicated that the alkyne was functionalized on the surface and CD results presented that during surface immobilization the α -helix and secondary structures were protected in the process. This research provides further insight into characterization of surface immobilized biomacromolecules

VIBRATIONAL AND ELECTRONIC PROPERTIES OF CHLORAMPHENICOL

Tabitha Batte, *Eric Nguyen*, and Dr. Elmer-Rico Mojica
Department of Chemistry and Physical Sciences
Pace University, New York, NY

Chloramphenicol, originally derived from the bacterium *Streptomyces venezuelae*, is an inhibitor of bacterial ribosomal peptidyl transferase activity. It is also known as Chloromycetine and Paraxin. In this study, the vibrational (Raman and infrared) and electronic properties (UV-Vis absorbance and fluorescence) of chloramphenicol were obtained. In addition, theoretical calculations were also performed and compared with the experimental results.

ANTIVIRAL ACTIVITY OF NATURALLY DERIVED COMPOUNDS

Lucie Chrastecka, and Dr. Karin Melkonian
Department of Biology
Long Island University, Post Campus, Brookville, NY

Influenza is a deadly disease that is particularly dangerous for those most vulnerable, including little children, senior citizens, pregnant women and people with prior health conditions. In 2010, influenza was listed as the 8th leading cause of death in 2010 killing almost 54,000 people that year. While vaccines are important for prevention of disease, they are not foolproof as seen with this year's flu vaccine which was 23% less effective than last year's vaccine. Antivirals are also available to the public but only serve to lessen the severity of symptoms when given within 48 hours infection. Therefore, new methods of prevention need to be identified. Several natural products/organisms appear to have innate antiviral activity, including Spirulina, (blue-green algae), chitosan (derived from the exoskeleton of shellfish) and hemp oil (from *Cannabis sativa*). I will examine the antiviral properties of each natural "antiviral" against the influenza H3N2 virus using Madin-Darby canine kidney cells as a model organism. This research may provide evidence for potential antiviral substances to be used in the medical and scientific communities, providing new possible protection against the influenza virus in various areas.

β -FIBRIL FORMING STRUCTURES FROM ISLET AMYLOID POLYPEPTIDE, MODIFIED FOR ENHANCED FIBRIL BINDING AND SOLUBILITY

Danielle M. Costanzo, Yara Elrashidy, and Dr. John W. Taylor
Department of Chemistry and Chemical Biology
Rutgers University, Piscataway, NJ.

Amyloid fibril formation and aggregation of the islet amyloid polypeptide (IAPP) is the leading cause of β -cell degeneration and pathogenesis in type II diabetes. IAPP hormone, containing 37 amino-acid residues, is a neuroendocrine regulator of glucose homeostasis that is secreted by pancreatic β -cells. Patients with type II diabetes ineffectively maintain regulatory blood-glucose levels, leading to formation of insoluble IAPP deposits in the pancreas. These misfolded protein deposits form cytotoxic β -fibrils aggregates at very low concentrations, which inhibit the beneficial actions of the hormone. The NFGAIL peptide sequence from IAPP was used to study β -fibril formation, binding, and solubility. It was found that NFGAIL, in branched and unbranched forms, rapidly forms insoluble aggregates at micromolar concentrations. However, when the modified sequence NFGAILKKK was studied, the cationic lysine tail increased the solubility of the peptide, resulting in very slow aggregation only at higher concentrations. Further analysis of these synthetic peptides will investigate the effects of the polylysine-modification, in branched and unbranched analogues, on the fibril formation and solubility of IAPP-derived structures.

EXPRESSION AND PURIFICATION OF CELB2, THE β -1,4- ENDOGLYCONASE, IN *ESCHERICHIA COLI*.

Margaret Morales and Dr. Natalya Voloshchuk

Department of Biochemistry and Microbiology

School of Environmental and Biological Sciences, Rutgers University, NJ

Cellulase, the β -1,4-endoglyconase, hydrolyses cellulose into smaller oligosaccharides. This enzyme presents scientific interest for cellulosic biofuel production as an alternative to petroleum based fuels. Catalytic subunit of the *Streptomyces lividans* cellulase β -1,4-endogluconase, CelB2, was expressed in *Escherichia coli* (*E.coli*) as N-terminal maltose binding protein (MBP) fusion to increase solubility and yield of the functional protein. Removal of MBP was carried out with factor Xa protease. Purification of CelB2 required separation of this protein from MBP and factor Xa. These three proteins, however, have similar molecular weights and pI values and cannot be separated by ion-exchange or size-exclusion chromatography. Therefore, we redesigned the expression vector by cloning in a six-histidine tag at the N-terminus of maltose binding protein. His₆-MBP-CelB2 fusion was successfully expressed in *E.coli*. New CelB2 purification procedure was developed for this expression system.

THE ANTIVIRAL ABILITIES OF NOVEL DABCO-MODIFIED CLOTHS

Elizabeth Stirling and Dr. Karin Melkonian
Department of Biology
Long Island University CW Post, Brookville, NY.

Viruses are internal parasites that hijack an organism's cellular machinery to produce more of itself. There are over 700 different types of viruses that infect humans. Many are responsible for a variety of contagious diseases that result in tens of thousands of deaths per year. Influenza virus alone is responsible for more than 200,000 hospitalizations and 24,000 deaths/year in the US. These numbers will continue to increase as evidenced by the recent Ebola and Enterovirus outbreaks. The ability to protect our healthcare workers, the general population and our military is critical. To this end, I have shown that a novel DABCO-hydrocarbon molecule covalently bound to cotton cloth has the ability to reduce the number of T4 virus particles available for infecting bacteria. Using detergents, I have shown that a charge interaction between the positively charged cloth and the negative tail fibers of the virus are responsible for this reduction in virus. Essentially, the cloth acts like a "virus-magnet", removing the virus from the environment. These cloths could provide a "first line of defense" protective measure for those in the medical field as well as the general public against viruses. In the medical field, these modified cloths could be used to attract viruses before they reach medical personnel beneath their gowns or scrubs. The modification could be added to airplane air filters to attract and trap respiratory virus particles that are re-circulated during a flight. In addition, these cloths could help protect our military forces from biological attacks.

PYROAURITE – STRUCTURAL AND TEXTURAL CHARACTERISTICS AS A FUNCTION OF CATION COMPOSITION

Jonathan Gabriel¹, Helen Quinones¹, Jessica Lopez¹, Aarti Patel¹,
Dr. Andrei Jitianu², and Dr. Mihaela Jitianu¹

¹Department of Chemistry, William Paterson University of New Jersey, Wayne, NJ

²Department of Chemistry Lehman College – City University of New York,
Bronx, NY

Pyroaurite-like compounds belong to the large class of anionic clays and are natural minerals with a layered double hydroxide structure with the general formula $[\text{Mg}(\text{II})_{1-x}\text{Fe}(\text{III})_x(\text{OH})_2](\text{CO}_3)^{2-x/2} \cdot m\text{H}_2\text{O}$. The naming of the family of these compounds derives from the mineral hydrotalcite, $[\text{Mg}_6\text{Al}_2(\text{OH})_{16}](\text{CO}_3)_4 \cdot 4\text{H}_2\text{O}$, a naturally occurring mineral which consists of brucite-like positively charged layers resulting from partial substitution of Mg(II) with Al(III), the positive charges being compensated by CO_3^{2-} ions, located in the interlayer region along with water molecules. Surface properties and morphology of different pyroaurite anionic clays have been studied as a function on their chemical composition. Nanostructured pyroaurite anionic clays have been synthesized for various cation ratios and characterized structurally by X-Ray diffraction, FTIR spectroscopy. Morphology and surface properties were assessed by transmission electron microscopy TEM and BET surface analysis.

SURPRISING ACTIVITY AND SELECTIVITY OF POLY(METHYLHYDROSILOXANE) INDUCED REDUCTION OF POLYBUTADIENES

Amanda Kolenski, Aarti Patel and Dr. Bhanu P. S. Chauhan*
Engineered Nanomaterials Laboratory, Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

Producing polymers with desirable physical and chemical properties and functional groups can oftentimes be difficult and/or expensive to achieve by conventional methodologies. Therefore, one-pot hydrosilylation of unsaturated polymers offers a convenient method for preparing silane-modified polymers that have found applications as rubber materials, adhesives, and drug delivery agents.¹ Additionally, studies have shown the effectiveness of selectively reducing polybutadienes to prepare various novel polymers.² Polybutadienes are a suitable and practical starting material for modifications because of their wide range of molecular weights and well-defined microstructures.³ Due to the important applications of such polymers, there is a need for better understanding the factors that influence the regioselectivity, catalytic activity, solubility, and tacticity of resulting modified materials.⁴

In this presentation, we disclose a systematic and high-yielding approach to selectively reduce polybutadienes in presence of green reducing agents such as, poly(methylhydrosiloxane) (PMHS). This catalytic process is achieved in the presence of palladium complexes. We have found that depending on the tacticity and stereochemistry of butadienes, PMHS induces the selective reduction of palladium complexes to Pd-nanoparticles. We have also observed that Pd-nanoparticles eventually are the real catalyst in the reduction of cis-polybutadienes. In addition, we have carried out a competitive experiment which show that only the cis-isomer of polybutadiene was predominantly reduced in presence of other isomers. These results including mechanistic implications, detailed NMR, IR, UV-Vis, and TEM analysis of the products will be discussed in detail. Furthermore, we will present a new method to produce cis-polybutadiene containing PMHS gel, which acts as a host material for palladium nanoparticles. This bodes well since such a nanocomposite can be used as a recyclable catalyst for industrial applications.

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*Indicates the Corresponding Author

ENVIRONMENTALLY FRIENDLY ALTERNATIVES TO CHLORINE BLEACHING IN LAUNDRY APPLICATIONS

Katherine Ness and Dr. Alessandra Leri
Department of Natural Sciences
Marymount Manhattan College, New York, NY

Fabrics are composed of natural and synthetic fibers consisting of chemically complex macromolecules, which are frequently laundered using chlorine-containing bleach. The use of chlorine-containing bleach in the United States dates back to the 18th century¹. This type of bleach contains hypochlorite, a powerful whitener and microbicide that is effective on a variety of surfaces in both industrial and residential settings¹. Chlorine bleach is widely used in the laundering of fabrics even though this form of laundering diminishes the longevity of the fabric, the brightness of the dyes and cannot be safely used on colored fabrics.

Although hypochlorite bleach has proven beneficial throughout many years of use, there is reason to explore alternative bleaching methods due to the harsh and reactive nature of chlorine. Chlorine bleach has been shown to produce both chloroform and carbon tetrachloride in the headspace of covered glass jars². Both chloroform and carbon tetrachloride have been shown to contaminate laundry effluent, which becomes part of municipal wastewater². Additionally, laundering cotton fabrics with chlorine bleach has been shown to produce organochlorine by-products³. These by-products were found to remain within fabrics for several months after washing with chlorine bleach under household conditions³. The existence of organochlorine in cotton fabric poses potential health hazards with consequences that are not fully understood.

A promising alternative to hypochlorite, ozone (O₃) bleaching, has been shown to effectively bleach cotton fabrics while causing less harm to the strength of the fabric⁴. In collaboration with textile engineers based in Turkey, we have embarked on an investigation into alternative methods of stain removal and sterilization. Cotton and polyester fabric samples were subjected to a variety of non-chlorine bleaching treatments, including treatment with ozone. Using chlorine-specific X-ray absorption spectroscopy (XAS), performed at the National Synchrotron Light Source at Brookhaven National Laboratory, we investigated the production of organochlorine by-products in fabrics following various treatments. Our results show that the alternative bleaching methods do not produce organochlorine by-products, in contrast with fabrics treated with conventional chlorine bleach. This suggests that alternative treatments, including ozone, provide effective bleaching without the formation of organochlorine residues.

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A NEW μ -NITRIDO BRIDGED CHROMIUM (V) SPECIES

Julie Niklas and Dr. Colin Abernethy
Department of Chemistry
Sarah Lawrence College, Bronxville, NY

Mono-Cp metal halide complexes, especially those of the early transition metals, serve as starting points for a wide range of elegant, controlled reactions. Nitrides of these complexes are incredibly rare, but can be used as N-atom transfer agents and catalysts, giving them a key role in organometallic chemistry. A new rational, high yield synthesis of $[\text{Cp}^*\text{CrCl}_2]_2$ was adapted from the syntheses of Cp^*TaCl_4 , Cp^*NbCl_4 , and $[\text{Cp}^*\text{VCl}_2]_3$, using Cp^*SnBu_3 as a mild Cp^* donor to form the desired half-sandwich complex, a Cl-bridged analogue of a previously characterized vanadium complex. In addition, a dinuclear Cr(V) complex, $[\text{Cp}^*\text{Cr}(\mu\text{-N})\text{Cl}]_2$, was formed upon reaction with $(\text{CH}_3)_3\text{SiN}_3$ and shows promising reactivity towards a variety of sterically demanding didentate ligands. Spectroscopic analysis of this compound has indicated a product mixture with unexpected structures.

SYNTHESIS OF NEW MONO(INDENYL) COMPLEXES OF VANADIUM

Sheila Pollozi and Dr. Colin D. Abernethy
Department of Chemistry
Sarah Lawrence College, Bronxville, NY

Mono(cyclopentadienyl) complexes of vanadium have been prepared and studied, since the cyclopentadienyl ligand serves to stabilize vanadium in a variety of oxidation states and also imparts solubility in common organic solvents. However, in contrast to cyclopentadienyl, indenyl complexes of vanadium have received much less attention. This is surprising as the indenyl ligand, through the *Indenyl Effect*, has demonstrated to enhance the reactivity of many metal complexes, compared to its cyclopentadienyl analogue. The research has focused on the preparation and characterization of new mono(indenyl) vanadium complexes, formed by the reactivity of bis(indenyl) vanadium with imidazolium chlorides, pyridinium tribromide and dipp-BIAN. The poster will discuss how the η^5 -to- η^3 coordination shift of cyclopentadienyl and indenyl occurs in vanadium complexes and how this rearrangement contributes to faster reaction rates and smaller activation energies when it comes to indenyl and its well-known effect, implying further reactivity for the reactions performed during this senior thesis compared to previously known ones with cyclopentadienyl ligands.

BIAN COMPLEX OF NIOBIUM

Tianjie Zheng and Dr. Colin Abernethy
Chemistry Department
Sarah Lawrence College, Bronxville, NY

There is currently great interest in the use of bis[*N*-(2,6-diisopropylphenyl)imino]acenaphthene (dipp-BIAN) as a didentate ligand for the synthesis of catalytically active transition metal complexes. However, despite the extensive use of BIAN ligands in both main group and late transition metal chemistry, BIAN complexes of early transition metals still remain rare. To date, only a handful of BIAN complexes of titanium, vanadium, and tantalum have been characterized. Importantly, there is still no example of a BIAN complex of niobium reported in the literature. In this poster, the reaction of dipp-BIAN towards a number of Lewis acidic niobium halides will be discussed and the synthesis and structure of the first ever characterized example of a (BIAN)niobium complex will be reported.

AMYLOID-PERTURBING DYES INHIBIT ADHESION OF *CRYPTOSPORIDIUM PARVUM* TO THE HUMAN ILEOCECAL ADENOCARCINOMA HCT-8 CELL LINE

^{1,2}Dustin Lee and ^{1,2}Dr. Cho X.J. Chan

¹Haskins Laboratories, Pace University, New York, NY

²Department of Chemistry and Physical Sciences, Pace University, New York, NY

The waterborne intestinal parasite *Cryptosporidium parvum* causes a life-threatening disease in immunocompromised people with no effective treatment available. Cryptosporidiosis is found worldwide and is only self-limiting in immunocompetent individuals. Bioinformatics analyses indicate that there is one amyloid-positive sequence in *C. parvum*'s mucin-like adhesion protein. Surface amyloid-forming sequences in *Candida albicans* mediate intercellular binding and cell-substrate adhesion; additionally, amyloid-perturbing dyes inhibit *C. albicans*' binding and adhesion (Lipke et al. 2014). *C. parvum*-infected host HCT-8 cells undergo an endoplasmic reticulum stress response (Morada et al. 2013). Intracellular putrescine levels of infected host cells increase 2.5-fold after 15 hours. Polyamines, such as putrescine, are cationic molecules that are crucial for the growth of all living cells. Attachment is essential for the infection of host cells; therefore we tested whether anti-amyloid dyes would decrease adhesion of the parasite *C. parvum* to host ileocecal HCT-8 cells, resulting in a reduced endoplasmic stress response of infected HCT-8 cells. We stained *C. parvum* sporozoites with amyloid-reporting compound thioflavin S and ascertained the sporozoites' amyloid dye fluorescence. We treated the parasite's sporozoites with amyloid-binding compounds thioflavin S, thioflavin T, and Congo red. Merifluor *Cryptosporidium*/*Giardia* Direct Immunofluorescence Assay (DFA) was used to detect oocysts following a 15-hour infection and high-performance liquid chromatography (HPLC) was used to measure intracellular polyamine levels after a 19-hour infection. Infected HCT-8 cells emitted a twofold increase in fluorescence compared to uninfected HCT-8 cells. HCT-8 cells with Congo red- and thioflavin T-treated sporozoites showed a similar fluorescence to uninfected HCT-8 cells. In comparison, HCT-8 cells infected with Congo red- and thioflavin S-treated sporozoites displayed unchanged putrescine and spermidine levels. These results report an effect of the amyloid-binding compounds on parasitic adhesion to host cells, as well as on the stress response of infected host cells. A deeper understanding of the role amyloids play in *C. parvum*'s adhesion to its host can aid in the development of a targeted therapy against this disease.

INVESTIGATING THE ROLE OF CPAR-1 IN CELL DIVISION

Gabriel Makar and Dr. Joost Monen
Theoretical and Applied Sciences
Ramapo College of New Jersey, Mahwah, NJ

CENP-A is a highly conserved Histone-H3 like protein, critical to centromere specificity and kinetochore assembly in all eukaryotes. Failure to properly produce or localize CENP-A leads to aneuploidy and cell death. In most organisms CENP-A has a single variant; however, in the nematode *C.elegans* CENP-A has two homologs, HCP-3 and CPAR-1. Based on previous studies, HCP-3 is responsible for specifying the centromere and thus critical for chromosome segregation in mitosis. CPAR-1's role however remains to be elucidated, albeit CPAR-1 is known to be essential as CPAR-1 mutants are embryonic lethal. The first step in understanding the role that CPAR-1 plays in embryonic development is to characterize where CPAR-1 localizes endogenously. To this effect, we are utilizing an immunofluorescence assay, which allows us to visualize chromosomes, microtubules, and the CENP-A homologs in the developing embryo to get a sense of where these proteins localize in the dividing cells. To date, we have an HCP-3 specific antibody that localizes to the centromere, and we are in the process of developing a CPAR-1 specific antibody for comparison. To test the functional role of CPAR-1, we are utilizing time-lapse microscopy to visualize microtubules and chromosomes in a dividing embryo and comparing wild-type to CPAR-1 deficient embryos. Here, we will describe our current progress, future molecular strategies and experimental design to assess the role of CPAR-1 in cell division. Through these studies, we will better understand what role CPAR-1 plays in embryonic development, and perhaps gain insight into a divergent role for CENP-A not yet characterized.

THE ROLE OF THE INSULIN SIGNALING PATHWAY IN DETERMINING GENITALIA SHAPE IN DUNG BEETLES

Michelle Martinez and Dr. Harald F. Parzer

Department of Biological & Allied Health Sciences
Fairleigh Dickinson University-College at Florham, Madison, NJ

Male insect genitalia exhibit high phenotypic diversity between even closely related species and are thought to play an important role in speciation. However, little is known about the development of size and shape of these organs.

Nutrition is a well-understood common factor in determining the overall size as well as the trait size in animals and shape of an organism. The insulin signaling pathway has been shown to mediate such growth patterns through a variety of mechanisms, including controls multiple factors of organisms, such as metabolism, lipid and protein synthesis. This pathway also plays a role in the size of mating traits in species such as insects, whose size is mainly dependent on their nutrition. In fish and insects, it is responsible for the proportion of body size and also the size of mating organs in these species. Finally, the insulin signaling pathway is responsible for the proportion of body size and studies have been done to attempt to show the relationship between this pathway and genitalia size in male insects. The mechanism by which an organism modulates these functions is through an important regulator of the insulin signaling factor. The Forkhead Box O transcription factor (known as FOXO), serves as a regulator of growth in the organism through inhibitory or excitatory pathway modulation. However, even though evidence is accumulating that the insulin signaling pathways plays an important role in the development of trait size, little to nothing is known about its role in the development of trait shape. To address this question, we used the dung beetle species *Onthophagus taurus* which were exposed to reduced expression of FOXO (through RNAi). A previous study using the same method has shown that the insulin signaling pathway is affecting genital size of this species. To further our understanding of genital development through the insulin signaling pathway (and thus nutrition), we compared these results with potential changes in genital shape. To do so, we used geometric morphometrics which allows us to distinguish between shape and size. We predict that genital shape will be similarly affected by the insulin signaling pathway.

CELLULAR RESPIRATION AS A TRIGGER FOR MULTICELLULAR BEHAVIOR IN *Staphylococcus Aureus*

Adriana van de Guchte, Ameya A. Mashruwala, and Dr. Jeffery M. Boyd

Department of Microbiology and Biochemistry
Rutgers University, New Brunswick, NJ

Staphylococcus aureus is a health concern worldwide and a leading cause of biofilm related infected. The bioavailability of oxygen in the human body and infected issue varies and we hypothesized that *S. aureus* would sense and respond to the presence of oxygen by altering its multicellular behavior. We find that multiple *S. aureus* clinical isolates form robust biofilms when cultured in the absence of oxygen. Although oxygen is a cell diffusible signal our data suggest the effect of oxygen on biofilm formation is a result of its role as a terminal electron acceptor (TEA). We find that decreased concentrations of TEA result in an impaired ability of *S. aureus* to respire and this causes the bacterium to switch to a multicellular lifestyle mode. Consistent with this hypothesis we find that supplementation of anaerobic biofilms with nitrate, an alternate TEA, results in reduced biofilm formation. Biofilm formation can be the result of either stochastic or deterministic cellular processes. We find that biofilm formation under conditions of impaired respiration is a deterministic process and the lack of a TEA is sensed by a membrane bound two-component regulatory system called SrrAB. Our data suggest that respiratory flux through electron transport chains alters the redox status of the cellular quinone pool thereby altering SrrAB activity. Finally, we show that upon sensing the cellular respiratory status SrrAB sets in motion a programmed cell death (PCD) response, which results in the release of extracellular DNA and increased biofilm formation.

ANALYZING EXTRACELLULAR VESICLE RELEASE IN *C. ELEGANS* COELOMOCYTES

Aayush Visaria, Dr. Anne Norris, Dr. Barth Grant
The Department of Cell Biology & Neuroscience
Rutgers University, Piscataway, NJ

Increasing evidence is accumulating suggesting that most cells, ranging from bacterial cells to mammalian cells, release extracellular vesicles (ECVs). These vesicles can be produced by budding off the plasma membrane, becoming induced by apoptosis, or by fusion of multivesicular bodies with the plasma membrane. *C. elegans* sensory neurons have been shown to release extracellular vesicles into the exterior environment, but there is yet to be documented evidence of ECV release from non-mammalian, sub-epithelial cells (Wang et al., 2014). The objective of this study is to analyze large, previously uncharacterized ECVs (>1000 nm) that are found to be released from *C. elegans* coelomocytes. Coelomocytes are scavenger cells that continuously endocytose pseudocoelomic fluid but do not have a vital, known function. There are three pairs of coelomocytes. Each pair is localized in each of the anterior, middle, and posterior regions of the worm. Using epi-fluorescent imaging with various transgenic strains, ECV production was analyzed as a function of age, exposure to specific bacterial contaminants, and localization within the worm. It was found that SNX-1, a BAR-domain protein that is part of the core retromer complex, affects ECV production. Certain bacterial contaminants, specifically *Stenotrophomonas maltophilia*, are able to increase ECV production. Furthermore, there is an aging phenotype with regards to ECV release. Not only do the number of ECVs as a function of age exhibit a bimodal distribution, localization of the ECVs within worms also show a distinct pattern. These results indicate that ECV production changes under specific conditions and may serve a purpose, such as for proteotoxic waste regulation or intercellular communication.

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CAUSES OF *BROMELIA PINGUIN* DOMINANCE IN LOWLAND WET FORESTS AND ITS EFFECTS ON PLANT DIVERSITY IN COSTA RICA

Katherine Andrade, Alessa Vindas-Cruz, and Dr. Daniela Shebitz
Environmental and Sustainability Sciences
Kean University, Union, NJ

Bromelia pinguin is a plant species found in the northern area of Costa Rica at the Maquenque National Wildlife Refuge (MNWLR), where the lowland wet forests are severely threatened. *B. pinguin* transforms the understory by growing in dense patches. This study determined what environmental variables contribute to *B. pinguin* forming dense monocultures and how its dominance influences other plants. A survey was conducted to measure the dimensions of each *B. pinguin* patch within 1 km² of primary forest. The recorded *B. pinguin* patches ranged from 6.7m² to 2082m². Abiotic variables and plant data suggest that *B. pinguin* dominant patches (BDPs) are most pronounced on south facing slopes. Ten randomly selected BDPs were extensively studied in their center, edge and outside of the plot. Center plots had significantly less species diversity while simultaneously having a greater total percent cover of understory. Interestingly, diversity recovered immediately at the edge and outer plots, suggesting that the effects of *B. pinguin* are restricted just to where it is the dominant species.

TAXONOMIC APPROACH TO STUDYING THE IMPACTS OF VISITATION AND SPACE ON THE BEHAVIOR OF CAPTIVE PRIMATES

Megan Cody and Dr. Brian Olechnowski
Department of Biological and Allied Health Sciences
Becton College , Fairleigh Dickinson University, Madison, NJ

Zoological parks provide benefits to the public in terms of education and conservation awareness. Despite these benefits, it is important to continuously monitor and scrutinize the well-being of the animals on exhibit. This research examines the effects of visitor density and exhibit space on primate behavior. This study focuses on various captive primate species representative of four primate families: Lemuridae, Callitrichidae, Cercopithecidae, and Hominidae. We hypothesize that the most basal primates, lemurs (Lemuridae), will exhibit the fewest number of behaviors; while, the species representative of the most derived family, Hominidae, will exhibit the widest range of behaviors in captivity (most complex behavioral patterns). Additionally, we hypothesize that great apes will exhibit the most pronounced change in behavior as a result of their captive environment. Alternatively the Prosimians, the most basal group of primates, are expected to have more programmatic behaviors less affected by external factors. We expect to see an increase in stress related behaviors as the number of visitors increases and space decreases. These negative (agonistic) behaviors include hair pulling, teeth clenching, body rocking, intragroup aggression, and audience directed aggression. Individual subjects were sampled for ten minutes each at ten second intervals using the focal observation rule. Social interactions and object use were exhibited significantly more among Hominidae species compared to the more primitive primate families. Movement was significantly reduced in Hominidae species when visitor density was high, while autogrooming behavior was expressed significantly more. Excessive autogrooming in the presence of many visitors may be considered an agonistic behavior. Results from this study will continue to enhance our understanding of captive primate behavior, and will guide zoo managers in establishing an ideal environment for both animals and visitors.

ARE OVERWINTERING TADPOLES MORE TOLERANT OF ROAD SALT RUNOFF?: ASSESSING THE ACUTE EFFECTS OF SODIUM CHLORIDE (NaCl) AND CALCIUM CHLORIDE (CaCl₂) EXPOSURE ON LARVAL AMPHIBIANS IN NORTHWESTERN NEW JERSEY

Mariano J. DelValle and Dr. Meagan L. Harless
Department of Mathematics and Natural Sciences
Centenary College, Hackettstown, NJ

Chemical deicers are commonly used to remove and prevent the formation of ice on roadways. Two of the most commonly used deicers are sodium chloride (NaCl) and calcium chloride (CaCl₂). Once applied, these chemicals often wash away into nearby water bodies and may harm freshwater species. Sensitive species such as amphibians are likely to be one of the most vulnerable creatures in the water. American bullfrog (*Lithobates catesbeianus*) tadpoles typically take more than one year to complete metamorphosis. Thus, they are likely at greater risk of exposure to high concentrations of chemical deicers when using roadside habitats. Little is known about the sensitivity of this species during this period of development. We exposed overwintering larvae to a range of concentrations of both NaCl and CaCl₂ in order to estimate the median lethal concentration (LC₅₀) for each of these deicers. We also monitored the salinity, pH, and conductivity in local water bodies that were both close to and far from salt treated roadways from November to January. Larvae were more sensitive to short term exposure to CaCl₂ (LC_{50-96h}: 5.38 mg/L) than NaCl (LC_{50-96h}: 8.54 mg/L). Our water chemistry analysis suggests local water bodies receive deicer runoff in winter months and this may negatively impact the survival of *L. catesbeianus* larvae. This analysis suggests that larvae adopting this life history strategy may be at greater risk of lethal exposure to these deicers as overwintering tadpoles.

ANALYSIS OF ARABIAN SEA DEEP-WATER SEDIMENT TRAP PARTICULATES VIA MICROSCOPY AND IR SPECTROSCOPY

Austin Gellis and Dr. Alessandra Leri
Department of Natural Sciences
Marymount Manhattan College, New York, NY

We are conducting a biological and chemical analysis of marine particulates in order to better understand changes in composition and decomposition rate. Sediment traps were deployed throughout the 1990s at various depths in the Arabian Sea to collect sinking particulate organic matter (POM)^{1,2}. Through microscopic analysis of these samples, we reveal an abundance of coccolithophores, including *Emiliana huxleyi* and siliceous microorganisms like diatoms. All samples examined under the light microscope were collected from Mooring Station 1, on a shelf close to the coast of Oman. An abundance of coccoliths, diatoms and silicoflagellates were present in most samples; intact coccolithophores were found in one sample. Coccolith plates and foraminifera composed a majority of the identifiable calcareous detritus under 12.5 μm in diameter. Diatoms composed a majority of the siliceous phytodetritus with traces of silicoflagellates.

We also analyzed these samples by IR spectroscopy to find relationships between organic structure and depth, seasonal processes like monsoons, and location in the Arabian Sea³. FT-IR spectroscopy reveals composition of sinking POM on a molecular level. A dominant peak around 1412-1440 cm^{-1} reveals an abundance of carbonate. Lipids and proteins appear as an amide I peak around 1654 cm^{-1} , which may represent the remnants of membranes of various microorganisms. Aliphatic hydrocarbons appear at 2918 cm^{-1} to 2852 cm^{-1} in varying abundance among samples. Many marine plankton have mineralized SiO_2 or CaCO_3 shells; thus, quantifying silica and carbonate levels at various locations and depths may reveal the rates of biological productivity and organic matter degradation. Using the FT-IR spectra, we calculated carbonate to silica ratios, giving insight into relative rates of decomposition as POM sinks down the water column. Further analysis will give us a greater understanding of composition as a function of depth, seasonal patterns, and locations. Our data will ultimately clarify these variables within the marine carbon cycle and illuminate molecular-level transformations of marine organic matter.

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²Honjo, Susumo *et al.* "Monsoon-controlled export fluxes to the interior of the Arabian Sea" *Deep-Sea Research II: Tropical Studies in Oceanography* **46** (1999): 1860-1897.

³Hatcher, Patrick G. *et al.* "Diagenesis of Organic Matter in a 400 m Organic Rich Sediment Core from Offshore Namibia Using Solid State ^{13}C NMR and FTIR." *Organic Geochemistry* **75** (2014): 8-23.

RECONSTRUCTING SEAWATER Sr/Ca THROUGH THE LATE PHANEROZIC FROM FOSSIL SHARK TEETH

Bryan Gonzalez and Dr. Michael Griffiths

Department of Earth and Environmental Science

William Paterson University of New Jersey, Wayne, NJ

Rutgers, The State University of New Jersey, School of Environmental and Biological Science, Institute of Marine and Coastal Science, New Brunswick, NJ

Constraining past seawater Sr/Ca ratios is an important and challenging task to scientists, because the chemical evolution of these two cations is fundamentally tied to various geologic and biogeochemical processes related to plate tectonics, weathering, diagenesis, and the carbon cycle. On geologic timescales, shifts in seawater Sr/Ca (Sr/Ca_{sw}) are thought to reflect variations in either the sources of Sr and Ca—which include riverine inputs via weathering, hydrothermal circulation, and calcium carbonate dissolution—or the output flux via carbonate sedimentation. By improving our understanding of seawater Sr/Ca evolution, we can thus potentially gain a deeper understanding of how these processes (controlling these fluxes) have operated on geologic timescales. Ancestral sharks are unique in that they have a globally robust and continuous fossil record since the late Cretaceous. This fossil record is comprised largely of teeth due to: 1) rapid and continuous replacement throughout an animal's lifetime; and 2), their dense, biogenic apatite composition which is highly resistant to chemical and physical erosion. Over the past decade, marine biogenic apatite—specifically enameloid (comprising the dense crown tissue) in modern and fossil shark teeth—has exhibited some success in providing a new tool for reconstructing the evolution of the world's oceans. This is largely due to the fact that enameloid has been shown to accurately preserve the aqueous conditions of the seawater (i.e. isotope and elemental composition) at the time of tooth formation. Preliminary results of this study demonstrate that the Sr/Ca_{sw} has overall declined since the late Cretaceous (~75 million years ago), a finding that is echoed in other marine fossil assemblages. Whilst this work is still in its infancy, we tentatively interpret the decline Sr/Ca_{sw} to be a regionally (and potentially global) coherent signal, and as such, provides a new record of Sr and Ca flux to the paleo-ocean.

PARASITE COMMUNITIES ALONG A RIVER CONTINUUM IN THE NEW JERSEY PINELANDS

Ryan W. Koch and Dr. Michael V. K. Sukhdeo
Ecology, Evolution and Natural Resources
Rutgers University, New Brunswick, NJ

Free-living community composition changes along a river gradient from upstream to downstream, and the River Continuum Concept (RCC) predicts shifts in macroinvertebrate communities that are linked to the physical characteristics of the river. While this idea has been developed for free-living communities, it is largely unknown how parasite community composition also changes along the river continuum. This study will test the hypothesis that parasite diversity correlates with host communities along the continuum. We sampled two rivers, the Mullica and the Batsto, located in Wharton State Forest in the New Jersey Pinelands, in August and September of 2014. Three sites were selected from each river based on variation in stream depth, width, and canopy cover. Sunfish (family Centrarchidae) were collected (n=20) from each site and necropsied for macroparasites. Macroinvertebrate samples were collected from each site using a dip net (n=3), sorted into functional feeding groups (FFG), and examined for parasites. A total of 8 parasite species were recovered from these sampling locations, and most sites were dominated by parasitic nematodes. Shannon's diversity index was used to evaluate parasite diversity among sites. In the Mullica River, parasite diversity declined as we sampled downstream (upstream = 1.36, midstream = 1.06, downstream = 0.6). The invertebrate community of the Mullica River followed the RCC and consisted of 35% shredders and 20% collectors upstream and 3% shredders and 92% collectors downstream. However, in the Batsto River, parasite diversity increased as we sampled downstream (upstream = 0.88, midstream = 1.12, downstream = 1.5), and the invertebrate community did not follow the RCC. Shredder abundance was positively and strongly correlated with acanthocephalan abundance ($R^2 = 0.8352$, and $p \leq 0.05$). These results suggest that macroinvertebrate functional feeding groups may be important in structuring parasite communities along these two rivers. This study measured both biotic and abiotic factors along rivers, and the data suggests that the biotic component is the dominant force controlling parasite communities in these rivers.

DEFYING ALL ODDS: UNDERSTANDING THE ABILITY OF HEAVILY CONTAMINATED SOIL TO SUSTAIN LIFE

Danielle Le Roux, Thamanna Misbah, and Eleanor Ojinnaka and Dr. Nina Goodey

Department of Chemistry and Biochemistry
Montclair State University, Montclair, NJ

Liberty State Park (LSP) was formerly a rail yard and dumping ground for chemical waste. Now, the park sustains a flourishing variety of vegetation, and a vibrant and diverse ecosystem. This means that the soil at LSP successfully produces the enzymes that catalyze ecological reactions necessary for forest growth. In fact, preliminary data show that the site with the highest heavy metal concentration at LSP has the highest enzyme activity compared to other less contaminated sites and a control site with no history of heavy metals. This presents an interesting anomaly because research shows a negative correlation between the concentration of heavy metals and enzyme activity. This experiment aims to understand the unprecedented ability of the contaminated soil to foster growth despite its history of severe heavy metal contamination. Properties of the soil are analyzed with respect to distinct particle sizes: coarse sand (425 – 2000 μm), fine sand (75 – 425 μm), silt (2 – 75 μm) and clay (< 2 μm). The properties studied were the exchangeable metal concentration, percent organic matter and pH measurements. Exchangeable metals are the metals that are loosely bound to the soil and their extraction can provide insight into the location of the metals in the different size fractions. Organic matter is essential for the health and productivity of the soil. Additionally, both the organic matter and the pH correlate with the presence and movement of heavy metals in the soil. Collectively, these properties examine the function of each particle size fraction in the enzyme activity of the soil. Two other soil sites with the same natural succession as LSP 14/16 were analyzed for comparison. Hutcheson Memorial Forest (HMF), located in Franklin Township, NJ was used as the control site with no history of heavy metal concentration and Site 43 of LSP was used as the site with mid-range levels of contamination. The results of the experiments should show significant differences among the sites, since each site is unique in its concentration of metals and enzyme activity. By examining the implications of exchangeable metals, percent organic matter and pH measurements on the particle size fractions of the soil, we hope to gain insight into the unusually high enzyme activity of LSP site 14/16.

GENOTYPICALLY DIVERSE PLANTINGS OF AMMOPHILA BREVILIGULATA SHOW GROWTH AND ALLOCATION DIFFERENCES UNDER WATER STRESS

John F. Sferruzza, Paige Appleton, and Dr. Michael S. Peek
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

The current practice of vegetating the coastal dunes utilizes only one genotype of American beachgrass referred to as 'Cape' (*Ammophila breviligulata*). Therefore, genetic diversity of the restored dunes is low, which in turn can or influence short- or long-term dune establishment, performance and stability. Genetic diversity often increases population and community performance in mixture relative to that of monoculture due to niche complementarity. We therefore hypothesized mixed pots of American beachgrass would outperform monocultures under similar conditions. We evaluated this hypothesis using mixed pots with 3 strains per pot compared to monoculture pots with one two and three plants per pot. No significant effects in growth or allocation were observed. We then evaluated mixture and monoculture performance under water limiting conditions. Mixture biomass increased significantly under water limiting conditions suggesting more efficient resource utilization. These findings help to give a better understanding of how genetically diverse plants can influence dune restoration.

**EFFECT OF HIGH LIGHT INTENSITY ON POLYKETIDE SYNTHASE
GENE EXPRESSION IN THE FLORIDA RED TIDE DINOFLAGELLATE,
*Karenia brevis***

Unnati Chauhan, Daniel Lupo, and Dr. Emily A. Monroe
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Karenia brevis is the toxic dinoflagellate endemic to the Gulf of Mexico that causes detrimental human health, environmental, and economic impacts through the production of brevetoxins. Brevetoxins are polyketide compounds produced by polyketide synthase enzymes (PKS), but no gene or protein has been linked to their biosynthesis. Previous work on a PKS protein, KB2006, suggests a link between chloroplast physiology and toxicity. To test the effect of high light (HL) intensity on PKS gene expression in toxic *K. brevis* (GB) and non-toxic *K. brevis* (NTB), 1-liter cultures were exposed to HL treatment ($\sim 100 \mu\text{mol photons m}^{-2}\text{s}^{-1}$) after reaching mid-log phase in control light intensity ($\sim 60 \mu\text{mol photons m}^{-2}\text{s}^{-1}$). Samples for cell counts and gene expression were taken at T0 (prior to HL treatment) and T5 (5 days post HL treatment) for control and HL cultures. HL treatment had no effect on growth of the toxic strain (GB). However, NTB cultures entered stationary phase directly after the HL treatment while control NTB cultures remained in log phase for six days after T0. There were no differences in expression of KB2006 between the control and HL cultures at the transcript level analyzed by qPCR. At the protein level analyzed by western blotting, KB2006 decreases in abundance over time, between T0 and T5, in both GB and NTB *K. brevis*. Under HL treatment, KB2006 protein abundance increases in GB but not in NTB. Additional analyses are underway to examine effects of HL on brevetoxin production. Developing a better understanding of biosynthetic pathways involved in brevetoxin production will play a pivotal role in management of future algal blooms.

CREATING A *CLAMP* NULL USING THE *CRISPR/Cas9* SYSTEM IN VITRO

Caroline Doherty, Dr. Erica Larschan and Dr. Jennifer Johnson
Department of Molecular and Cell Biology
Brown University, Providence, RI

In all organisms, gene regulation is crucial for proper cell function and development. Dosage compensation is one such mechanism of gene regulation. In *Drosophila melanogaster*, dosage compensation is mediated by the MSL (Male Specific Lethal) protein complex. The MSL complex allows for the two-fold up-regulation of the X chromosome in males (XY), in order to equalize the disparities in amount of genetic information with females (XX). Since none of the known MSL components are sufficient for direct DNA recognition in vitro, the Larschan laboratory has identified an additional DNA binding protein as a key player in MSL complex recruitment. This previously unstudied zinc-finger protein, CLAMP, (Chromatin Linked Adaptor for MSL Proteins), co-localizes to the X chromosome with MSL complex in vivo. In order to fully investigate the role of CLAMP in dosage compensation, it is necessary to generate a null or mutant of CLAMP. The aim of my project is to generate a CLAMP null mutant using the CRISPR/CAS9 system. With this cutting edge technique, I have site-specifically mutagenized CLAMP in vitro in *Drosophila melanogaster* S2 and Kc cells and in vivo in *Drosophila melanogaster* flies

REGULATION OF Clp PROTEASES BY SrrAB IN *STAPHYLOCOCCUS AUREUS*

Carly Earle and Dr. Jeff Boyd
Department of Biochemistry and Microbiology
Rutgers University, New Brunswick, NJ

Reactive oxygen species are spontaneous byproducts of aerobic respiration that cause substantial damage to cellular macromolecules such as DNA and proteins. Studies have found that exposure of cells to constitutive levels of oxidative stress can result in the misfolding of proteins. In the human pathogen *S. aureus* the Clp proteolytic system is responsible for the processing (refolding or degradation) of misfolded proteins. We have recently found that a two component regulatory system (SrrAB) positively influences aerobic respiration as well as the ability of cells to metabolize ROS upon the onset of respiration. In this work we tested the hypothesis that SrrAB positively regulates the Clp system upon the onset of respiration to ensure that cells are capable of turning over damaged or unnecessary proteins. Consistent with this hypothesis we found that an *srrAB* mutant is sensitive to growth with puromycin, a compound that results in the premature abortion of protein translation and leads to protein misfolding stress. A prior proteomics analysis identified a putative Clp protein to be under the SrrAB regulon. Basic Local Alignment Search Tool (BLAST) analyses against the genetic background in which we conduct our experiments identified *clpC* and *clpL* as genes potentially regulated by SrrAB. Growth analyses found that a *clpC* mutant is sensitive to growth with puromycin, while a *clpL* mutant is not. Transcriptional analyses found that the *clpC* gene is part of the SrrAB regulon. We reasoned that decreased transcription of the *clpC* gene leads to the puromycin sensitivity of the *srrAB* mutant. We found that the phenotypes displayed by *clpC* and *srrAB* mutations are only partially additive and that expression of *clpC* in an *srrAB* mutant decreases the sensitivity of the *srrAB* mutant to puromycin. The data presented led us to propose a model wherein SrrAB increases transcription of the *clpC* gene upon the onset of respiration allowing the cell to refold or turnover proteins damaged by ROS.

THE NuA4 AND Swr1 CHROMATIN MODIFICATION COMPLEXES FOR RNA SPLICING

Nikita Paripati, Daniel Sprague, Jordan Martinez, Aron Moazamian, Ryan Moazamian, and Dr. Tracy L. Kress.

Department of Biology
The College of New Jersey, Ewing, NJ

The ability to quickly and precisely regulate gene expression is a fundamental biological process of paramount importance to cell survival. Two important steps in gene expression are transcription and splicing. These steps are coordinated to ensure accuracy and efficiency, yet very few proteins that function in this coordination have been identified. Recent high throughput genetic interaction studies using *Saccharomyces cerevisiae* revealed that splicing factors interact with factors that are important for transcription. We have utilized a targeted genetic screen to identify novel interactions between splicing factors and factors that modify chromatin to modulate transcription. Using both qualitative and quantitative growth assays we identified negative genetic interactions between genes encoding splicing factors and both *SWR1*, a component of the Swr1 chromatin remodeling complex, and *HTZ1*, which encodes the variant histone inserted into chromatin by Swr1. In addition, our screen revealed novel negative genetic interactions between splicing factors and *EAF7*, a component of the NuA4 histone acetyltransferase complex. Notably, both the NuA4 and Swr1 complexes function together to regulate transcription. Using quantitative RT-PCR we have shown that mutation of individual components of the NuA4 or Swr1 complexes or Htz1 causes a modest block in RNA splicing and exacerbates the splicing defects observed in a yeast strain lacking a splicing factor, as predicted by our genetic analysis. Taken together, these data support a model in which the NuA4 and Swr1 chromatin modification complexes interact with the splicing machinery to coordinate transcription and splicing.

THE ROLES OF DIATOM NRAMP USING KINETICS & REVERSE GENETICS

Konrad Stelmark, and Dr. Adam Kustka
Department of Environmental Sciences
Rutgers, Newark, NJ

NRAMP is a divalent metal transporter ubiquitous among eukaryotes and is most often associated with iron or manganese transport. We investigated the role of this protein in the marine diatom, *Thalassiosira pseudonana*, as previous reports have shown its transcripts to be among the most highly upregulated under low Fe, yet other lines of evidence suggest such a divalent transporter might not be involved in Fe uptake. Diatom clones expressing antisense RNA to NRAMP were generated, which should lead to reduced NRAMP levels. Antisense clones in low iron conditions exhibited the same extent of growth rate depression as that of the wild-type cells, yet growth was severely depressed under low manganese conditions; this suggests a possible interaction between Mn demand and Fe status whereby low Fe cells require more Mn. To further evaluate the role of NRAMP in Mn metabolism we grew the antisense clones and wild-type cells in low manganese conditions with a manganese 54 radiolabel. This approach allowed us to explore the interrelationships among intracellular Mn quota, growth and steady state uptake. The data revealed that antisense clones exhibited the same Mn uptake rates as wild-type cells, despite the pronounced growth rate depression for low Mn grown clones. These results suggest that NRAMP may not play a role in manganese transport at the cell surface, but rather that NRAMP plays a vital role in intracellular manganese trafficking. Furthermore, this may be more important under low Fe conditions. These possibilities will be explored with experiments focused on Fe-Mn interactions as well as confocal-based localization of NRAMP in the cell.

REV1 HAS A POLYMERASE ZETA INDEPENDENT ROLE IN DNA REPAIR

Michael Turadek, Dr. Mitch McVey and Dr. Varandt Khodaverdian
Department of Biology
Sarah Lawrence College, Bronxville, NY

DNA damage occurs frequently and requires constant maintenance by repair machinery. There are multiple repair pathways that can be followed depending on how a DNA template was damaged. Translesion synthesis occurs when a bulky adduct makes an addition to DNA and causes a replication fork stall. The replicative polymerase is switched out for a repair polymerase which extends past the lesion. Polymerase zeta and Rev1 are thought to play crucial roles in this process. It is hypothesized polymerase zeta extends past DNA lesions and Rev1 acts as a scaffold and recruits other repair polymerases. The role of these two proteins was investigated in *Drosophila melanogaster*. We bred mutants with gene knockouts for Rev1 and Rev3, the catalytic subunit of polymerase zeta, and ran a sensitivity assay on them using the mutagen MMS which inserts bulky adducts to DNA bases. The number of surviving flies was counted and used to calculate the relative percent survival. The assay revealed that Rev1 mutants were much more sensitive to MMS than Rev3 mutants, indicating Rev1 might have a role independent from recruiting polymerase zeta during DNA repair.

THE USE OF BIFIDOBACTERIUM LONGUM TO ALLEVIATE AUTISTIC-LIKE SYMPTOMS IN THE *BTBR T+ tf/J*

Devon Atkinson, Danielle Mazowiecki, Patricia Bush, Norman Schanz,
and Dr. Robert Benno
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Autism Spectrum Disorder is a behavioral abnormality characterized by reduced social interaction, impoverished social communication and repetitive behaviors. The *BTBR T+ tf/J* mouse strain is commonly used in research as a model organism for ASD, as they exhibit irregularities in these key areas. There have been numerous attempts to alleviate these symptoms, and some of the more successful studies have utilized approaches to decrease levels of anxiety in the strain. Recent studies have shown that the probiotic *Bifidobacterium longum* has been able to diminish anxiety related behaviors in mice. In this study we sought to decrease anxiety, in the *BTBR* mouse using *B. longum*, in an attempt to alleviate the autistic-like phenotypes of this strain. The results of this study show that *B. longum* was able to moderately decrease the repetitive behaviors as observed through grooming. However, it was ineffective in altering other anxiety related behaviors, or improving deficits in social behavior.

COPPER HOMEOSTASIS OIN *STAPHYLOCOCCUS AUREUS*

Sakshi Gandhi and Dr. Jeffrey Boyd
Department of Microbiology and Biochemistry
Rutgers University, New Brunswick, NJ

Staphylococcus aureus is of imminent concern to public health officials worldwide because of its ability to cause severe infections and resist the efforts of a growing number of antibiotics. Recent studies have shown that human macrophages accumulate copper (Cu) during phagocytosis as a mechanism of bacterial killing. While *S. aureus* does require Cu in trace amounts, excess Cu can be toxic. In order to successfully cause infections, *S. aureus* must be able to tightly control intracellular Cu concentrations. To do this, *S. aureus* employs CopA, a P-type ATPase copper exporter, together with CopZ, a Cu-specific chaperone protein. However, the genome of the *S. aureus* USA300 strain also encodes for an additional putative Cu exporter, provisionally named CopB. To study the role of CopB, a *copB* mutant was built and found to be more susceptible to Cu than the wild-type strain. Like *copA*, *copB* is induced under Cu stress conditions and under the transcriptional control of the Cu-dependent repressor CsoR. A *copAB* double mutant was constructed and found to be more sensitive to Cu than the parent strains, suggesting a functional overlap between CopA and CopB. Overexpression of the *copA* gene via plasmid successfully remediated the phenotype of the *copAB* mutant, while *copB* overexpression did not. Altogether, these results provide new insights about additional factors involved in copper homeostasis in the human pathogen *S. aureus*.

IDENTIFYING CANDIDATE REPRODUCTIVE GENES FROM APOMICTIC PISTILS OF *CENCHRUS CILIARIS* (*Buffelgrass*) USING GENOMIC METHODS

Victor Leon, Jermin Adrawy, and Dr. Terry L. Kamps
Biology Department
New Jersey City University, Jersey City, NJ

Apomixis is a mechanism of clonal reproduction through seeds which occurs in a wide variety of plant species. From a practical perspective, researchers are interested in apomixis in order to utilize it to rapidly fix desirable genetic characters in cultivated plants. From the perspective of evolutionary biology, apomixis is of interest because it is an unusual mode of reproduction considered by some to be an evolutionary dead end, despite the fact that it is a not uncommon process in several species of plants. *C. ciliaris* is valuable as a forage grass, and the existence of sexual and apomictic genotypes makes this species an important resource for investigating the genetics and mechanisms determining modes of reproduction. Apomictic reproduction in *C. ciliaris* is through aposporus apomeiosis. BLASTx to the Uniprot database was performed using 10318 sequences previously derived by the assembly of an EST library constructed from young ovaries of obligate apomictic buffelgrass plants. *C. ciliaris* candidate genes involved in general reproduction and apomixis were identified by Gene Ontology (GO) results in combination with a syntenic cross species in silico mapping strategy. Thirty-two of a GO-based selected subset of ESTs mapped within rice chromosome 12 region known to be syntenic with the apomictic region of *Paspalum simplex*. Among these were genes involved in auxin signaling pathways, methionine biosynthesis, endoreduplication, and programmed cell death. Significant BLASTn hits to a *Panicum maximum* apomictic pistil cDNA library has provided additional candidates for consideration. Future studies will include comparative expression assays of the identified candidate genes and tBLASTx analysis of ESTs that failed to match known proteins in the Uniprot database.

FORAGING AND COMPETITIVE INTERACTIONS OF PASSERINE BIRDS AT FORESTED HABITAT EDGES

Alex Smith and Dr. Brian Olechnowski

Department of Biological and Allied Health Sciences, Becton College
Fairleigh Dickinson University, Madison, NJ

Habitat edges have been extensively studied in ecology, and the nature of interactions between organisms at edges are only partially understood. Edges can act as areas of higher competition and predation, but also as areas of higher productivity and diversity. Due to human-induced habitat fragmentation, understanding this duality is paramount to leading successful and responsible restoration and land management efforts. This research aims to determine the effects habitat edges have on foraging and competitive behaviors in passerine bird species. This will be achieved by directly comparing interactions at forest-habitat edges with those at forested cores (managed open fields are adjacent to the forested patches). Feeders were set up at edge and core habitats in a large scale natural area (Duke Farms, in Hillsborough, New Jersey) (1100 hectares) and a small scale natural area (Primrose Farms in Harding, New Jersey) (50 hectares). At each feeder the following data was recorded: species, duration of visit, and whether or not a competitive interaction took place. Competitive interactions were determined by the displacement of a bird from a feeder or the denial of a bird's access to a feeder by another bird. We hypothesize that species richness and total number of visits to the feeders will be more numerous at the edge, but individual visits will be shorter than those at the core because of both the increased risk of predation and competition with other birds at the edge. We also expect these same patterns to be more pronounced in the small scale natural area (Primrose). This is due to the smaller patch providing fewer resources (greater competition) and less refugia from predators. Preliminary results indicate that at habitat edges, species richness is higher, birds visit feeders more often and for longer periods, and there are higher levels of competition than at forest cores. This research is currently in progress and will be completed after Summer 2015. The results of this research will increase our knowledge on behavioral interactions at habitat edges as well as provide additional insight for adaptive land and wildlife management practices, especially in areas with high levels of habitat fragmentation.

MODIFICATION OF ACUTE STRESS INDUCED ALCOHOL CONSUMPTION BY CANNABINOID CB2 LIGANDS

Sneha Tammareddy, Norman Schanz and Dr. Emmanuel S. Onaivi
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Alcohol use disorders affect about 18 million Americans. Addiction to alcohol and other drugs is influenced by genetic and environmental factors such as stress. It is evident that excessive stress may lead to alcohol consumption. The connection between the two is not fully known, and it varies from person to person as it depends on exposure time and pre-consumption stress levels. Studies have been performed to study specific aspects of the stress response that aid drug seeking and there is evidence of the involvement of the endocannabinoid system. The endocannabinoid system is ubiquitous in the central nervous system and peripheral tissues. It is known to have some role in the behavioral effects of ethanol, especially ethanol drinking behavior. It consists of receptors, endocannabinoids, and enzymes for the synthesis and degradation of endocannabinoids. There are two endocannabinoid receptors (CBRs), CB1 and CB2 receptor. CB1 receptor is mainly found in the central nervous system and CB2 was previously thought to be in immune cells in the periphery, but new research indicates their presence in neurons in the brain. The stress response involves the hypothalamic-pituitary-adrenal (HPA) axis. Stressed activated HPA axis releases CRF from the paraventricular nucleus of the hypothalamus. Then it is transported to the anterior pituitary, where it stimulates the release of adrenocorticotrophic hormone (ACTH). ACTH further stimulates the adrenal cortex to release of glucocorticoid hormones, corticosterone or cortisol depending on rodents or humans respectively. Endocannabinoids are involved in this pathway and seem to take part as both a regulator and effector of the stress response. The goal of the study was to determine the effects of CB2 cannabinoid receptor ligands on acute stress induced alcohol consumption in mice. The experiments were conducted in C57BL/6J mice that have been widely used in alcohol studies and in serotonin transporter (SERT) knockout mice for their impact in cannabinoid effects. SERT ko mice are associated with an increase vulnerability to stress and was used to investigate the influence of acute stress induced alcohol consumption and modification by CB2R ligands. Both the C57BL/6J and SERT ko mice were weighed, divided into 3 groups with appropriate control groups. The experimental groups 1 and 2 in both strains were injected with CB2R agonist, JWH133 or the antagonist AM630 with 2.0 mg/kg doses before being subjected to acute stress by placement in a 50 ml conical tube for one hour. After one hour all groups were returned to their cages and exposed to 8% alcohol and water as a choice model.

The C57BL/6J animals that were given CB2 agonist JWH133 consumed similar amounts of alcohol and water, while the control animals mainly consumed water. The SERT animals that were given JWH133 did not consume as much alcohol as they did water, similar to their control animals. The C57BL/6J animals that received the CB2 antagonist AM630 consumed more water than alcohol, especially the third day of measurement. The cause is unknown. The control animals consumed similar amounts of alcohol and water. The SERT ko animals that received the antagonist consumed more water than alcohol, as seen with the control animals as well. From this initial view of the data obtained, the C57BL/6J of both groups was not affected by the stress as alcohol consumption was not increased. Also, comparing the results of the C57BL/6J and SERT ko, we can possibly conclude that serotonin is not involved in stress induced mechanisms as there was no significant difference between the data of the two strains. Future studies will use other transgenic mice.

MOLECULAR BASIS FOR CHRONIC MILD STRESS INDUCED DEPRESSION: ROLE OF CB2 CANNABINOID RECEPTOR GENE EXPRESSION

Ndeah Terry, Norman Schanz and Dr. Emmanuel S. Onaivi
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Major depressive disorder is the leading cause of disability in the United States in the age group 18-44., and affects 6.7% of the U.S. population in a given year. Symptoms of depression include persistent sadness, loss of interest or pleasure in hobbies and activity, called anhedonia, loss of appetite, and irritability. Although it is not known exactly what causes depression individual factors include, brain chemistry, biological differences, hormones, inherited traits, life events and environmental factors. Chronic stress often precipitates and increases the risk for developing major depression. Major depression also has a high comorbidity with alcoholism. A study of comorbidity with anxiety and depressive disorders in four geographic areas found that individuals with alcohol abuse or dependence generally experienced a twofold to threefold increased risk of anxiety and depressive disorders. Alterations of the endocannabinoid system (ECS) are involved in the pathophysiology of neuropsychiatric disorders depression, anxiety and drug addiction. The ECS consists of the cannabinoid receptors (CB1Rs and CB2Rs), endocannabinoids (eCBs), and the synthesizing and degradation enzymes of eCBs. Recent evidence suggests that CB2Rs are implicated in neuropsychiatric disorders. In a recent study, transgenic mice overexpressing the CB2 receptor (CB2xP) were exposed to acute and chronic mild stress (CMS) to evaluate their response to depressive-like behaviors. It was found that the overexpression of CB2 receptors produced an endophenotype resistant to depressive behaviors produced by acute and chronic mild stress. The objective of this study is to evaluate the role of CB2 receptors in the regulation of depressive and addictive-like behaviors mice using CMS to establish anhedonia, a symptom of depression that can be modeled in animals, and alcohol consumption in a choice model. The choice model was chosen because repeated exposure to stress increases alcohol consumption in a 2-bottle choice model and can trigger the reinstatement of alcohol seeking in experimental animals.

C57BL/6Js were subjected to weekly CMS regime and anhedonia was measured by consumption of 2% sucrose solution. The experimental protocol was the same for the control mice housed in a different room but were not subjected to CMS. The stressed mice consumed an average of 4 ml of sucrose solution, while the controls consumed an average of 13 mls. During the first week of the 2 bottle alcohol/water choice model the stressed animals consumed an average of 22.4 mls of water and 25.8 mls of alcohol, the controls consumed an average of 18 mls of water and 25.4 mls of alcohol. However, during the second week of the alcohol choice model when the stressed animals were injected with sub-acute doses of the CB2 antagonist JWH133, the stress animal's alcohol consumption increased, while their water consumption decreased. They consumed an average of 18mls of water and 37.6mls of alcohol, while the alcohol/water consumption remained consistent. At different critical points, mice and their controls were sacrificed and the brains harvested for the determination of CB2 cannabinoid receptor gene expression. The results obtained indicate that CB2 cannabinoid receptors may be associated with CMS model of depression and alcohol consumption. Further studies are required to determine the role of the different elements of the endocannabinoid system in depression and alcohol dependence.

EXPLORING THE ROLE OF REDOX METALS IN THE NITRIC OXIDE AND H₂O₂ SYNERGISTIC EFFECT TOWARDS *E.coli*.

Rahab Basher, Wendy Lee, Layla Tashmin, Mohamed O. Nasef and Dr. Uri Samuni.

Department of Chemistry and Biochemistry
Queens College, City University of New York, Flushing NY

We studied the effect of nitric oxide on the kinetics of prokaryote cell survival in the presence of oxidative stress. The results show a mild cytostatic effect of nitric oxide when added alone. However, when nitric oxide is added in the presence of H₂O₂, a strong synergistic killing of *E. coli* was observed, as compared to the effect of H₂O₂ alone. This may represent a new therapeutic avenue given the differing effects on prokaryote vs. eukaryote cells. The addition of the antioxidant TEMPOL has abrogated the pro-oxidative synergy of NO/H₂O₂ suggesting a role of metal redox chemistry. In order to further elucidate the mechanism, cell proliferation and cell survival experiments were performed testing the effects of metal ions, chelators and hydroxamates.

TRANSPLANTATION OF ISLET OF LANGERHANS CELLS IN STZ-INDUCED DIABETIC MICE TO TEST FOR ALTERED NEUROPATHIC PAIN BEHAVIOR

Alec DeGraaf, Neal Joshi and Dr. J. W. Lee
Department of Biology
William Paterson University of New Jersey, NJ

Diabetes mellitus is the seventh leading cause of death in the United States. Type 1 diabetes mellitus (T1DM) is a very debilitating autoimmune disease characterized by immune cells destroying pancreatic beta cells. Most common manifestations of T1DM are hyperglycemia, (high blood glucose) and weight loss. Untreated T1DM will cause development of peripheral diabetic neuropathy (DN). Currently there is no cure for T1DM and DN but studies have shown possible allotransplantation of islet cells to reverse hyperglycemia.

This study examined; i) a possible treatment for T1DM and DN by xenotransplantation of islet of Langerhans cells from rat to mouse, and ii) pain behavior tests in diabetic BTBR T+ tf/J mice to test for DN. In experiment 1, adult male C57BL/6J (n=18) were injected with streptozotocin (STZ) to induce T1DM (≥ 350 mg/dl). STZ is a drug that mimics T1DM by selectively destroying pancreatic beta cells. C57 mice were transplanted with islets or received cell culture media only as a control. In experiment 2, naïve-BTBR and diabetic BTBR (n=10) were used to measure diabetic neuropathy with paw-licking durations for 60 minutes using 5% formalin. For diabetic C57 mice, the glucose levels were 544.25 ± 13.96 mg/dl (1wk post-transplantation) and 542.83 ± 26.98 mg/dl (2wk post-transplantation); whereas C57 control was 564.33 ± 33.90 mg/dl (1wk) and 563.50 ± 26.14 mg/dl (2wk). The STZ-BTBRs displayed shorter paw-lick duration at phase II (12.0 ± 9.71 sec) compared to naïve-BTBRs (83.5 ± 36.85 sec; $p < 0.02$).

Immunohistochemical analyses labeled healthy living beta cells with primary insulin antibody post-transplantation at days 0, 1, and 14. Data suggest hyperglycemia in transplanted diabetic mice may be related to the number of surviving islet cells. Transplantation of islets may be a viable method to alleviate or prevent DN pain.

ANTIOXIDANT ACTIVITY IN EDIBLE BROWN SEAWEEDS

Marisa Dunigan and Dr. Alessandra Leri
Department of Natural Sciences
Marymount Manhattan College, New York, NY

Seaweeds are photosynthetic macroalgae that grow in the littoral zone of the ocean. Consequently they are exposed to high sunlight radiation and oxygen concentrations. Although these are optimal conditions for free radical production, seaweeds do not tend to express serious photodynamic damage (S. Gupta 2011). This suggests that seaweeds are natural and potentially edible sources of antioxidants. We employed diverse assays to measure different types of antioxidant activity in the edible brown seaweeds: *Laminaria digitata* (Atlantic kelp), *Fucus vesiculosus* (bladderwrack), *Pelvetia canaliculata* (sea sprigs), and *Saccharina latissima* (sweet kelp), all collected from Scottish shores.

To measure radical scavenging antioxidant activity, we used the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay. DPPH is a stable free radical that is quenched in the presence of an antioxidant (W. Brand-Williams 1995). We observed a decrease in absorbance at 520nm as a function of time when reacting our seaweed extracts with DPPH, indicating radical scavenging activity by antioxidants in our samples. For each seaweed, we calculated the concentration of antioxidant at which 50% inhibition of free radical activity is observed (IC₅₀).

To measure antioxidant activity in the form of reducing power, we used the potassium ferricyanide assay (G.C. Yen 1995). We observed an increase in absorbance at 700nm when reacting our seaweed extracts with iron compared to a control, indicating reducing power. We quantitatively expressed the reducing power of each seaweed in ascorbic acid equivalents.

Polyphenol groups are often implicated as antioxidants because they can function as metal chelators and radical scavengers. To measure polyphenol content in our seaweeds, we used Folin-Ciocalteu's polyphenol assay (M.S. Taga 1984). We observed substantial increase in absorbance at 720nm when reacting our seaweed extracts with the Folin-Ciocalteu reagent compared to a control, indicating high polyphenol content in the seaweeds. We quantitatively expressed the polyphenol content of each seaweed in gallic acid equivalents.

Our results demonstrate radical scavenging and reducing power as well as high polyphenol content in all four edible brown seaweeds. Such edible sources of antioxidants could play a role in supplementing the human body's natural antioxidant defense system to combat oxidative stress.

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IDENTIFYING TARGETS OF THE ANIT-MICROBIAL AGENT TRICLOSAN ON *C. ELEGANS* EGG-LAYING BEHAVIOR

Katelyn Giordano and Dr. Edith M. Myers
Department of Biological and Allied Health Sciences
Fairleigh Dickinson University, Florham Campus, Madison, NJ

Triclosan is an antibacterial agent used in countless consumer products that enter the environment after use by the general population. Studies have shown that triclosan can affect organisms, although not much is known about the molecular targets of triclosan. In order to identify the targets of triclosan a model organism, the *C. elegans* was used. *C. elegans* are microscopic nematodes with a fully sequenced genome that has a great amount of homology with the human genome. Due to this high homology, *C. elegans* is a great choice to study some potential targets of triclosan, such as serotonin and ryanodine receptors, which are also found in mammals.

Studies from our lab have shown that triclosan likely affects *C. elegans* survival and egg-laying. The purpose of this project was to try to determine whether triclosan targets serotonin or ryanodine receptors to affect *C. elegans* egg-laying behavior. The neurotransmitter, serotonin is important for regulating *C. elegans* egg-laying, while ryanodine receptors are important for function of skeletal muscles, similar to the egg-laying muscles. An egg in worm assay was performed using *ser-7* (a serotonin receptor) and *mod-5* (a serotonin reuptake transporter) mutants to determine whether the presence of these receptors/ transporters is necessary for the effect of triclosan on egg-laying. Triclosan (2.5µg/ml) had no effect on the number of eggs retained in either wild-type or mutant worms. However, a majority of the worms exposed to triclosan retained eggs longer (eggs retained were at a later stage of development) than the non-exposed worms. To examine this effect an early stage egg assay was performed using wild type, *ser-7*, *mod-5*, and *unc-68* ryanodine receptor mutants. Worms exposed to triclosan laid a large percent of late-staged eggs. However, the effect of triclosan was not different between wild type worms and serotonin or ryanodine receptor mutants. This suggests that triclosan causes *C. elegans* to retain eggs for a longer period of time in a *ser-7*, *mod-5*, and *unc-68* independent manner.

STABILIZED SERUM AMINE OXIDASE. TOWARDS ENHANCED ELECTRON TRANSFER KINETICS

TaeHoon Kim, Anna Braun, Dr. Mihaela Leonida and Dr. Ish Kumar
School of Natural Science
Fairleigh Dickinson University, Teaneck, NJ

Serum amine oxidase (SAO) is among enzymes known to have cardioprotective effect, hence they are potential therapeutic agents. Amine oxidases were also proposed in several reports for use as sensing agents in biosensors for clinical laboratory and food industry applications

SAO is an oxidoreductase and has a limited stability. The present project targets the stabilization of SAO by modifying its structure using a green reagent, a room temperature ionic liquid (RTIL).

It is known that enzymes are more stable in the presence of their substrates. Therefore the enzyme was suspended in 1-ethyl-3-methylimidazolium tetrafluoroborate (RTIL) in the presence of pyrroquinoline quinone (PQQ), the prosthetic group of the enzyme. After removal by dialysis of the denaturing RTIL, SAO refolded entrapping some of the PQQ present in the denaturing mixture. Assays before and after the modification procedure demonstrated a successful procedure and measured the activity of the modified SAO (ME).

Other modifiers were tested in parallel procedures: copper ions (SAO is a copper enzyme), lipoic acid (LA) - beneficial in therapy due to its antioxidant effect and intrinsic to some redox enzymes, and combinations thereof. Activity assays were done periodically on MEs and the starting SAO to assess the effect of the modification on enzyme stability.

Antioxidant assays were also conducted on MEs and the results were compared with those for the initial SAO. "Wiring" SAO with electroactive species (PQQ, LA, Cu ions) is expected to enhance the electron transfer rate of SAO as well. A biosensor using SAO modified with PQQ and copper ions was built in which the modifiers served as mediating, enzyme-friendly species. The biosensor was evaluated for catalytic effect, linearity in amine concentration, and stability.

ENDOCANNABINOID SYSTEM ALTERATIONS IN AN ANIMAL MODEL OF AUTISM SPECTRUM DISORDERS

Kevin Penkoski, Norman Schanz, Sue Sgro, Dr. Claire M. Leonard,
and Dr. Emmanuel S. Onaivi
Department of Biology
William Paterson University of New Jersey, Wayne, NJ

Alterations of the endocannabinoid system (ECS) are involved in the pathophysiology of neuropsychiatric disorders including autism spectrum disorders (ASDs). The causes of ASDs which are complex heterogeneous neurodevelopmental disorders are incompletely understood. However, the interaction between genes and environmental factors including immune system dysregulation are associated with ASDs. The ECS consists of the cannabinoid receptors (CB1Rs and CB2Rs), endocannabinoids (eCBs), and the synthesizing and degradation enzymes of eCBs. The ECS are involved in embryo neurodevelopment and growth and is a key regulator of the immune system via CB2Rs which are expressed on macrophages, microglial cells and neurons. We used the BTBR T+tf/J mice that have been shown to exhibit autism-like behavioral phenotypes to 1). Determine brain expression of CB2Rs throughout neurodevelopment in BTBR T+tf/J in comparison to C57BL/6J mice and 2). Evaluate the neurochemical and molecular basis of cannabinoid-induced behavioral effects in the mouse model. We report that CB2Rs are present and essential during neurodevelopment and its enhanced brain expression in the adult BTBR mice might be associated with the differential cannabinoid-induced behavioral effects in motor function and emotionality tests when compared to the C57BL/6J mice. eCBs, anandamide (AEA) and 2-arachidonoyl glycerol (2-AG) were measured in frontal cortex, cerebellum and the rest of the brain by LC-MS using isotopic dilution method. AEA but not 2-AG levels in the BTBR mice were reduced in the brain areas analyzed. The data indicate that dysfunction in the ECS may in part contribute to ASDs. Further studies are required to determine the contribution of the different elements of the ECS involvement in the etiology of ASDs.

PLASMA TREATMENT ACCELERATES TAIL REGENERATION IN TADPOLES

Adonis Rivie, William Manzo, Dr. Kevin Martus* and Dr. Jaishri Menon
Departments of Physics* & Biology
William Paterson University of New Jersey, Wayne, NJ

Atmospheric pressure plasmas have found large application in regenerative medicine. Presently, we investigated the effect of plasma on wound healing and tail regeneration of tadpoles, *Xenopus laevis* especially role of reactive oxygen species (ROS).

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. Here we report faster rate of growth of the regenerating tail following plasma exposure. By comparing results on *in situ* staining for ROS, nitric oxide (NO) and mitochondria between experimental and control groups, there is increased ROS (hydrogen peroxide and superoxide but not NO) production at 2h, 4h, 12 h and 24 h post amputation at the wound site in plasma treated tadpoles.

However, these ROS species were not derived from mitochondria evident from double immunostaining. Growth of the blastema (5 days post amputation) in experimental group was higher than control with increased ROS, NO and catalase in plasma exposed group compared to control.

Microscopically, in plasma treated tadpoles, cells of wound and blastemic epithelium showed blebbing of plasma membrane, increased cellular lipid droplets, hypertrophy of the cells, increased mitochondrial density, and reduced intercellular connections.

These findings demonstrate that some of the free radicals might be acting as signalling molecules and these tadpoles possess sophisticated mechanisms to respond to stress of plasma and yet hastening the dynamics of wound healing and tail regeneration.

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DIETARY EFFECTS ON DRUG TOXICITY IN DROSOPHILA

Ariana Safi and Dr. Theodore Brummel

Department of Biology

Long Island University, Post Campus, Brookville, NY

Dietary restriction (DR) in rodents has been shown to increase longevity, reduce the rate of cancer and protect against cognitive decline. Similar benefit of DR have been described or proposed to exist in other organisms ranging from yeast to primates. The fruit fly, *Drosophila melanogaster*, is a powerful model organism that has been used to uncover mechanism of behavior, development and disease. Studies in *Drosophila* have shown that manipulation of diet can dramatically extend longevity. This study aims to address whether alterations in diet can modulate the toxic effects of drugs. Using caffeine and nicotine, two common social drugs, we have found that dietary restriction protects against these drugs. One complication in this work is that both drugs alter food consumption, making a clear interpretation of the results more difficult. We have acquired flies that are deficient in the ability to taste caffeine and are using these to determine whether the alterations in food consumption are mediated by the aversive taste of these compounds or whether the changes in feeding are due to appetite suppressive effects of these drugs. The possibility that diet can block or enhance the effects of drugs could have fundamentally critical consequence when evaluating medication to be taken by elderly patients, since these often have greatly reduced dietary intake relative to younger patients

THE ROLE OF NMDA RECEPTORS IN CANCER

Mina Youssef, **Jan Osea**, and Dr. Natalia Coleman

Department of Biology

New Jersey City University, Jersey City, NJ

Despite intensive research efforts and promising discoveries, cancer still is the leading cause of death in the US. There is growing evidence of the importance of glutamate signal transduction in cancer. N-methyl-D-aspartic (NMDA) receptors are one of the three glutamate receptors found in the mammalian central nervous system. While it is common knowledge that NMDA receptors are essential for spatial learning and memory, little is known about its function in cancer. We previously showed that NMDA receptors are expressed by human prostate, breast and lung cancer cells. The aim of the current study is to evaluate the NMDA receptor antagonist memantine as a potential target for cancer treatment. The cancer cells growth inhibition was determined by using a 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. Our study indicates that memantine inhibits the growth of breast cancer cells.

BUTYL-3-METHYLIMIDAZOLIUM THIOCYANATE)

Nadia Abbas¹, Ruel Z.B. Desamero², and Dr. Elmer-Rico E. Mojica¹

¹Department of Chemistry and Physical Sciences, Pace University,
New York, NY

²Department of Chemistry, York College, Jamaica, NY

Ionic liquids are a new class of purely ionic, salt-like materials that are liquid at unusually low temperatures. These materials manifest physiochemical behaviors quite unlike water or organic solvents. They possess high ionic conductivity, high ion concentrations, and excellent oxidative stability making them ideal materials for demanding applications at elevated temperature. Ionic Liquids have many applications, such as powerful solvents, electrolytes (electrically conducting fluids) and in power sources (batteries, capacitors, and fuel cells). In order to better understand the unique properties of ionic liquids we measured the Raman spectra of 1-butyl-3-methylimidazolium thiocyanate or [BMIM][SCN] in different environments. Raman spectra were correlated to the results of *ab initio* calculations. The data obtained will be discussed in terms of their implication to the function of ionic liquids.

DESIGN AND SYNTHESIS OF NEW CHIRAL PHOSPHORYL CHLORIDES AS CATALYSTS FOR HENRY REACTION

Mary Abdulkarim and Dr. Parminder Kaur
Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

A new class of chiral N-phosphonyl chloride was designed and synthesized using usual synthetic protocols. The newly synthesized catalysts were characterized using modern characterization techniques and utilized successfully in asymmetric Henry reaction. The reaction is convenient to perform to give excellent yields and good stereoselectivities.

TRANSITION METAL CATALYZED FUNCTIONALIZATION OF TERMINAL ALKYNES

Bryant Catano and Dr. Yalan Xing
Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

The transition metal-catalyzed functionalization of carbon-carbon multiple bonds is an important synthetic strategy. The need for efficient, atom-economical methods to synthesize certain synthetic intermediates under mild conditions with inexpensive reagents has led to the increased investigation of iron catalysts. It has been discovered that both aromatic and aliphatic alkynes can be halo-functionalized to α,α -dihalodimethyl ketals, catalyzed by iron (III) in excellent yields using methanol as a solvent and N-halosuccinimide as the halogen source. This efficient, rapid transformation is highly regioselective and can be run in mild conditions. The deacetalization to α,α -dihaloketones using 8% iron (III) chloride in silica was also observed and can be performed in a one-pot reaction. Direct conversion to an α -haloketone is also observed using isopropanol as the solvent. An investigation into the possible mechanism of this novel reaction is currently underway.

SOLID PHASE EXTRACTION OF ILLICIT DRUGS (AMPHETAMINE AND METHAMPHETAMINE)

Normisha V. Evans, Robert L. Marvin; and Dr. Elmer-Rico E. Mojica
Department of Chemistry and Physical Sciences
Pace University, New York, NY

Analysis of illicit drugs such as amphetamines and its derivatives is usually done by chromatographic methods like gas chromatography (GC) and liquid chromatography (LC). Solid phase extraction (SPE) methods aim to isolate illicit drugs and their metabolites in complex biological samples like urine. They have become commercially available to improve drug analysis. Among these materials is a molecularly imprinted polymer (MIP), a class of polymer-based recognition elements tailored to target a specific chemical or a class of structurally related chemicals. In this study, two commercially available MIPs were used in extracting a mixture of amphetamine and methamphetamine from synthetic urine and water. Their performance was compared with one another and quantified using high performance liquid chromatography (HPLC).

ENANTIOSELECTIVE SYNTHESIS OF ANTICANCER NATURAL PRODUCT ACTINOPOLYMORPHOL B AND ANALOGS

Claudia Kim and John Lee and Dr. Yalan Xing

Department of Chemistry

William Paterson University of New Jersey, Wayne, NJ

Natural product actinopolymorphol B was isolated from *Actinopolymorpha rutilus* and shows potential anticancer activity. A synthetic strategy and the progress of synthetic efforts towards Actinopolymorphol B and analogs will be presented. Noyori's asymmetric hydrogenation of ketone will be utilized to install the stereochemistry of the secondary alcohol. Our recently developed Iron (III) catalyzed functionalization of alkyne could allow the generation of the ketone functional group and its derivatives from alkynes, which provides the access to many analogs of Actinopolymorphol B. The natural product and its analogs will be screened for their biological activity to study the medicinal chemistry of the structure and their activity relationship

CATALYSIS AND MECHANISM OF FORMATE TO OXALATE: A CRUCIAL STEP IN THE CONVERSION OF CARBON DIOXIDE INTO C2 AND HIGHER ORDER VALUE ADDED PRODUCTS

Charles Ryan^a, Mikhail Askerka^c, Victor Batista^c, Heidie Beyer^a, Christina Gili^a, Jerry Kaczur^b, Michael Marino^a, Brittany Olejarz^a, Brittany Piercy^a, Robert Wetzel^a and Dr. Prasad Lakkaraju^a

^aDepartment of Chemistry and Biochemistry,
Georgian Court University, Lakewood, NJ

^bLiquid Light Inc., Monmouth Junction, NJ

^cDepartment of Chemistry, Yale University, New Haven, CT

Our interest in the formate to oxalate conversion stems from the fact that this process offers us a unique route from carbon dioxide to a C2 compound which can be subsequently subjected to further reactions including carbon-carbon bond formation reactions. In this sense, the conversion of carbon dioxide to formate by aqueous electrochemical methods and the thermal conversion of formate to oxalate offer a paradigm shift in CO₂ utilization.

The following high temperature coupling equation shows the reaction:



Our initial efforts are focused on the following aspects:

- (a) Establishing the optimal conditions for the maximum yield of oxalate for a specific catalyst,
- (b) Finding the catalyst that gives nearly quantitative yield of oxalate.
- (c) Proposing a reasonable mechanism for the reaction, investigate it by DFT methods.

The results obtained from our experiments and computations will be presented.

SILVER NANORASPBERRIES

Saadia Chaudhry, Aarti Patel, and Dr. Bhanu P. S. Chauhan*
Engineered Nanomaterials Laboratory, Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

Nanoscale particles display exquisite quantum mechanical properties because of their large surface areas compared to their bulk material counterparts. It has been demonstrated that transition metal nanoparticles exhibit unique optical, conductive, catalytic, and SERS properties. Naked metallic nanoparticles are unstable due to the changes in the band gap energies that result when transitioning from bulk to nanoscale; this results in a high surface energy that causes them to aggregate back into bulk if they are not stabilized with a surface ligand. In our laboratory, we are investigating a family of silicon based systems, in particular siloxanes with repeating Si-O-Si linkages. Siloxanes can function as tailoring agents for nanoparticle size, shape, stability, solubility, density, and crystallinity [1, 2]. We have also demonstrated that the cyclic and linear siloxanes provide unique stabilization, which does not compromise the activity of the resulting nanocomposites. However, investigations of cyclic siloxanes for the generation of nanoparticles have not been thoroughly explored.

In this study, we present a bottom-up approach to synthesize silver nanoparticles using the oligomeric cyclic siloxane 1, 3, 5, 7 tetramethylcyclotetrasiloxane (D_4^H), as a reducing and stabilizing agent. D_4^H is a reactive siloxane containing silicon-hydrogen bonds that are known to undergo oxidative addition/reductive elimination cycles in the presence of noble metals. Our hypothesis theorizes that the use of SiH bonds of D_4^H will reduce metal complexes and produce siloxane functionalized metal nanoparticles [3, 4]. For the first time, we will demonstrate that the four silicon vertices of D_4^H allow it to create distinctive nanoparticle morphologies, which we call “raspberry nanoparticles”. It is our belief that such nanoparticle morphologies can be widely used as silicon-based building blocks for hybrid nanomaterials and crosslinking reagents [5]. In addition, a study to examine the effect of the silicon-hydrogen bond mediated reduction process, a cyclic siloxane 1, 3, 5, 7-tetramethylcyclotetrasiloxane (D_4^V) that is devoid of SiH bonds was also studied. The resulting nanoparticle assemblies in presence of D_4^H and D_4^V were thoroughly characterized via UV-vis, FT-IR, IR mapping, SEM and TEM techniques.

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* Indicates Corresponding Author

NANOTECHNOLOGY AND ITS APPLICATION IN TEXTILE INDUSTRY

Sankalp Chauhan

Staten Island Technical High School, Staten Island, NY

Nanotechnology has impacted our everyday life in a significant manner. New technological advances are achieved using nano-technological principles in drug design, coatings, electronics communication and green chemistry. One area which is poised to achieve tremendous growth is nano-textile field. The age of designer nanomaterials based fabrics has major repercussions in R&D and technological innovations. Textile industry is the first manufacturing industry to make nano based finished products.

In this presentation, a detailed study of global impact of nanotechnology on the textile industry will be discussed. We will demonstrate that an interactive and innovative processes which exist between the two industries. Nanotechnology applications in garment industry includes manufacturing of stain resistant, wrinkle resistant, antimicrobial, and UV protected fabrics. United States textile industry has faced fierce competition due to labor intensive manufacturing processes. The global economic crisis has resulted in down turn of worldwide demand for textile and clothing. The key challenges faced by the textile industry in South East Asia is shrinking export demands, rising costs, currency fluctuations and financing constraints. In addition, in this presentation, current trends, social and economic impacts of nanotechnology in the textile industry with a particular emphasis on South East Asia will also be discussed.

YEAST CELLS-DERIVED HOLLOW CORE/SHELL HETEROATOM-DOPED CARBON MICROPARTICLES FOR SUSTAINABLE ELECTROCATALYSIS AND RENEWABLE ENERGY APPLICATIONS

*Xiaoxi Huang*¹ and Dr. Tewodros Asefa^{1,2,*}

¹ Department of Chemistry and Chemical Biology,

² Department of Chemical and Biochemical Engineering
Rutgers University, Piscataway, NJ

The use of renewable resources to make various synthetic materials is increasing in order to meet some of our sustainability challenges. We show that yeast cells can be thermally transformed into hollow, core-shell heteroatom-doped carbon microparticles that can effectively electrocatalyze the oxygen reduction and hydrazine oxidation reactions, reactions that are highly pertinent to fuel cells or renewable energy applications. We also show that yeast cell walls, which can be separated from the cells, can produce carbon materials with electrocatalytic activity for both reactions, albeit with lower activity compared with former one. The results reveal that the intracellular components of the yeast cells are indirectly responsible for the latter's higher electrocatalytic activity, by providing it with more heteroatom dopants. The synthetic method we report here can serve as a general route for the synthesis of (electro)catalysts using microorganisms as raw materials.

FACILE SYNTHESIS OF CARBON NANOTUBE SCAFFOLDED NANO-GELS

Qiaxian Johnson[^], Chinara Feizullayeva⁺, Dr. Moni Chauhan⁺, Swetha Matam[^],
and Dr. Bhanu P.S. Chauhan^{^*}

[^]Engineered Nanomaterials Laboratory, Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

⁺Department of Chemistry
Queensborough Community College of City University of New York, Bayside, NY

The unique aspects of fullerenes and their derivatives such as carbon nanotubes have been well documented since their discovery in 1985 [1]. Of these, carbon nanotubes possess many desirable properties that can be exploited. Carbon nanotubes are known to impart electrical conductivity through the propagation of an interconnected nanotube network inside of the polymer matrix (percolation), making them usable for conductive coatings, electrostatic dissipation, electromagnetic interference (EMI) shielding, printable circuit wiring, and conductive coatings [2]. In addition, their relative light weight coupled with their high tensile strength and elastic moduli can be employed to bestow a framework for various materials [3,4].

In our previous work, we synthesized and analyzed the successful self-assembly of silver nanoparticles using tris[3-(trimethoxysilyl)propyl] isocyanurate [5]. Building off this research, we present a synthetic strategy for the generation of a silyl functionalized nano-gel utilizing hydroxyl functionalized carbon nanotubes as scaffolding. To accomplish this, tris[3-(trimethoxysilyl)propyl] isocyanurate (TTPI) was grafted onto hydroxyl functionalized carbon nanotubes. The TTPI molecule was chosen for its ability to reduce salts to nanoparticles, stabilize them, and its ability to act in producing stable self-assembled nanoparticles [5]. Analysis of these materials was conducted via UV-Vis, Transmission Electron Microscopy (TEM), Secondary Electron Microscopy (SEM), Fourier Transform Infrared (FT-IR), and Electron Disruptive Spectroscopy (EDS).

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ULTRASMALL PALLADIUM NANOPARTICLES SUPPORTED ON AMINE-FUNCTIONALIZED SBA-15 AS EFFICIENT CATALYSTS FOR HYDROGEN EVOLUTION FROM FORMIC ACID

***Katherine Koh*¹, Jung-Eun Seo³, Jin Hee Lee³, Anandarup Goswami^{1,2*},**

Dr. Chang Won Yoon^{3*} and Dr. Tewodros Asefa^{1,2*}

¹Department of Chemistry and Chemical Biology

²Department of Chemical and Biochemical Engineering

Rutgers University at New Brunswick, NJ

³Fuel Cell Research Center, Korea Institute of Science and Technology
Hwarangno14-gil 5, Seongbuk-gu, Seoul 136-791, Republic of Korea

The success of the so-called “hydrogen economy” for large-scale applications will ultimately depend on efficient and sustainable production, storage and distribution of hydrogen. Owing to its low toxicity, high volumetric H₂ storage capacity and availability both from renewable resources (e.g., biomass) as well as nonrenewable resources (e.g., fossil fuel feedstocks), formic acid is one of the most favorable chemical hydrogen storage media for large-scale energy storage applications. However, for FA to become a viable hydrogen storage medium, efficient catalysts that enable it to release H₂ at low cost are necessary. Herein we show a facile synthetic route to amine-functionalized nanoporous silica-supported ultrasmall Pd nanoparticles (SBA-15-Amine/Pd) that were highly active catalysts for formic acid dehydrogenation, producing hydrogen at ambient temperature with a high turn-over-frequency (TOF) of 293 h⁻¹—which was among the highest TOFs ever reported for the reaction by a heterogeneous catalyst. We also show that the material is easily recyclable multiple times, without losing its catalytic activity. So, the catalyst we developed might contribute to some of the solutions of our sustainability challenges.

NEW HOST MATERIALS FOR WATER SOLUBLE SILVER AND GOLD NANOPARTICLES AND THEIR SELF-ASSEMBLY

Kelly Moran, Aarti Patel, Saadia Chaudhry, Qiaxian Johnson, and Dr. Bhanu P.S. Chauhan*
Engineered Nanomaterials Laboratory, Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

In recent years, nanosized particles of noble metals have experienced an increased attention due to their utility in the biological, pharmaceutical, and technological arena. The shape and size of these nanostructured materials are significant features that affect their applicability [1]. Studies have shown that the stability, particle size, and properties of nanoparticles are strongly dependent on the specific method of preparation and the experimental conditions applied [2]. In recent years, it has been proposed that silylated polymers due to the size of silicon and the freedom of rotation and flexibility with silicon heteroatoms bonds provide a degree of control over self-assembly systems [3]. In particular, we are interested in examining the effect of silylation of poly(ethylenimines) (PEI), which are known to exhibit high water solubility which makes them ideal vehicles for drug delivery applications. An added bonus is that PEIs have a high transfection efficiency, which allows PEI-stabilized metallic nanoparticles the ability to permeate through the cell membrane for targeted drug delivery [4].

In this poster, we present a facile method for synthesizing noble metal nanoparticles where silylated PEI are used as host materials. We theorize that both PEI and silylated PEI polymers will differently affect the formation, size, and morphology of the resulting nanoparticles. We will also present a comparative study of the ability of PEI versus trimethoxysilylpropyl-polyethylenimine (TMSP-PEI) for hosting the nanoparticles under identical reaction conditions. We have observed that TMSP-PEI can provide further tailoring of nanoparticle composites because of the reactivity of silicon moiety to further polymerize to produce sol-gel type materials. Detailed analytical studies indicate that trimethoxysilylpropyl-polyethylenimine imparts a tight control over nanoparticle agglomeration and passivation [5]. In this work, we will present evidence related to such an effect via detailed analyses of resulting materials using UV-Vis spectroscopy, FT-IR, NMR, TEM, and SEM/EDS.

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* Indicates Corresponding Author

LIGHT INDUCED TOXICITY OF SILVER NANOPARTICLES PRODUCED BY LASER ABLATION

J.J. Naddeo^{1,2}, *Matthew Ratti*^{1,2}, Dr. Eric Klein^{2,3}

¹Department of Physics, Rutgers University, Camden, NJ

²Department of Biology, Rutgers University, Camden, NJ

³Center for Computational and Integrative Biology, Rutgers University, Camden, NJ

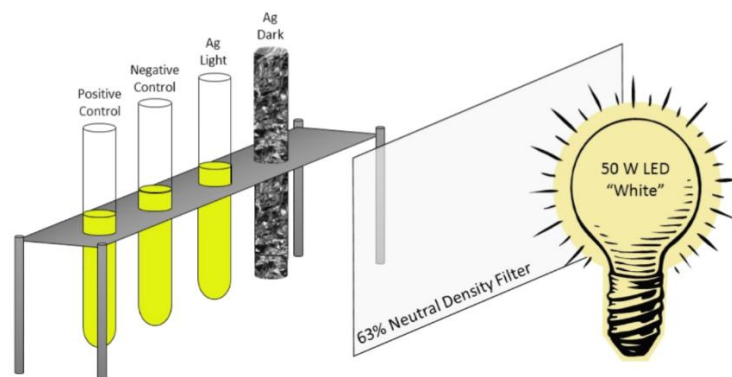


Fig. 1. *E. coli* cultures supplemented with silver nanoparticles, exposed to light

Silver is one of the most studied metals in the biomedical field and has been used for centuries in various forms as an antimicrobial agent dating back to Chaldean dynasty c.a. 4,000 B.C.E. [1]. Silver nanoparticles (AgNP) are of particular interest due to their physical properties, which have been shown to strongly influence antimicrobial activity. Our lab used laser ablation in liquid to synthesize AgNPs, giving us the ability to make “bare” particles, free from precursors that are typically associated with chemical synthetic methods. [2] A Nd:YAG laser at the fundamental wavelength ($\lambda=1064$ nm) was used to ablate a pure silver target immersed in a 60 mM sodium dodecyl sulfate solution. As some pathogenic bacteria form resistances to antibiotics, understanding the mechanisms behind AgNPs antimicrobial activity is paramount. A major problem that is preventing the universal application of AgNPs is their possible toxicity to higher organisms. Our current work supports the hypothesis that colloidal suspensions of silver nanoparticles produced by laser ablation, when irradiated with visible light, release a higher concentration of silver ions. Currently the consensus is that AgNPs are toxic due to their ability to release Ag^+ ions. Therefore, an increase in ion release will cause an increase in antimicrobial activity that may allow for lower levels of AgNPs required when treating bacterial infections, thus, limiting off-target toxicity. Our group showed that ablating a pure silver target immersed in a SDS solution produced very concentrated colloidal silver nanoparticle solutions, with hydrodynamic radii of approximately 40 nm. We also showed that this antimicrobial activity was greatly enhanced when the solutions were exposed to visible light at power of approximately 0.7 W. Using the optical properties of the DZ- Ag^+ complex, it was shown that particles exposed to light release ions at a much higher rate relative to particles kept in the dark. The reduced antimicrobial activity of the AgNP in the presence of L-cysteine showed that ions play a major role in the antibacterial effectiveness of AgNPs. As stated above we hope that paired with light, these silver nanoparticles can be employed at a low enough concentration that no adverse effects to mammalian cells will occur, or at the very least the mammalian cell death will remain localized.

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ANTIMICROBIAL ACTIVITY IN NANOCOMPOSITES BASED ON CHITOSAN

John-Michael Punla and Christie Tjie, Dr. Mihaela Leonida and Dr. Alice Benzecry

School of Natural Science
Fairleigh Dickinson University, Teaneck, NJ

The cosmetic industry is very interested in antibacterial agents active against Gram positive and Gram negative bacteria which are significant for skin conditions. Broad activity, stability, and sustained release properties are of special interest. Chitosan, a biocompatible polymer, active against many such species, can be used to make nanosized cationic matrices, using an entirely green process.

In this study several nanoparticulate materials based on chitosan were prepared: nanochitosan, nanocomposites containing chitosan and β -acid and, in a parallel procedure, chitosan and nisin. Nisin is a hydrophilic, small peptide, a biocin – species secreted by some microorganisms to protect themselves. It is typically used as food preservative but has the tendency to leak out from meat products too soon. Nanoparticulate chitosan is known for its capacity to encapsulate proteins. Lupulone (β -acid) is a component of hop (*Humulus lupulus* - a species of flowering plant in the *Cannabaceae* family, native to Europe, western Asia and North America). It was chosen for its strong antimicrobial activity (beer preservative). Its shortcoming is a very low bioavailability due to its lipophilicity. Sodium tripolyphosphate was used as a cross-linker and several ratios chitosan to cross-linker were used to make different nanocomposites. The particles were characterized by: ratio of free amine groups, content of additive (β -acid/nisin), IR spectra, encapsulation efficiency, loading capacity, and release kinetics.

The nanocomposites were tested against *Pseudomonas aeruginosa* and *Staphylococcus aureus* pathogens important for the skin and for the storage of cosmetic formulations. Turbidimetric assays were conducted in Mueller-Hinton broth and the activity of the composites was compared to that of the starting chitosan, of nanochitosan, and of the additives, taken separately. Synergistic effects were evaluated. Two other series of antimicrobial assays were conducted on a moisturizer containing nanocomposites and on a hand cream containing nanocomposites, respectively. The influence of diffusion was also evaluated.

MODELING CYP3A4-SPECIFIC INHIBITORS THROUGH RATIONAL INHIBITOR DESIGN

Janine Almale, Vicklyn Datilus and Dr. Parminder Kaur
Department of Chemistry
William Paterson University of New Jersey, Wayne, NJ

Cytochrome P450 3A4 (CYP3A4) is the most abundant metabolizing enzyme present in human body. It interacts with wide variety of molecules and some of these molecules were found to be inhibitors of CYP3A4. In our continuing effort for the design of new inhibitors, we have synthesized a series of simpler analogs as inhibitors. In this study, we did a systematic study of various structural aspects of these inhibitors such as backbone flexibility, aromaticity and side groups on the affinity of inhibitors.

EFFICIENT INVESTIGATIONS OF LIGAND-PROTEIN INTERACTIONS AT THE ATOMIC LEVEL WITH THE MOLECULAR DOCKING METHOD

Ryan Dugan and Dr. Yang Yang
Department of Chemistry and Biochemistry
Rowan University, Glassboro, NJ

Molecular docking is a computational modeling method that seeks to explore the best binding compatibility between a ligand and a target protein receptor. The method efficiently samples the conformational space of a ligand binding into the active site of the target protein. It further evaluates the “binding affinities” for various ligand-protein complexes with a well-optimized scoring function, and predicts the most probable binding position, conformation and orientation within the protein active site. In this current study, with Schrodinger’s Small Molecule Drug Discovery Suite, we benchmark the Glide molecular docking algorithm with two specific ligand-protein systems. For both of the cases, our calculations successfully reproduce the experimentally-determined crystal structures, supported by the low root-mean-square deviation (RMSD) of the computed ligand structure in comparison with the cocrystallized ligand in the protein active site. Molecular docking, an efficient and accurate modeling technique, is being implemented in our research group to facilitate high throughput drug design.

GREEN CHEMISTRY PRINCIPLES INCORPORATED INTO THE UNDERGRADUATE ORGANIC LABORATORY

Akram Hussain, Henry Herrera, and Dr. Sarah Carberry
Department of Chemistry
Ramapo College of New Jersey, Mahwah, NJ

Three new and/or improved undergraduate laboratory experiments will be discussed. The first is a standard column chromatography experiment with 1:1 mixture of acetylferrocene and ferrocene using heptane and acetone instead of hexane and diethyl ether to introduce the concept of Green Chemistry, by reducing the use of hazardous substances. Hexane-ether trials gave an average percent recovery of 74% for ferrocene and 89% recovery for acetylferrocene. This is comparable to the hexane-acetone trials where the average percent recovery for ferrocene was 70% and for acetyl ferrocene was 93.72%. For the second experiment, sequential oxidation-reduction reactions were investigated. This sequence should allow for recycling of the products for the use in subsequent experiments. The systems that were tested were 9-fluorenone/9-fluorenone and benzhydrol/benzophenone. Both systems were oxidized using bleach and acetic acid and reduced using NaBH₄, with yields of 86-98%. The third experiment was an Olefin Metathesis of styrene to (E)-Stilbene using Grubbs second generation catalyst. This product was then purified by then filtering through alumina followed by recrystallization. Studies to determine optimal conditions for this experiment are still under way.

COMPUTATIONAL STUDIES AND RAMAN SPECTRA OF TEN SULFA DRUGS

Alexis R. Javornik, Ashley E. Kuptsow, Maximillian P. Baria

and Dr. Elmer-Rico E. Mojica

Department of Chemistry and Physical Sciences

Pace University, One Pace Plaza, NY

Sulfa drugs are commonly used in aquaculture as agricultural herbicides and in the treatment of respiratory and urinary tract infections in humans. These drugs remain one of the most popular active antimicrobial agents used in animal food production due to their relative low cost. The aim of the work is to identify chemical bonds, unique to the sulfa drugs, which are not only key in understanding its antimicrobial properties but will also provide a way to quantitate amounts of each drug in a given mixture. We applied computational methods to ten sulfa drugs, namely sulfamethazine, sulfamethoxazole, sulfachloropyridazine, sulfadimethoxine, sulfathiazole, sulfamerazine, sulfisoxazole, sulfamethizole, sulfameter, sulfadiazine and sulfadiazine. Results of the simulation studies were then compared to the measured Raman spectra of the ten sulfa drugs. Vibrational bands that are both unique and common to the sulfa drugs were identified. The data obtained will be discussed in terms of their implication to the function and the quantitative analysis of the sulfa drugs.

VIBRATIONAL SPECTROSCOPY OF FLUOROQUINOLONE ANTIBIOTICS

Ashley E. Kuptsov, Alexis R. Javornik, Maximillian P. Baria and Dr. Elmer-Rico E. Mojica
Department of Chemistry and Physical Sciences
Pace University, New York, NY

The fluoroquinolones are a family of broad spectrum, systemic antibacterial agents that have been used widely as therapy of respiratory and urinary tract infections. They are among the most commonly prescribed class of antibiotics in the United States and active against a wide range of aerobic gram-positive and gram-negative organisms. The aim of the work is to identify chemical bonds, unique to the fluoroquinolones, which are not only key in understanding its antimicrobial properties but will also provide a way to quantitate amounts of each drug in a given mixture. We applied computational methods to four antibiotics, namely ciprofloxacin, enrofloxacin, norfloxacin and sarafloxacin. Results of the simulation studies were then compared to the measured Raman and IR spectra of the four drugs. Vibrational bands that are both unique and common among the four drugs were identified. The data obtained will be discussed in terms of their implication to the function and the quantitative analysis of the fluoroquinolones

QSAR—A POWERFUL COMPUTATIONAL TECHNIQUE FOR ACCURACY AND EFFICIENCY IN DRUG DESIGN

Cody Prettyman, Dr. Yang Yang
Department of Chemistry and Biochemistry
Rowan University, Glassboro, NJ

Quantitative Structure-Activity Relationship (QSAR) modeling is a powerful computational technique which predicts the biological activity of new drug candidates based on the quantitative relationship between chemical structures and molecular properties for a set of training molecules. In contrast to the traditional drug design, where each drug candidate is synthesized and tested experimentally, QSAR is able to screen out the potentially unsuccessful compounds in a high throughput manner *in silico*. It is a tremendous leap forward in the field of drug design as it saves time and resources while leading to a more precise description of activity. In the present study, a QSAR model system based on the Gaussian fields of a set of ligands is established and tested with Schrödinger's Small Molecule Drug Discovery Suite to determine the effects of various functional groups on biological activity. Specifically, we explore how different ligands in the study set relate to variances in activity (e.g., pIC₅₀). A specific case where two different ligands with nearly identical structures demonstrated dramatically distinct pIC₅₀ values is investigated in detail. With QSAR, we are able to modify the structure of one of these ligands to better resemble the other and predict how such changes affect the bioactivity correspondingly, through which the contribution of individual functional groups towards bioactivity is revealed quantitatively. QSAR, proven to be extremely useful in drug design, is being established as a routine practice in our research group to facilitate experimental drug optimization.

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FACULTY PARTICIPATION

Dr. Colin Abernethy Sarah Lawrence College cabernethy@sarahlawrence.edu	Dr. Mihaela Jitianu William Paterson University jitianum@wpunj.edu	Dr. Elmer-Rico Mojica Pace University Emojica@pace.edu
Dr. Alice Benzecry Fairleigh Dickinson University Benzecry@fdu.edu	Dr. Terry Kamps New Jersey City University tkamps@njcu.edu	Dr. Emily Monroe William Paterson University monroe@wpunj.edu
Dr. Robert Benno William Paterson University bennor@wpunj.edu	Dr. Parminder Kaur William Paterson University Kaurp6@wpunj.edu	Dr. Edith Myers Fairleigh Dickinson University edmyers@fdu.edu
Dr. Ted Brummel Long Island University Post Campus tbrummel@liu.edu	Dr. Swayamjot Kaur Rutgers University Kaursw@rci.rutgers.edu	Dr. Brian Olechnowski Fairleigh Dickinson University bolech@fdu.edu
Dr. Sarah Carberry Ramapo College sbolton@ramapo.edu	Dr. Ish Kumar Fairleigh Dickinson University ikumar@fdu.edu	Dr. Emmanuel S. Onaivi William Paterson University onaivie@wpunj.edu
Dr. Bhanu P.S. Chauhan William Paterson University chauhanbps@wpunj.edu	Dr. Prasad Lakkaraju Georgian Court University Lakkaraju@georgian.edu	Dr. Harald Parzer Fairleigh Dickinson University
Dr. Moni Chauhan Queens County College - CUNY Mchauhan@qcc.cuny.edu	Dr. Mihaela Leonida Fairleigh Dickinson University mleonida@fdu.edu	Dr. Pradeep Patnaik William Paterson University Patnaikp@wpunj.edu
Dr. Eileen Gardner William Paterson University gardnere@wpunj.edu	Dr. Alessandra Leri Marymount Manhattan College Aleri@mmm.edu	Dr. Michael Peek William Paterson University peekm@wpunj.edu
Dr. Michelle Hersh Sarah Lawrence College mhersh@sarahlawrence.edu	Dr. Kendall Martin William Paterson University martink@wpunj.edu	Dr. James Salierno Fairleigh Dickinson University Salierno@fdu.edu
Dr. Andrei Jitianu Lehman College - CUNY Andrei.jitianu@lehman.cuny.edu	Dr. Patricia Melloy Fairleigh Dickinson University pmelloy@fdu.edu	Dr. Norman Schanz William Paterson University schanzn@wpunj.edu

FACULTY PARTICIPATION

Dr. David Slaymaker William Paterson University slaymakerd@wpunj.edu	Dr. Carey Waldburger William Paterson University waldburgerc@wpunj.edu	
Dr. Joseph Spagna William Paterson University spagnaj@wpunj.edu	Dr. Yufeng Wei Seton Hall University Yufeng.wei@shu.edu	
Dr. Natalya Voloshchuk Rutgers University voloshchuk@aesop.rutgers.edu	Dr. Yalan Xing William Paterson University xingy@wpunu.edu	

PARTICIPATING INSTITUTIONS

Entree	Name
1	CENTENARY COLLEGE
2	CITY COLLEGE OF NEW YORK
3	EDISON HIGH SCHOOL
4	FAIRLEIGH DICKINSON UNIVERSITY
5	GEORGIAN COURT UNIVERSITY
6	HARVARD MEDICAL SCHOOL
7	KEAN UNIVERSITY
8	KOREA INSTITUTE OF SCIENCE & TECHNOLOGY
9	LEHMAN COLLEGE
10	LONG ISLAND UNIVERISTY - POST
11	MARYMOUNT MANHATTAN COLLEGE
12	MONMOUTH UNIVERSITY
13	MONTCLAIR STATE UNIVERSITY
14	NEW JERSEY CITY UNIVERSITY
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28	UNIVERSITY OF SÃO PAULO
29	WILLIAM PATERSON UNIVERSITY
30	YALE UNIVERSITY

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