

Fall 2009



**Proceedings of the Thirtieth Annual
Sigma Xi
Student Research Symposium
and
Third Annual
Scholars' Celebration Student Research Symposium**

The University of Toledo



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The following people are being recognized for outstanding presentations during the 30th Annual Sigma Xi Student Research Symposium and 3rd Annual Scholar's Celebration Student Research Symposium. Please note that the categories for recognition are based on the fields in which the majority of presentations occurred.

Biological/Medical Sciences

First Place: Michael Bekier

Honorable Mention: Dipali Date

Environmental Sciences

First Place (Tie): Kristopher Barnswell and Osvaldo J. Sepulveda-Villet

Engineering

First Place: Jayanth Malatkar

Honorable Mention: Thehazhnan K. Ponnaiyan

Posters

First Place: Leah Rider

Honorable Mention (Tie): Andrew Wash and Thehazhnan K. Ponnaiyan

Undergraduates (Posters and Oral Presentations)

First Place: Hannah West

Honorable Mention: Kristin Stroud

Please note the following!! You are invited to be present for the Annual Meeting and Lecture tomorrow evening (October 28th) - see a copy of the announcement, below.

Congratulations to all of our presenters. You helped to make the Symposium an interesting and wonderful experience!

The abstract proceedings are attached.

Daryl Dwyer

Announcement

The University of Toledo Chapter of Sigma Xi will formally recognize the 2009 recipients of the *Dion D. Raftopoulos/Sigma Xi Award for Outstanding Research* (Saleh Jabarin, Professor of Chemical and Environmental Engineering) and the *Young Faculty Award* (Surya Nauli, Assistant Professor of Pharmacology) as well as the winners from this year's upcoming student research symposium.

Dr. Saleh Jabarin **will be delivering a lecture entitled, "The Roles of Structure, Morphology, and Processing of Polymers in Meeting Rigid Packaging Expectations."**

The event will be held on **October 28th** at **7:00pm** in the College of Engineering Seminar Room (**Nitschke 1027**). Light refreshments will be served starting at 6:30 pm.

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Length of mitotic arrest induced by microtubule-stabilizing drugs determines cell fate after mitotic exit

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Cell death induced by agents that disrupt microtubules can kill cells by inducing a prolonged mitotic block. This mitotic block is dependent on the spindle assembly checkpoint, a surveillance system that ensures the bipolar attachment of chromosomes to the mitotic spindle before the onset of anaphase. Under some conditions, the spindle assembly checkpoint can become weakened, allowing cells to exit mitosis despite the presence of chromosomes that are not properly attached to the mitotic spindle. Here, we use an Aurora kinase inhibitor to drive mitotic exit and test the effect of mitotic arrest length on death in the subsequent interphase. Cells that are blocked in mitosis for >15 h die shortly after exiting from mitosis, whereas cells that exit after being blocked for <15 h show variable fates, with some living for days after exiting mitosis. Cells blocked in mitosis by either Taxol or epothilone B are acutely sensitive to the death ligand tumor necrosis factor-related apoptosis-inducing ligand, suggesting that prolonged mitosis allows the gradual accumulation of internal death signals, rendering cells hypersensitive to additional prodeath cues. Death under these conditions is initiated while cyclin B1 is still present, indicating that cells are in mitosis. Our experiments suggest that there is a point of no return during prolonged mitotic block after which mitotic exit can no longer block death.

Post-translational Modifications of Chromosomal Passenger Protein Borealin

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Cancer is one of the leading causes of death in the United States of America. Cancer is characterized by abnormal cell growth and uncontrolled cell division. The cell cycle is a series of events that results into growth of a cell, duplication of its contents and division into two daughter cells. The chromosomal passenger complex (CPC) plays an important role in the co-ordination of essential cell cycle events. The CPC is made up of Aurora B the enzymatic core, and regulatory subunits INCENP, Survivin and Borealin.

Borealin is expressed in a cell cycle dependent manner and is phosphorylated at S219 during mitosis. Phosphorylation is an important form of posttranslational modification that regulates protein stability, function and localization. Cells expressing Borealin mutant S219A exhibit defects in mitosis, however the kinase phosphorylating S219 is unknown. Cdk1 belongs to a family of Ser/Thr kinases that exert their effects on cell-cycle events by phosphorylating a large number of proteins in the cell. Over expression of a constitutively active Cyclin B1/CDK1 complex resulted in an elevated level of phosphorylated Borealin species. However, purified CDK1 did not efficiently phosphorylate full length GST-Borealin in vitro. Hence CDK1 may not directly phosphorylate Borealin at S219 during mitosis. An alternative is that Cdk1 regulates phosphorylation status of Borealin by regulating its phosphatase. Borealin is dephosphorylated after mitotic exit. Cdc14s belong to a novel family of dual specificity Ser/Thr phosphatases that are active during interphase and inactive during mitosis. We observed that over expression of Cdc14B resulted in a reduced amount of slow migrating phosphorylated species of Borealin. Also Cdc14B and Borealin were seen to co-localize to the nucleolus of interphase cells. In addition over expression of Cdc14B affected the kinetics of Borealin dephosphorylation on mitotic exit. We hypothesize that Cdc14B may be involved in the dephosphorylation of Borealin after cells have exited mitosis.

Analysis of Sororin Phosphorylation

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Cancer is characterized by the uncontrolled growth of aberrant cells and kills over half a million people a year in the United States. Many cancers are aneuploid; therefore, an understanding of how chromatids are linked together and separate at the appropriate time may shed light on the origins of cancer. Cohesion of sister chromatids is maintained by the multi-protein complex cohesin, consisting of Smc1, Smc3, the kleisin family protein Scc1, and the accessory subunit Scc3. Sororin associates with the cohesin complex and regulates the segregation of sister chromatids but little is known regarding the regulation of sororin. We observed that Cdk1 phosphorylates sororin *in vitro*. Further, sororin is phosphorylated in mitosis where Cdk1 is most active. We created a mutant that cannot be phosphorylated by Cdk1 by converting all serines/threonines followed by proline to alanines (nine mutations in total). Unlike wild-type, the mutant remains associated with the chromosomes and the cohesin complex throughout prometaphase. We tagged the mutant with GFP and unlike the wild-type, it associates with the chromatin in prometaphase. Also, we isolated the cohesin complex by immunoprecipitating with an antibody to Smc3. Wild-type sororin is associated with Smc3 in G2 but not prometaphase. In contrast, the mutant is associated with the Smc3 in G2 and mitosis. Therefore, Cdk1 phosphorylates sororin and is required to release sororin from the chromatin.

Neuropeptides are essential for the serotonergic stimulation of sensory mediated aversive behaviors in *Caenorhabditis elegans*.

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In mammals, serotonin (5-HT) regulates diverse behaviors, including, mood, anxiety, perception and aggression (1,2). Mood disorders, such as depression, are among the most common mental illness and are often treated with drugs that elevate monoamine levels, leading to the “monoamine hypothesis” of depression. However, other signaling cascades, including those mediated by peptides are also important. For example, substance P, neurokinin A, corticotrophin-releasing factor, neurotensin, neuropeptide Y and galanin have all been identified as candidates for antidepressant drug development (3). In *Caenorhabditis elegans* behavioral state or “mood” is dependent on food availability and is translated by both monoaminergic and peptidergic signaling in the fine-tuning of most behaviors (4,5). We have used this simple model to examine the interaction of monoamines and peptides in the modulation of aversive behaviors mediated by a pair of polymodal, nociceptive ASH sensory neurons. Serotonin sensitizes the ASHs and stimulates aversive responses through a pathway requiring the $G\alpha_s$ -dependent-release of neuropeptides encoded by *nlp-3*. Peptides encoded by *nlp-3* released from the ASHs appear to stimulate aversive responses through the C06G4.5 receptor, as sensory and locomotory phenotypes associated with *nlp-3* over-expression are absent in *c06g4.5* null animals. These studies are continuing to functionally characterize the role of this peptide receptor in mediating the effects of serotonergic modulation on the ASH-mediated circuit. Together, they highlight the utility of the *C. elegans* model for defining interactions between monoaminergic and peptidergic signaling at the level of single neurons.

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4. R. Wragg *et al.*, *J. Neuro Sci* **27**, 13402-13412 (2007).
5. G. Harris *et al.*, *J. Neuro Sci* **29**, 1446-1456 (2009).

Monoamines and peptides interact to modulate sensory-mediated glutamatergic signaling in *Caenorhabditis elegans*

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Monoaminergic signaling is involved in a number of behaviors and disorders, such as anxiety, addiction, depression, obesity, Parkinson's disease and schizophrenia (1). However, due to the extreme complexity of the mammalian nervous system, the mechanisms underlying the monoaminergic modulation of these behaviors are still only poorly understood. In *C. elegans*, monoamines partially define "behavioral state" and modulate key behaviors, with octopamine (OA) often opposing the action of serotonin (5-HT). Aversive responses to environmental stimuli are modulated by monoamines, facilitating the development of a simple model system to define the sensory-mediated aminergic circuits mediating behavioral plasticity. The polymodal ASH sensory neurons are necessary and sufficient for detection of 30% octanol, while responses to 100% octanol also involve the AWB and ADL sensory neurons (2, 3, 4). OA inhibits responses to both 30% and 100% octanol, but through different OA receptors. OCT-1 mediates the OA inhibition of 5-HT stimulated aversive responses (3). OCT-1 couples to $G\alpha_o$ and functions directly in the ASHs to inhibit aversive responses to 30% octanol. In contrast, the putative OA receptor, SER-6, is essential for aversive responses to 100% octanol and functions in the ADLs and AWBs, not the ASHs, to stimulate the release of inhibitory neuropeptides, based on neuron-specific RNAi knockdown and rescue. The ADLs and AWBs express multiple peptide-encoding genes. For example, aversive responses in *nlp-7* or *nlp-9* null animals are not inhibited by OA, in contrast to wild type animals, and the overexpression of either *nlp-7* or *nlp-9* dramatically inhibits basal responses. Together, these results suggest that OA, acting through SER-6, stimulates the release of inhibitory peptides encoded by *nlp-7* and *nlp-9* that in turn inhibit ASH mediated aversive responses. These studies are continuing with characterization of SER-6 mediated G-protein signaling in both the AWBs and ADLs and the identification and functional localization of the putative G-protein coupled receptors activated by peptides encoded by *nlp-7* and *nlp-9* in the ASH mediated locomotory circuit. The *C. elegans* model system has proven to be ideal for defining monoaminergic/peptidergic interactions in the behavioral modulation of neuronal plasticity.

1 Lanni et al. Cell. Mol. Life. Sci. 66, 2985-3008 (2009).

2 Chao et al. PNAS, 101, 15512-15517 (2004).

3 Wragg et al. J. NeuroSci. 27, 13402-13412 (2007).

4 Harris et al. J. NeuroSci. 29, 446-1456 (2009).

Influence of Gold Nanoparticle-modified Electrode on Binary Self-Assembled Monolayers composed of 3-mercaptopropionic acid and 1-tetradecanethiol

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Immobilization of different organic molecules on various substrates is important in many research areas. Modification of surface of metal electrodes at a molecular order can be performed by Self-assembled monolayers (SAMs) of alkanethiols and their derivatives (1). Techniques using organized SAMs provide several interesting characteristics and can be applied for many applications, such as biosensors, bioelectronics, and patterning (2).

In this report we present electrochemical studies of binary self-assembled monolayers (SAMs) consists of 3-mercaptopropionic acid (MPA) and 1-tetradecanethiol (TDT) on a gold nanoparticle (AuNP)-modified electrode. The comparison of assembly structure and property of binary SAMs on AuNP-modified electrode with that on Au planar electrode were examined by Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS). The overall surface area and average size of AuNP would be controlled by varying concentration and deposition time and were investigated by Field Emmission-Scanning Electron Microscope (FE-SEM) (3,4). The reductive desorption in 0.5 M KOH was carried out and it was shown that AuNP-modified electrode would enhance the electrochemical properties (5).

Keywords

Self-assembled monolayer, Gold nanoparticles, Reductive desorption, Cyclic voltammetry, Electrochemical Impedance Spectroscopy

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2. K. Zhang et al., Fabricatoin of a sensitive impedance biosensor of DNA hybridization based on gold nanoparticles modified gold electrode. *Electoanalysis* 20, 2127, (2008)
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4. T.R. Soreta et al., Electrochemical surface nanopatterning by selective reductive desorption from mixed metal surfaces. *Electrochimica Acta* (2009)
5. S.F. Liu et al., The influence of gold nanoparticle modified electrode on the structure of mercaptopropionic acid self-assembly monolayer. *Electrochimica Acta* 51, 427, (2005)

Investigating Rhamnose as a Tumor-Antigen Immunogen

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Cancer antigens represent a class of poor immunogens that are often unsuccessful in generating a significant immune response in mammals. One technique used to enhance the immunogenicity of tumor-related epitopes involves the coupling of tumor-associated antigens to known immunogenic substances. Rhamnose, a biosynthetic sugar found in a number of plants and bacteria, was evaluated in our study as a novel candidate for tumor-antigen conjugation. In related studies, a structurally similar sugar, α -galactose, has been shown to enhance the immune presentation of influenza virus, HIV, as well as smaller molecules including BSA. In our study, BALB/c mice were primed with rhamnose-conjugated KLH to generate anti-rhamnose antibodies. The mice were subsequently vaccinated with rhamnose-conjugated ovalbumin to evaluate immune presentation. Our experimentation revealed that rhamnose did not enhance the immune presentation of ovalbumin. Further studies are planned to determine the reasons for the observed differences between rhamnose and α -galactose as enhancers of immunogenicity.

*This project acknowledges fiscal support through The University of Toledo Office of Undergraduate Research.

Total Synthesis of (\pm) Vestitol

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Because of their antioxidant properties, isoflavonoids have been implicated in the treatment of free radical mediated disorders such as cancer, Alzheimer's, Parkinson's, and certain cardiovascular diseases (1). Isoflavans, a comparatively smaller subgroup of isoflavonoids, also show a broad range of physiological activity. Vestitol (1,2,3) and related isoflavans are considered to be useful chemopreventive agents for peptic ulcer and gastric cancer in *H-Pylori* infected individuals (4). Because of its therapeutic potential as a cancer preventive agent, our lab has undertaken a multi-step total synthesis of (\pm) vestitol. Experimental results and important chemical details will be described during the presentation.

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**What Role Does Handedness Play in Endowment Effects?
The Mechanism behind the Endowment Effect: Loss Aversion or Egocentric Empathy***

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Previous research has found that the endowment effect is demonstrated when a person is willing to sell an object for more than they are willing to buy the same exact item. The current study was aimed at figuring out why this effect takes place and which theory, loss aversion, (i.e., not being able to part with something that has been part of oneself) or egocentric empathy (i.e., not being able to take the perspective of others) is the driving force behind the effect. More specifically, we asked 72 undergraduate students at the University of Toledo to fill out a short packet of questions containing the current study. Half were given a University of Toledo pencil to keep while others were only shown the pencil. They rated the pencil on its qualities and how much they thought it was worth. The purpose of this study was to look at the strength of handedness, the degree to which a person uses one (strong hander) or both (mixed hander) hands for a variety of everyday tasks as a prediction and an explanation for the effect. The anticipated result was that the endowment effect would have handedness differences and that these results would show that the effect is driven more by egocentric empathy than loss aversion. The overall results did show an overall endowment effect but in the opposite direction as predicted. Also, it seems as if there is in fact a handedness difference in that mixed-handers are driving this opposite effect, although these particular results were not significant.

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**Elaborating the Theme of Gender using the German Language as Inspiration
An Exploration of Different Materials and Techniques***

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My creative project took place over the span of a ten week period, where I developed artwork inspired by gender and the German language. I began by gathering information in the form of art magazines and scholarly articles that related to issues regarding gender and German or a combination of the two. Using both the work of other artists and the articles as inspiration, I began planning and developing ideas. I narrowed my focus by creating a list of 13 specific words that were systematically chosen from a German-English dictionary. I worked to create new ways to express my thoughts using various media including the computer, vellum paper, MRIs, and acetone transfers. I used the knowledge I gained from research and the list of words along with their gender according to the German language to create three main pieces of art. The products of this research indicate how very diverse approaches can be taken to address an issue or idea

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Field Water Balance for Evapotranspiration Covers in Northwest Ohio

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The overall goal is to design final covers for landfills that produce allowable rates of percolation and that use native plants restore habitat. Evapotranspiration (ET) covers are a potential strategy to achieve this goal, but have produced unacceptable rates of percolation in regions that receive greater than 40 cm of precipitation per year. An overview of published studies suggests that increasing plant transpiration will enhance the performance of the ET cover. The objectives of this study were to evaluate the rates of percolation produced by ET covers using immature and mature vegetation and determine their suitability for landfills in northwest Ohio (annual precipitation of 83 cm; target rate of percolation is 32 cm per year). The experiment was conducted in two lysimeters (1.52 m diameter x 1.52 m depth) that permitted the components of the water balance equation (applied water = ET + soil water storage + percolation) to be quantified. A soil mixture containing sediments dredged from the Toledo Harbor shipping channel dredged sediment was placed into each lysimeter to a depth of 60 cm; this base soil was amended with peat moss (6.5% FWT, a greenhouse study demonstrated this rate was able to increase the water storage capacity) and placed into the overlying 60 cm. The ET cover using immature vegetation consisted of a native seed mixture that was sown into topsoil (20 cm), while the ET cover using mature vegetation consisted of sod (20 cm) that was excavated from a native prairie (5 to 10 years old). Water was applied (AW) three times weekly to simulate the months of the wettest year on record (116 cm in 2006) from 11 June to 8 October in 2009. Moisture sensors were placed in a triangular array at two depths (0.30 m and 1.12 m) during construction to quantify the soil water storage (SWS), and water that reached the bottom of a lysimeter was collected using peristaltic pumps to quantify the rate of percolation (PER). The rate of ET was determined from the difference between AW and the sum of SWS and PER. There was no PER produced from the ET cover using mature vegetation, while the ET cover using immature vegetation produced 2.62 cm (7.97 cm per year). The mature vegetation had greater ET (52.68 cm) than the immature vegetation (40.81 cm), which increased the SWS during the experiment. The rates of PER produced by both ET covers are well below the target rate for Ohio landfill covers. The data collected do not support conclusions from other studies, and indicate that ET covers are suitable for humid regions.

The effect of the ant, not the mutualism: *Azteca instabilis* impacts herbivore and tropical tree in Chiapas, Mexico

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Ants are predators of herbivorous insects. The effect of ants on herbivores and indirect effect on plants are strongest on plants that form strong mutualisms with ants. However, there are only few examples documenting the importance of ants that are only incidentally associated with plants, although some of these ant species are extremely aggressive. Here we show the presence of the ant, *Azteca instabilis* reduced the abundance of herbivorous flea beetles ~75 fold on base leaves and ~12 fold on the canopy leaves of *Conostegia xalapensis* shade trees in a coffee agroforestry system. Additionally, in the presence of *Azteca* the amount of herbivore damage was reduced ~25 fold on base leaves and ~22 fold on canopy leaves. Further, the tree does not bare domatia, extra-floral nectary, or food body ant rewards, and we found no correlation between beetle damage and the presence of honeydew-producing insects, suggesting it was the ant not a mutualism that caused the strong indirect positive effects for this particular tropical tree.

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**A complex trophic interaction in a coffee agroecosystem:
Effects of a parasitic phorid fly on ants and the coffee berry borer**

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The *Pseudacteon* sp. phorid fly parasites have a negative direct effect on *Azteca instabilis* ants, thereby creating a positive indirect effect on ant prey. However, it is unknown of the influence of habitat factors on ant-phorid interactions or to what effect phorid flies have on the coffee berry borer, a pest to coffee farms. For two months, I performed research on the three species in two field sites in Finca Irlanda, a high shaded area and a low shaded area in Chiapas, Mexico. I conducted lab and field experiments to test the following hypotheses: 1) The phorid fly effects on *A. instabilis* ants differ between sun coffee and shade coffee habitats and 2) The presence of phorid flies near *A. instabilis* colonies has a positive, indirect effect on the coffee berry borers by allowing them more access to coffee berries.

To test hypothesis 1, I observed the influences of phorid flies on ant activity in both field sites. I randomly selected *Alchornea latifolia* trees with *A. instabilis* nests, and placed five tuna baits on the tree. I then recorded the number of *A. instabilis* ants present at each bait every two minutes for thirty minutes and the phorid arrival time.

I performed a lab experiment to determine hypothesis 2. I set up twenty-six insect arenas consisting of three treatments. Treatment one contained a coffee branch with ten berries and twenty CBB. Treatment two contained a coffee branch with ten berries, twenty CBB, and twenty ants. Treatment three contained the same components as treatment two, but two phorid flies were added. The insect arenas were left unattended for 24 hours, and then I counted how many berries were occupied by the CBB.

My field results indicate that the phorid flies have a bigger impact on the *A. instabilis* in the low shaded area. Also, the phorid fly arrives to the nest in the low shaded area almost twice as fast as the restoration area. My lab results show that treatment 1 and treatment 3 are significantly different from treatment 2.

My results prove that the *A. instabilis* ants control the CBB population, and that since the phorids have a greater impact on the ants on a low shaded farm, the ants will be more effective in controlling the CBB in densely shaded areas.

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Viral Hemorrhagic Septicemia (VHS) Immersion Challenge in Juvenile Muskellunge Using StaRT-PCR: A Quantification Study

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Viral hemorrhagic septicemia (VHS) is a very contagious fin fish disease, of which a unique and especially virulent strain (IVb) outbreaked in 2005 in the Great Lakes, killing several economically prominent freshwater fishes; yellow perch (*Perca flavescens*), muskellunge (*Esox masquinongy*), and freshwater drum (*Aplodinotus grunniens*); with outbreaks in subsequent years. Despite efforts to reduce detection time with DNA diagnostics, cell culture - which is a weeks long laborious process - is the only currently approved method to detect VHS. Over the past year, our laboratory has been developing a new Standardized reverse transcriptase polymerase chain reaction (StaRT-PCR) assay to detect and quantify VHS. This method will significantly speed detection time (to hours), lower detection threshold, uniquely identify among VHS strains, and provide intrinsic quality control via a standardized mixture of internal standards (SMIS). To date, our test has been optimized to detect lower levels of infection for all VHS strains (and specifically strain IVb) in fish 0-12 hours post infection. We partnered with Drs. Mohammed Faisal and Robert Kim (Michigan State University) to conduct an immersion challenge experiment using four doses of VHSv-IVb in juvenile muskellunge: control (0 plaque forming units (pfu)/mL), low (100 pfu/mL), intermediate (4,000 pfu/mL), and high (100,000 pfu/mL). Duplicates of 45 fish were immersed in the separate doses, and kidney and spleen tissues were removed from two fish per tank at different time points for testing. MSU conducted cell culture to determine if samples tested positive or negative and plaque assay/qRT-PCR for viral quantification; which we are comparing with our StaRT-PCR test results. Our test is projected to benefit aquaculture, hatchery, and baitfish facilities and Great Lakes fishery managers in accurately detecting the presence of the virus within hours.

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Genetic structure of Lake Erie yellow perch: A landscape genetic approach to test management unit congruency

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The yellow perch is a key sport and commercial fish whose abundances and distribution center in the lower Great Lakes, and particularly Lake Erie. Lake Erie populations have fluctuated historically due to unstable recruitment patterns and exploitation. Discerning the genetic basis underlying population structure and its relation to current fishery management units (MUs) are critical for effective conservation. Specifically, MUs should reflect the genetic structure of stocks. Our study tests the correspondence of the population genetic structure of yellow perch *Perca flavescens* across Lake Erie to its 4 MUs, which span 2 countries and 5 states/provinces. Fourteen nuclear microsatellite loci are analyzed for 594 spawning individuals from 13 Lake Erie sites, representing all current MUs and physiographic basins, with reference to their differentiation from outgroups in Lake St. Clair and Lake Ontario. Analyses include pairwise divergence comparisons, AMOVA partitioning, Mantel regression of genetic and geographical distances, genetic distance trees, Bayesian assignment, 3-dimensional factorial correspondence, and Monmonier geographic networks. Results show fine-scale genetic structure distinguishes some spawning groups in Lake Erie, with those spawning in eastern Lake Erie appearing more closely allied to groups in Lake Ontario than to western Lake Erie. Results further show fine-scale genetic structure distinguishes some spawning groups in Lake Erie, with little relationship to the MUs. Yellow perch spawning groups along the southern shores of Lake Erie also exhibit genetic divergence from those spawning along the northern shores. There is preliminary evidence of some temporal variation at spawning sites that contain multiple stocks, whereas others appear to comprise single stock and remain stable, meriting further testing.

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Effects of silicon on uptake and toxicity of arsenic and copper in *Lemna minor*

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Arsenic and copper commonly co-occur in mining and/or industrial wastes. Aquatic plants in free water surface wetlands (FWSWs) might be useful for removal of those metals from contaminated water. One potentially useful plant species, *Lemna minor*, has been shown to accumulate concentrations up to 1496 mg As kg⁻¹ (unpublished data) and 647 mg Cu kg⁻¹ (1) when cultured in arsenic- or copper-laden solutions, respectively. Silicon is the second most common element in the earth's crust and has been shown to affect plant responses to some abiotic stressors, including metals. The objective of this study was to determine the effects of silicon on uptake and toxicity of arsenic and copper in *L. minor*. Plants were grown in a greenhouse (25°C, 60% humidity, 12-h day, 500 μmol m⁻² s⁻¹) in modified Hoagland's solutions (1 L) amended with arsenic (either 0 or 1.5 mg L⁻¹) and/or copper (either 0.13 or 5 mg L⁻¹) and/or silicon (either 0 or 50 mg L⁻¹). After two weeks of growth, plant tissues were harvested, oven-dried (65°C; 72 h), and dry masses were recorded. Subsamples were collected from each treatment, prior to drying, for determination of total chlorophyll content. Dried plant tissues were acid-digested and silicon, arsenic, and copper contents were determined by inductively coupled plasma-optical emission spectrometry (ICP-OES). Tissue concentrations of silicon, arsenic, and copper increased with increasing treatment concentrations. The highest arsenic concentrations (387 mg As kg⁻¹) were in *L. minor* plants treated with arsenic and copper, regardless of silicon treatment. Silicon did, however, affect the biomass of *L. minor*; replicates treated with copper but without silicon had the lowest dry biomass (0.32 g) of all treatments, regardless of arsenic level. Similarly, plants treated with copper, without silicon had the lowest chlorophyll content (301 μg chl g⁻¹ fresh mass) of all treatments. Overall, silicon had little or no effect on arsenic uptake and toxicity, but did mitigate toxicity of copper in *L. minor*. There were significant interactions between silicon, arsenic, and copper which could affect the long-term uptake of those contaminants by *L. minor* in FWSWs.

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Modeling Arsenic Remediation in Wetlands

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Arsenic contamination of ground and drinking water is causing an endemic of disease across the world, and is listed as the number one contaminant of concern in the United States. Moreover, current methods of arsenic remediation are expensive, produce contaminant by-products, and are inaccessible to some regions. Although treatment wetlands provide a solution to treat arsenic-laden wastewater effectively, certain processes are in need of extensive research, including plant uptake, microbial transformations, and soil adsorption. In the effort to develop a model for field-scale systems, these processes are currently being researched at the University of Toledo by the use of a mesocosm experiment. Since these processes are functions of the system's hydrology, current experiments set to characterize the flow of water containing a conservative tracer through constructed wetland cells (6.1 m x 1.2 m x 1.5 m). Flow-data will be assessed for reproducibility by comparison of multiple cells and a computer model. A reproducibly successful outcome will be the first step in sizing and developing field-scale systems in collaboration with other researchers that are involved in the project.

Interannual variability of soil respiration in managed forests in Missouri

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Interannual soil respiration (R_S), soil temperature (T_S), and soil moisture (M_S) were measured to investigate the long term (5-year) variability of R_S and its controlling factors in forests subjected to different harvesting methods in 1996-1997. The three MOFEP treatments used in this study included: control no-harvest (NHM), even-aged clear-cut harvest (EAM), and uneven-aged single-tree harvest (UAM). Soil properties, including soil ammonium content, nitrate content, microbial biomass, total organic carbon and pH were also measured to assess the treatment effects. My results showed that, T_S was the best predictor of R_S daily and seasonally. R_S in all treatments increased from January to July and decreased afterwards, sharing a similar seasonal trend in T_S ; Interannually, total summer precipitation (PPT_S) was highly related to summer mean R_S in all the treatments. The interannual comparison demonstrated the trend that R_S in EAM and UAM were higher than that in NHM in wet years and lower in dry years, but the differences were only statistically significant in 2007 when the area suffered a severe summer drought. The less interannual R_S variability in NHM suggested that NHM are more resistant to disturbance than the harvested treatments. There existed thresholds in the relationship between T_S and R_S ($\sim 23^\circ\text{C}$) over the five years observation. R_S increased exponentially with T_S when T_S was lower than this threshold, but decreased together with M_S as T_S increased beyond this threshold. The T_S threshold changed monthly from May to August, with the lowest threshold in May ($\sim 19^\circ\text{C}$) and the highest in July ($\sim 26^\circ\text{C}$) with stable monthly M_S , suggesting that the monthly threshold is controlled by substrate supply from aboveground plant photosynthesis. Moreover, the threshold changes annually, with R_S in 2007 the lowest ($\sim 20^\circ\text{C}$) and 2008 the highest ($\sim 25^\circ\text{C}$). The low M_S and depleted substrate supply at high T_S is probably the reason for this T_S threshold. The annual Q_{10} values for each treatment showed that over the five years, NHM had the highest Q_{10} and UAM had the lowest.

Transportation and degradation of selected pharmaceuticals in soils applied with biosolids

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Biosolids are recognized as a major sink for pharmaceutical compounds introduced into the wastewater stream (1). As biosolids are rich in nutrients and organic matter, they are commonly used beneficially as a soil amendment to improve soil quality and ultimately increase plant yield (2). These compounds can potentially be transported into the environment following land application of biosolids. However, limited information is available with regards to their fate and transport once in soils. In this research, standard methodology was used to conduct laboratory column and degradation experiments. Both experimental setups simulated biosolids application on three soils with differing properties in order to study the transportation and dissipation of five pharmaceutical compounds frequently detected in biosolids (carbamazepine, diphenhydramine, clindamycin, fluoxetine, and diltiazem). The column leaching experiment showed poor mobility for all compounds in all three tested soils, likely due to their strong sorption characteristics. In the degradation experiment, no change was observed for carbamazepine, diphenhydramine and fluoxetine, while the amount of clindamycin and diltiazem decreased over time with varied dissipation rates in tested soils but no specific trend was observed. The results from this work suggest that these compounds commonly detected in biosolids are likely to be retained in applied surface soils and several can persist for extended amounts of time. This poses a potential environmental risk, although continued research is needed in this research area.

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An analytical model for predicting trajectories of droplets ejected by a centrifugal atomizer (fuel slinger)

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Since their development, gas turbines have seen many advances in the design, performance and extent of applications for commuting, military and space research purposes. One of these is the Small Gas Turbine. A Small Gas Turbine is a scaled-down version of the typical gas turbine, designed for lower cycle pressures and temperatures because of smaller blading and cooling limitations. Consequently, they are used for low-power applications (1). In conventional gas turbine engines, the fuel is atomized with the help of a high-pressure fuel pump. For compact applications, appropriately smaller pressure pumps cannot be used for small gas turbines. The replacement of typical fuel injection systems with the centrifugal atomizer design allows for high-speed operation, low-cost, reduced weight and simple design requirements for the purpose of fuel atomization. Due to rotary motion of the fuel slingers, the liquid is forced out of the radial channels by centrifugal forces in the form of cylindrical jets. These jets then disintegrate into droplets due to wave disturbances and physical forces. The trajectory of the jet and the droplets is observed to be curved due to rotation of the atomizers.

An analytical model which can predict spatially and temporally, the droplet trajectories of liquid jets atomized by centrifugal atomizers or rotary fuel slingers used in Small Gas Turbines has been developed. This model is aimed at establishing mathematical expressions for the governing parameters of the liquid jet flow outside the slinger, such as velocity and displacement, which may define the trajectory of the liquid jet outside the slinger (2). The relations for droplet trajectories are derived using the concept of equilibrium between the droplet's inertial force and the aerodynamic drag forces acting on a single drop during the course of the secondary breakup phase of atomization. The results of the model were compared with visual data acquired experimentally by Sescu et. al. (1) by plotting trajectories for droplets using data calculated from the mathematical relations and overlaying them on the actual trajectories at corresponding operating conditions. Sufficient close correspondence was observed with regards to parameters governing the spatial and temporal position of the drops and the data calculated from the model was used to further analyze the complex mechanism of drop disintegration with successful results.

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Finite Element Simulation of the Thermomechanical Behavior of Shape Memory Alloys

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Shape Memory Alloys (SMA), such as Nickel Titanium (or Nitinol), undergo a phase transformation in their crystalline structure when transformed from Austenite into Martensite. This inherent phase transformation is the basis for the unique properties of shape memory (SM) and superelasticity (SE) which obtained SMA widespread attention from various fields of engineering sciences. The SM is attributed to the recovery of large mechanically induced deformations upon raising the temperature up to a specific level (A_f). The SE is the ability of the material, at a temperature above Austenite start A_f , to recover mechanical deformations upon unloading. Thanks to superelasticity, shape memory effect, high damping capacity, corrosion resistance and biocompatibility, NiTi SMA alloys have been implemented in biomedical fields for the past 40 years (1). Namely, Nitinol is used in minimally invasive surgery, cardiovascular applications, and orthopedics. The Nitinol's shape memory effect, for instance, can be employed to activate medical devices in operation through body heat or external sources of heat. Such designs cannot be realized with conventional alloys.

In order to provide a framework for SMA simulation purposes in the field of biomechanics and orthopedics, the thermomechanical behavior of shape memory alloys was modeled through a representative beam structure in COMSOL Multiphysics Finite Element software (Figure 1). The functionality of different biomedical devices that utilize the SM and SE effects can be studied via this FEM model as a future work and the outcomes of the simulation can be compared with experimental tests on the prepared sample of the designed device.

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Saccharification of Ionic Liquid Pretreated Biomass with Commercial Enzyme Mixtures

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The high crystallinity of cellulose poses an impediment to hydrolysis enzymes for the cellulosic portion of biomass (1). The present work focuses on the evaluation of the performance of Spezyme CP, a commercial cellulase system, and Primafast Luna CL, a textile bio-finishing enzyme, on substrates following ionic liquid pretreatment. Ionic liquid pretreatment of lignocellulosic biomass produces amorphous or partially crystalline cellulose and enhances its saccharification (2). Target substrates for hydrolysis of glucan and xylan components include poplar, switchgrass and Avicel, a highly crystalline cellulose substrate. Spezyme was found to hydrolyze glucan and xylan components completely in 24 hours with modest enzyme loadings. Primafast was found to selectively hydrolyze glucan components of biomass.

Fabric biofinishing enzymes are often formulated to hydrolyze amorphous cellulose for fabric softening, to prevent fabric pilling and fibrillation, for surface fiber removal, and for preserving the strength of fabric. They are expected to have high endoglucanase activity (3, 4, 5). Both commercial enzyme mixtures were supplemented with β -glucosidase to limit end product inhibition. The present work focuses on the evaluation of the performance of these cellulase enzyme mixtures for hydrolysis of glucan and xylan components of pretreated poplar, switchgrass and Avicel, a highly crystalline cellulose substrate. This work provides further evidence that enzymatic hydrolysis cocktails can be specifically tailored to the lignocellulosic biomass feedstock.

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Surface Functionalization of Novel Polybenzimidazole Nanofiltration Membranes for forward osmosis

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Forward osmosis (FO) is an emerging membrane technology that, like reverse osmosis (RO), uses a semi-permeable membrane to separate water from dissolved solutes. The semi-permeable membrane acts as a barrier that allows water to pass through while blocking salts. Generally, any dense, non-porous, selectively permeable material can be used as a membrane for FO. Our collaborators at the National University of Singapore have developed a novel porous nanofiltration (NF) for FO. However, this NF membrane has low monovalent salt rejection efficiency along with low fouling control, which makes it inadequate for desalination applications. This requires the development/improvement of the materials used for the NF membrane. To address this, we have functionalized the surface of PBI based NF FO membranes in a way that targeted surface charge and hydrophilicity. The goal will be to identify surface functional groups that will enhance monovalent salt rejection and fouling resistance while maintaining inherent high water flux.

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International Planning Visit to the National University of Singapore – Development of Collaborations in Forward Osmosis Research (co-Pis: I. Escobar & M. Coleman)
- NUS: Material Engineering and Fabrication of High-Performance Nanofiltration-based FO Membranes for Water Reuses (PI: N. Chung, co-PIs: K. Wang, Q. Yang, J. Qin, I. Escobar, M. Coleman)

Evaluation of Lake Erie Algae as Bio-Fuel Feedstocks

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Currently, transportation fuels are produced from depleting fossil fuel sources. This calls for additional renewable sources that could be used for the production of high quality transportation fuel. Bio-diesel or bio-ethanol are such alternatives. Soybean, a food crop, has been used in the past as a source of lipids for the production of bio-diesel and corn grain has been used in the US for ethanol production. Algae are an alternative non-food source of lipids for bio-diesel and/or carbohydrates for bio-ethanol. We have surveyed algae and phytoplankton in the western Lake Erie basin in collaboration with Department of Environmental Sciences to identify the predominant algae species. The lipid, carbohydrate and the protein content of lake species were determined. Sampling at selected lake sites was performed in an attempt to correlate lake conditions (i.e. temperature, phosphorus and nitrogen) with the selection and composition of species. Based on the results of these analyses, native species were identified as candidates for bio-diesel or bio-ethanol production.

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Hydrophilic enhancement of UF membranes through green chemistry applications

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Over the past several decades we have clearly observed the repercussions of releasing toxins into the environment. Though initial focus of treating this problem concentrated on treatment of wastes before their release into environment, since 1990 authorities concentrated on the prevention of the formation of waste at the source leading to the advent of green chemistry (1). The emphasis of the green chemistry aims at elimination or at least minimization of waste generation in a chemical process through environmentally benign choices of solvents, non-toxic chemicals and renewable materials (2).

Commercially available water filtration membranes are usually modified by various techniques to impart the desired properties to the selective layer, thereby improving their filtration capabilities. Graft polymerization is one of those techniques widely used to attach Poly ethylene glycol (PEG) to the membrane surface. Grafting of PEG to membrane surface was proven to reduce the membrane fouling susceptibility (3). In this project an environmentally friendly approach will be used to perform PEG grafting by minimizing the waste production by using enzymatic condensation.

Porcine pancreatic crude type II lipase, a commercially available inexpensive enzyme will be used to catalyze the PEG graft polymerization on cellulose acetate ultrafiltration membranes. This process would be an environmentally benign modification that would result in a green product through the reduction of waste stream product as well as an ability to recycle solvents and the catalyst (4).

The graft polymerization reaction was performed under mild reaction conditions. A mixture containing preferred solvent, membrane samples, PEG monomer and PPL were reacted in a round bottom reaction flask containing a reflux condenser. Various solvents will be used to promote different reaction media. A solvent free condition was tested to see the influence of enzyme in bulk conditions. The proposed approximate solvent to monomer weight ratio is 5 and monomer to enzyme ratio is 2. Reaction was performed for 50 to 55 hrs at a temperature of 45⁰C. Influence of various parameters such as solvent to monomer ratio, monomer to enzyme ratio, reaction time and temperature were explored.

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Low-Biofouling Polypropylene Feed Spacers for Reverse Osmosis

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Biofouling is the accumulation of microorganisms onto the membrane surface and on the feed spacer. Research and development of biofouling prevention has commonly focused on the pretreatment of the feed water, the improvement of cleaning solutions and procedures, and modifications to the membranes themselves. This research focuses on developing low-biofouling polypropylene (PP) feed spacers. This is particularly significant because membrane replacement due to fouling is the single largest operating cost in water separation. PP was functionalized via the addition of a spacer arm with metal chelating ligands. These ligands were charged with copper ions to allow for slow release of ions into the feed water in the membrane systems. Copper ions have been previously used to disinfect water against microbial life. In this work, functionalization of PP was achieved using a spacer arm (glycidyl methacrylate (GMA)), which was polymerized to the PP using benzoyl peroxide as a radical initiator. Iminodiacetic acid (IDA) was then added to the end of the GMA spacer arm to allow for the chelation of the copper ions. This functionalization was chosen as the focus because these chelating ligands are quite stable and easily synthesized, operate over a diverse range of conditions, have easily controlled binding affinities, and are well suited for model studies. Characterization of the PP modification was performed using Fourier transform infrared spectroscopic (FTIR), scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The effects on the biological content of water in the presence of the modified spacer were tested using a synthetic water matrix of E.coli and LB broth. Both modified and unmodified spacers were contacted with the feed water for extended periods of time to allow for growth and then placed in stomacher bags where the biofilm was removed. The cells making up the biofilm were then enumerated to show the affect of the modifications, and it was determined that the modified PP displayed consistently one order of magnitude less microbial growth than the unmodified PP. The effectiveness of the modifications was assessed through crossflow filtration experiments. Both modified and unmodified feed spacers were used with identical membranes in a full recycle mode. The feed water was dechlorinated tap water that had been supplemented with sodium acetate. Flux was measured over different time intervals, after which, the membranes were removed so that the biofilm could be quantified. The membranes that used the modified PP displayed a higher flux during operation and, again, one order of magnitude lower microbial growth as compared to the membrane that used the unmodified PP. Possible leaching of the copper from the spacer during the filtration was monitored by testing permeate and retentate by using inductively coupled plasma (ICP) spectroscopy.

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Pyrolysis of Algae (*Lyngbya Wollei*)

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Lyngbya wollei is a freshwater cyanobacteria found in lakes, rivers and water supply reservoirs capable of producing neurotoxins and dermatotoxic alkaloids(2). The main motive is to convert *Lyngbya wollei* into useful products (bio-oil and syn-gas (CO+H₂)).

Experimental measurements of the liquid and gas products produced by pyrolysis of algae, *Lyngbya Wollei* are reported. The experiments were performed using a packed bed reactor at a temperature of 600° C. The biomass was heated at rate of 30° C s⁻¹ with a sweep gas (Helium) flow rate of 0.220 L min⁻¹. The *Lyngbya Wollie* (1) feedstock is found widely in Lake Erie. The experimental apparatus consists of two furnaces which are used to convert raw biomass into valuable products, mainly bio-oils and bio-gases (H₂, CO, CO₂, and CH₄). The pyrolysis reactor is a fixed bed stainless steel tube (25 mm OD, 20 mm ID, and 15 cm long) with biomass packed at the center of the tube. Quartz wool is used to support the biomass on either side. The biomass is heated by contacting with the hot inert helium sweep. The sweep is preheated to 800°C in the preheater furnace before being introduced into the pyrolysis furnace. The temperatures of the pre-heater and the pyrolysis furnace are controlled using K-type thermocouples. The line carrying the effluent streams from pyrolysis are insulated to avoid any condensation. The liquid bio-oils produced by pyrolysis are condensed in a glass condenser and analyzed using a gas chromatography-mass spectrometry (GC-MS, Agilent Technologies). The gaseous products are analyzed using an online gas chromatograph (GC, Shimadzu Corporation) using Helium as carrier. The GC is equipped with a pulsed discharge helium ionization detector (PDHID) and a flame photometric detector (FPD). A known volumetric flow of Argon was fed simultaneously to the reactor using a mass flow controller (Alicat Scientific) to enable quantitative analysis of the gaseous products. Molar fractions of H₂, Ar, CO, CO₂, CH₄ and other light hydrocarbons were analyzed using PDHID while FPD was used to analyze sulfur products.

Reference: 1 <http://www.westernlakeerie.org/Lyngbyawollei.html>

Removal of Acetic Acid from Hydrolysate using a Membrane Extractor/Reactor

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Production of bioethanol from lignocellulosic biomass requires pretreatment of the biomass to hydrolyze hemicellulose, separate lignin and reduce cellulose crystallinity. During the pretreatment by dilute acid hydrolysis, acetic acid is generated in concentrations of up to several grams per liter. Before the subsequent enzymatic hydrolysis, acetic acid needs to be removed from the hydrolysate since it can dramatically reduce the efficiency of fermentation by inhibiting enzyme activity (1). Currently, detoxification is done by lime treatment of the hydrolysate, but it consumes large quantities of calcium hydroxide and does also not produce any valuable products (2, 3).

Therefore, we propose to remove the acetic acid with an alternative process whereby acetic acid is extracted into 1-octanol in a membrane extractor and reacted with 1-octanol *in situ* on the membrane or in a separate reactor yielding 1-octyl acetate. Acetic acid concentration in hydrolysate will be reduced from 12.5g/L to < 1 g/L. The extracted acid will be esterified with 1-octanol and the ester will be removed periodically from the organic phase (4). Thus, the membrane extractor/reactor removes the acetic acid and produces a valuable by-product in an environmentally friendly process.

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Evaporative Separation of Ionic Liquid following Biomass Pretreatment for Ethanol Production: Generation of Required Thermodynamic Data

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Plant (lignocellulosic) biomass is an abundant, inexpensive and sustainable source of organic carbon, for the production of renewable fuels and chemicals. However, many technical and environmental challenges exist in developing commercially viable processes for producing sugars from biomass that serve as precursors for fuel and chemical production. Pretreatment and enzymatic hydrolysis are critical steps, and most of the current pretreatment methods do not effectively disrupt the biomass structure, especially the crystallinity of cellulose, which is a major barrier for efficient enzymatic hydrolysis. Ionic liquids (ILs) being non volatile, non-flammable, recyclable and designer friendly, are gaining wide recognition as green solvents, and their unique solvating properties make them ideal for pretreating lignocellulosic substrates. Rates of enzymatic hydrolysis for cellulose (avicel) pretreated by ILs were found to be two orders of magnitude higher than that for untreated cellulose [1]. Enhanced enzymatic hydrolysis yields of glucan to glucose and xylan to xylose are observed for IL pretreated lignocellulosic biomass like corn stover (softwood) and poplar (hardwood). In IL-pretreatment, the IL is displaced from the biomass by washing the pretreated biomass with an anti-solvent (water/ethanol). The IL preferentially dissolves in the anti-solvent and hence can be completely recovered. However, from an economic stand-point it is important that the IL is separated from the IL/water mixture. This is also desirable to avoid any ecological consequences associated with the presence of IL in wash streams and be able to reuse the process water. This work addresses: (a) the pretreatment of lignocellulosic biomass using suitable ionic liquids, resulting in enhanced enzymatic hydrolysis for subsequent bio-ethanol production, and (b) a facile thermo gravimetric method for efficiently generating the required thermodynamic (vapor liquid equilibrium) data needed for designing evaporative separation of IL from the anti solvent.

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Influence of membrane surface properties on the rate of bio-fouling of ultra-filtration membranes

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Recent studies have shown that membrane surface morphology and structure influence permeability, rejection, and fouling behavior of different types of filtration membranes. This investigation attempts to identify the most influential surface membrane properties governing fouling rate, with a particular focus on bio-fouling of ultra-filtration membranes. Two types of ultra-filtration membranes were used including an unmodified membrane (UM-UF) of cellulose acetate with a molecular cut-off weight of 20,000 Daltons and a modified membrane (HPC-UF) prepared by grafting the UM-UF with a thermally responsive film layer that can collapse and expand when the temperature is oscillated below and above its low critical solution temperature (LCST), respectively. The two different membranes were characterized for physical surface morphology and chemical heterogeneity using atomic force microscopy (AFM) and chemical force microscopy techniques (CFM), respectively. Membrane bio-fouling data obtained in a laboratory-scale cross-flow unit were correlated to the measured membrane surface properties. Results showed that bio-fouling of HPC-UF membranes, filtered at temperatures below LCST, are nearly correlated with the membrane surface roughness and surface charge. For the UM-UF and HPC-UF bio-fouled membranes, it is further demonstrated that AFM images and bio-film surface area coverage analysis yield valuable insights into the mechanisms governing bio-fouling. The non-uniformity of the polymer brushes on the HPC-UF membranes, especially at temperatures below LCST, may create areas of valleys and hills on the membrane surface. In these local areas, the shear forces applied on the formed bio-film during the cross flow filtration is decreased, thus varying the bio-film development rate per area (aggregation). Our data suggest that the bio-film particles are more likely to deposit on rough membrane regions rather than smooth regions. However, membrane surfaces are chemically heterogeneous impacting particle transport and attachment processes, and membrane surface character is a function of both surface morphology and surface chemistry.

Agent-based model for diffusion in water and porous media

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Understanding fate and transport of contaminant in groundwater and wetlands is crucial for remediation. Fate and transport of contaminants has often been modeled in the past using various equation based methods (EBM) such as ordinary differential equations (ODE) and partial differential equations (PDE), which encompass rigorous mathematics and assume homogeneity over time, space, and among individuals. But individuals in real world are heterogeneous, and the equations used to describe the relation among parameters of interest are non-linear. ABM has proved to be effective in modeling such scenarios. An Agent-Based Model (ABM) for the transport of contaminant (2,4,6-trichlorophenol) in water and soil has been modeled. Among many ABM platforms, NetLogo was found to be the suitable platform for the current study. First, the diffusion of contaminant from contaminated water into the overlying uncontaminated water was modeled and second, the diffusion of contaminant from contaminated soil to the overlying uncontaminated water was modeled. The results obtained from both the models were compared with Hydrus 1-D for verification. The results obtained from ABM and Hydrus-1D for diffusion in water showed good agreement with each other. However, the results obtained for diffusion in soil using ABM and Hydrus 1-D were not in complete agreement with each other. The difference in the result obtained is due to the relation on which each model focuses upon. For example, Hydrus results were obtained by assigning diffusivity coefficient value and monitoring variability over time by using partial differential equations. However, NetLogo results were obtained by allowing each individual contaminant to move freely in the porous soil, which produce the given output. Another reason for the difference is due to tortuosity. In Hydrus, tortuosity depends on porosity (i. e. $\tau = \varepsilon^{-1/3}$), but NetLogo model does not have a specific relation between them, therefore, the results obtained differ.

Keywords: ABM; EBM; NetLogo; HYDRUS; Diffusion; Tortuosity; Contaminant; Water; Soil

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Modeling Conservative Solute Transport Through Wetland Microcosms Using HYDRUS

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Interest in constructed treatment wetlands is increasing as low-cost and low-energy alternatives to traditional methods are being sought for the sustainable treatment of both municipal and industrial wastewater. Constructed treatment wetlands are man-made systems that mimic the biogeochemical and hydraulic conditions present in natural wetlands and encourage the development of specific processes that can successfully treat a particular waste stream. In this laboratory and modeling study, several small-scale wetland microcosms were evaluated to determine their utility for further greenhouse studies and to aid in the design of larger treatment wetlands for the purpose of treating arsenic-laden wastewater.

The wetland microcosms were uniformly packed with a sandy loam soil. Inlet and outlet ports were placed at opposite ends of the cells. Flow through the cells was achieved by maintaining a constant head difference between the inlet and outlet ends. Gravel was placed at the inlet and outlet ends for a more uniform flow through the soil and to prevent short-circuiting. The cells were thus configured to mimic the hydraulic conditions present in horizontal subsurface flow wetlands. The microcosms received a constant pulse of a conservative tracer (NaBr, sodium bromide) at the inlet port in order to determine the flow pattern within the cells. Six pore water samplers were placed in each mesocosm and sampled at regular time intervals. The concentration of Br was determined as a function of time for each pore water sampler.

The flow pattern in the cells was modeled using HYDRUS, a software package that simulates water and solute transport in one- two- or three-dimensional variably saturated media. Several different simulations were performed to determine the expected flow pattern in the microcosm cells, the effects of the gravel placed at the inlet and outlet, and the effects of pore water sampling on the flow regime. The HYDRUS model output was then compared with the actual breakthrough curves for the sodium bromide tracer to elucidate any differences in flow patterns between the cells, to prepare for future arsenic treatment studies with the microcosms and to determine the best design parameters for larger-scale arsenic treatment wetlands.

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New Investigations into the Morphology of the particulate matter inside urban public transit bus in Toledo, Ohio

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This study compares the physical characteristics of fine particulates collected inside urban-public transit buses in Toledo, Ohio that run on ultra-low sulfur diesel (ULSD) and 20 percent biodiesel blend with ULSD (B20). The number size distribution, microstructure, and aspect ratio of fine PM filter samples collected in the urban-public transit buses are measured using an Scanning Electron Microscope (ESEM) coupled with energy dispersive X-ray spectrometry (EDX) for three years (2007, 2008 and 2009). The size distribution was generally multi-modal for the ULSD but uni-modal for the B20-fueled bus. The multimodality may owe to the agglomeration and/or presence of other sources.. The aspect ratio found for different filters collected inside the bus fueled by both the B20 blend and ULSD ranged 2.4-3.6 and 2.3-2.9 in average value with standard deviation range 0.9-7.4 and 1-7.3 respectively. The particle morphology was characterized by the 12 different shape clusters: square, pentagon, hexagon, heptagon, octagon, nonagon, decagon, agglomerate, sphere, triangle, oblong, strip, line or stick, and unknown, by quantitative order. The square and oblong-shaped particles represented the single inhalable particle's morphology characteristics in the air of a Toledo transit bus. The surface of most particles was coarse with a fractal edge that can provide a suitable chemical reaction bed in the polluted atmospheric environment. The three sorts of surface patterns of squares were smooth, semi-smooth, and coarse. The three sorts of square surface patterns represented the single inhalable particle's morphology characteristics in the air inside the bus in the Toledo, Ohio.

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Polyphenols as Antimicrobial and Antibiofouling agents against *Streptococcus mutans*

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Phenolic compounds found in many plants, fruits, and vegetables often have considerable antioxidant and antimicrobial effects. These natural polyphenols have demonstrated advantages in aiding benefits for human health by scavenging free radicals and microorganisms within the human body. The antimicrobial effects of polyphenols span from medical use to cosmetics and food preservatives. One of many benefits of using polyphenols in these applications is preservation and protection against microbial contamination, while simultaneously protecting the human body from carcinogenic free radicals.

The antimicrobial activity of the polyphenols has been investigated for protecting solid surfaces from microbial colonization. In this study, polyphenols were applied to solid surfaces to form a coating and tested for antifouling effect. Antimicrobial activities of the polyphenols were measured using *Streptococcus mutans*, a Gram-positive bacterium. The antimicrobial activities of polyphenols were assessed against *Streptococcus mutans* using minimum inhibitory concentration assay with the plate dilution technique. (1)

S. mutans is well known for causing dental caries. Dental caries are initiated by the potent, cariogenic *S. mutans* that forms plaque on teeth. Polyphenolic extracts have been observed to prevent dental plaque by inhibiting the activity of glucosyltransferase enzyme produced by *S. mutans* in vitro. Antibiofouling activities of polyphenols were measured using a modified microtiter plate assay. (2-4) We were interested in the effect of the molecular structures of the polyphenols on the antimicrobial and the antibiofouling activities. Natural phenols with distinct structure differences: numbers of phenol rings, OH groups, and carboxyl groups were strategically selected. Polyphenols examined in this study include: ascorbic acid, gallic acid, quercetin, tannic acid, and salicylic acid

The contents of this paper include the tests of sucrosyl transferase enzyme activity in the presence of polyphenols, antimicrobial and antibiofouling activities of polyphenols against *Streptococcus mutans*.

Keywords: Polyphenols, Antimicrobial activity, Minimum Inhibitory Concentration, Antibiofouling activity

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SH2B1 β is a Novel Actin Cross-linker

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The widely-expressed SH2 domain-containing adapter protein SH2B1 β was initially identified as a binding partner and substrate of JAK2 tyrosine kinase. SH2B1 β is a member of the SH2B family (SH2B (SH2B1), APS (SH2B2), and Lnk (SH2B3)), which contains a conserved N-terminal dimerization, central pleckstrin homology, and C-terminal SH2 domains. Deletion of the SH2B1 gene results in severe obesity and both leptin and insulin resistance, as well as infertility, suggesting that SH2B1 β may play a fundamental role in cell functions. SH2B1 β has also been previously implicated in the regulation of the actin cytoskeleton by growth hormone and PDGF and cell motility. SH2B1 β is also required for maximal actin-based motility of *Listeria monocytogenes*.

SH2B1 β increases the rate of bacteria propulsion in infected cells and in cell extracts in a VASP-dependent fashion. However, the mechanisms by which the effects of SH2B1 β on the actin cytoskeleton are mediated remain unknown. Here we report that SH2B1 β has two actin-binding sites. The first site contains amino acids 150-200 and binds F-actin with high affinity while the second site (amino acids 615-670) binds F-actin less strongly as assessed by high speed cosedimentation assay. Using a low speed pelleting assay and electron microscopy, we showed that SH2B1 β cross-links actin filaments *in vitro*. In cells, SH2B1 β localizes not only to cell ruffles as previously shown but also along the filopodia. Deletion of amino acids 150-200 leads to mislocalization of the mutant protein to the filopodia "tip complexes" where the mutant co-localizes with VASP. Using VASP-deficient MVD7^{-/-} cells and the same cells stably re-expressing GFP-VASP, we showed that proper intracellular localization of SH2B1 β depends on the presence of the first actin-binding site and the presence of VASP. Finally, we demonstrate that both actin-binding domains of SH2B1 β are required for maximal growth hormone-induced cell ruffling and for cell motility as assessed by phagokinetic assay. We hypothesize that SH2B1 β functions as an adapter protein that in response to JAK2 activation, cross-links actin filaments leading to modulation of cellular responses.

Antimicrobial Titania Nanofibers and Films for Wound Healing

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Infection of battlefield-acquired wounds and segmental bone/ tissue loss among military personnel in Iraq and Afghanistan are two common conditions which can have devastating consequences, both clinically and economically. Depending upon the circumstances, the wounds and fractures could be minor or debilitatingly severe. Even in the case of minor wounds and fractures, mitigation of infection is of prime importance and must be attended to at all times – right from the battle site where they were first inflicted, all the way to the facility where full-fledged medical attention is available to the injured service men and women.

Frequent association of combat-related wounds with significant bone loss is another challenging condition. Presently available bone grafting materials has limited success particularly in the presence of infection. By interposing an effective procedure based on nanotechnology, the bone healing can be made safer and take place at an accelerated pace, eliminating or mitigating the probability of wound infection.

In order to achieve this, we have taken a two-pronged approach: (i) the development of non-woven nanofibers of titanium dioxide (TiO_2) - possessing known photoactive antimicrobial attributes - either in pristine form or after impregnation with antibacterial agents, that can be used as disinfectant gauze for wound healing upon brief activation by a pocket UV/IR flashlight, and, (ii) the development of a procedure for treating the surface of the external fixator pins, bone replacement materials and implants (made of Ti or Ti-Al-V alloy, used for bone fractures healing) with nanoscale photoactive disinfectant in the form of a thin film or fibrillar structure. In the first case, technique of electrospinning has been used for fabricating non-woven TiO_2 mesh. Uniform coating of nanoscale TiO_2 on external fixator pins or implants has been achieved via hydrothermal processing under very mild and benign experimental conditions in the second case.

Enzyme systems for optimization of ionic-liquid pretreated biomass saccharification

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Biomass, which consists of cellulose, hemicellulose, and lignin, is being developed as a renewable carbon source for fuel and chemical production. The use of biomass as a renewable carbon source requires that it be hydrolyzed to monomeric sugars through efficient processes. The process which shows the most promise for the deconstruction of biomass is pretreatment via chemical processes followed by enzymatic hydrolysis. Enzymatic hydrolysis is preferred over mineral acid catalyzed hydrolysis because no sugar breakdown products, which often times act as inhibitors in downstream processes, are produced.

The continued optimization of the biofuel production from terrestrial biomass includes development of processes that takes advantage of fundamental understanding of the complex interplay between lignocellulose components. Ionic liquid (IL) pretreated biomass provides an opportunity to improve hydrolysis processes through increased understanding of the interactions between lignocellulosic components since it is a unique feedstock in that it provides amorphous cellulose while retaining the hemicellulose and lignin components. In addition, enzyme groups (cellulases and hemicellulases) which are critical for saccharification of this substrate are indentified. Some of these enzyme groups are endoglucanases, cellobiohydrolases, β -glucosidases, xylanases, and xylosidases. Selected cellulases and hemicellulases are expressed, isolated, purified and characterized for activity and substrate specificity. The identified enzyme systems are also examined for their synergistic effects on the hydrolysis of ionic liquid pretreated biomass.

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Determination of ethanol in ionic liquids using headspace solid phase microextraction-gas chromatography [1]

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Ionic liquids (ILs) being non volatile, non-flammable, recyclable and designer friendly, are gaining wide recognition as green solvents and efficient reaction media in process industries as potential replacements for volatile organic solvents. The application of ionic liquids as non-derivitizing solvents for the pretreatment and regeneration of cellulosic and hemicellulosic biomass for the production of biofuels is a growing area of research. Commercial viability materializes when the reaction media / green solvent is completely recovered and recycled in any processing stream. Anti-solvents such as water or ethanol are employed in the recovery process and it is of interest to quantify volatile components such as ethanol in the IL-water mix. This study reports the development of a rapid and simple method for the determination of residual ethanol content in ionic liquids. The method utilizes headspace solid phase microextraction (SPME) coupled to gas chromatography using elevated extraction temperatures resulting in rapid equilibration times. The effect of IL water content on the ethanol extraction efficiency is presented. Recovery experiments carried out in real samples gave recoveries ranging from 96.8 to 98.2%.

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Enantioselective Alcohol Oxidation with Binaphthyl-based Aminoxyl Radical

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The importance of enantioselective reaction in organic synthesis is hardly overstated. In fact, the number of chiral substrates in pharmaceutical, agrochemical, and material science has been growing rapidly in recent years. Coupled with the current interest in environmental issues, we became interested in developing a new enantioselective oxidation reaction, which is one of the most problematic transformations from a green chemistry standpoint.

We see aminoxyl radical catalyzed oxidations of alcohols as a developmental lead with great potential for our purpose. Aminoxyl radicals are small molecular catalysts that have recently demonstrated the ability to mediate a wide range of oxidative reactions. In particular, oxidation of alcohols with this catalyst is one of the most atom-efficient and scalable reactions with minimal use of toxic reagents. More importantly, mechanistic hypotheses of the known aminoxyl-radical catalysts suggested that chirality transfer from the catalyst to products should occur. In addition, it was suggested that the use of the same catalyst for other enantioselective process that involve electron transfer may also be possible.

We have designed several chiral aminoxyl radicals that are expected to retain their catalytic activity. Binaphthyl-based compounds, being axially chiral through space, are recognized as one of the privileged ligands for stereoselective reactions. Our catalyst design principles will be discussed and the progress in synthesis of the catalyst will be presented.

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Carbon, Water and Energy Implications of Rainwater Harvesting in Educational Buildings

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Rainwater harvesting to supply non-potable water demands has become a viable option to eliminate water shortages in the future and reduce the burden on municipal water treatment facilities, but what if a large amount of additional materials that emit an excessive amount of CO₂ during their manufacturing are needed to implement the system? It is possible that one's efforts to improve the environment could actually harm it greater than if no sustainability effort was implemented. The goal of this study was to address these questions. A life cycle assessment approach was used to estimate the CO₂ emissions and energy consumption associated with different rainwater management scenarios for the North Engineering building at the University of Toledo. The scenarios vary with respect to end use of the rainwater. The four scenarios are as follows:

1. Potable water used for irrigation and flushing toilets (no rainwater harvesting system).
2. Rainwater used for irrigation, potable water used for flushing toilets.
3. Potable water used for irrigation, rainwater used for flushing toilets.
4. Rainwater used for irrigation and flushing toilets.

The four scenarios were compared by calculating the amount of water sent to storm sewer, potable water required, energy usage, CO₂ equivalence and cost. The optimum scenario to be implemented for the North Engineering building will be discussed in detail during the conference.

This work was supported in part by a grant through the UT Office of Undergraduate Research and the Lake Erie Protection Fund (LEPF).

Random Subsample Ensemble: Classification in High-Dimensional Feature Spaces

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Classification as in machine learning is a procedure in which individual data points are placed into classes (groups) based on the quantitative information on the characteristics inherent in the data points (referred to as features, attributes, variables, etc). Inventions and advancement in technology and science have resulted in the collection of data sets with high dimensional feature spaces in fields like biomedical, finance, satellite imagery, customer relationship management, network intrusion detection etc. (1-4). High dimensional feature spaces cause scalability problems for machine learning algorithms because the complexity of a high dimensional space increases exponentially with the number of features. This effect is called as the curse of dimensionality (1, 5).

Although it is not possible to eliminate the adverse effects of the curse of dimensionality completely, we propose that the divide-and-conquer methodology can be used to manage its onset. Within the machine learning context, the divide-and-conquer methodology is best modeled by the ensemble learner. Ensemble learning is a form of machine learning which works with the aggregation of predictions of multiple classifiers with the goal of improving accuracy and other figures of performance. We present the application of machine learning ensembles to classification problems of algorithm scalability, data sparsity and information loss with high dimensional feature spaces. The original high dimensional feature space is randomly projected onto a number of lower-dimensional feature subspaces. Each of these subspaces constitutes the domain of a classification subtask, and is associated with a single learning algorithm within an ensemble machine-learner context. Such an ensemble conceptualization is called as random subsample ensemble. Simulation results performed on data sets with up to 20,000 features indicate that the random subsample ensemble classifier performs comparably to other benchmark machine learners based on performance measures of prediction accuracy and cpu time.

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Colonization of rotting wood by ground-foraging ants in coffee agroecosystems: Does diversity and coffee management matter?

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Introduction. The coffee shade canopy is important for preserving the biodiversity and ecological interactions within coffee agroecosystems. However, management intensification of this agroforest has showed decline in species richness of several taxa that utilize resources related to the shade trees (1). For example, shade tree pruning, resulting in increases in rotten logs on the ground, could have important impacts on organisms that use rotten logs as nest sites including arthropods such as beetles, ants, and spiders (2). Furthermore, pruning could affect habitat quality with drastic management changes such as changing the density or diversity of shade trees (3). Ants are useful insects for studying the effects of coffee management, and further, ants occupy many different ecological niches. We worked in a series of coffee farms and a forest with different management and availability of rotten logs to examine how adding artificial nesting resources would impact ant richness and composition. Specifically, we measured whether: 1) Habitat differences influence biodiversity of the colonizing log-nesting ants; and 2) if composition of log-nesting ants differs in different habitats or log species.

Methodology. Our study was carried out in two coffee farms in Chiapas, Mexico. Finca Irlanda is a large farm with two management types: 1) organic traditional polyculture (TP) and 2) commercial polyculture (CP). Finca Hamburgo is a conventional monoculture shade farm (SM). Both farms are connected by a patch of forest (F). We choose the six most common species of canopy trees in those farms and forest: *Albizia* sp. *Alcornea latifolia*, *Cecropia obtusifolia*, *Inga micheliana*, *Schizolobium* sp., and *Trema micrantha*. On February 2008, we cut logs to a standard size (50 cm diameter x 50 cm length) and put the six logs, one of each species (conforming an experimental group) in plots in the different sites. We placed 9 groups in each site (SM, CP, TP and F). Every six months (July 08, February 09 and June 09) we harvested three of groups of logs from each habitat type. We then cut open logs with axes collecting all the ants seen inhabiting logs.

Results and conclusions. We collected 139 ant individuals distributed in 7 subfamilies, 28 genera and 47 species. Ant species richness was higher in CP (29), second TP (24), followed by SM (17). Surprisingly, the forest logs had the lowest ant richness (8). The species found in all sites included: *Brachymyrmex* sp. 1, *Pachycondyla stigma*, *Pheidole* sp. 1 and *Solenopsis* cf *globularia*. Some species, *Taturdris* sp. 1 and *Probolomyrmex*, were only found in CP, and *Apterostigma* sp. 1 was only found in TP. These results show that ant species differed among habitats differing in management. The effect of the intensification is a negative factor for the biodiversity and some coffee agroecosystems are important areas for preserving biodiversity.

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Analysis of natural and synthetic hormones in surface water by solid-phase extraction and liquid chromatography-tandem mass spectrometry

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Natural and synthetic steroidal hormones are reported as the most potent endocrine disruptors for many biological species at nanogram per liter levels (1,2,3). A method for the analysis of 4 natural steroidal hormones, estrone (E1), 17- α -estradiol (17 α), 17- β -estradiol (E2), and estriol (E3), and 3 synthetic steroidal hormones, progesterone, melengestrol-acetate, and 17- α -ethinylestradiol, in surface water by solid-phase extraction followed by liquid chromatography-electrospray injection tandem mass spectrometry was developed. Post extraction derivatization with dansyl chloride was necessary and was optimized for analytical rigor. Using hormone spiked samples ENVI-18, tandem ENVI-18 and Florisil, LC-18 and Evolute reverse phase solid-phase extraction cartridges were compared for extraction from waters with differing matrices. The ENVI-18 was chosen based on overall analyte recovery (>77% for all), performance, and cost. Sample pH, cartridge conditioning, wash and elution steps were further optimized to increase recovery. The composition of the wash step was an important factor in reducing matrix effects without reducing the recovery, and 20% acetone in water was chosen in the final method. The developed method was validated using surface water samples from several streams in Northwest Ohio impacted by both agricultural and urban runoff, with many of the targeted hormones present. This method will be used in the future to determine hormone fate and transport in wetland systems.

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Entomophages associated with inflorescences of mango Ataulfo in the Soconusco region, Chiapas, Mexico

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Introduction. The mango Ataulfo is the most important crops in the Soconusco region, Chiapas with a planted area of about 18,334 hectares (4) that generate economic income of 4 billion pesos annually (2). Although this variety is originally from Chiapas, producers of the eight states that exist in Mexico, Chiapas ranks last in productivity to 9.4 tons per hectare (3). One of the reasons that have been mentioned to explain the low yields is the presence of the genus *Frankliniella* thrips and other pests (1). The lack of basic studies on these insects in the region aggravated the problem, because there are no known natural enemies or the intensity with which they are acting. Synthetic insecticides are the main measure of combat that carried them out without following economic criteria and / or organic. In this context, the objective of this study was to determine the presence of natural enemies (parasitoids and predators) in the inflorescences of mango orchards Ataulfo in two different agricultural management.

Methodology. Fieldwork was conducted in two orchards of mango Ataulfo located on the Coastal Plain of Chiapas: Huerto "Tres-A", characterized by having intensive management of agrochemicals and "Rancho La Escondida", featuring only an agroecological management. The samples were randomly every 5 days between 08:00 and 10:00, since the beginning of flowering (25/11/08) even when presented the latest (19/02/09), (18 samples / site). Each sampling consisted of collecting 5 inflorescences (one from each tree) located at a height not exceeding 2.5 m, same that were placed individually in plastic bags. The identification of the specimens was conducted in the laboratory of Ecoetología de Artrópodos of ECOSUR.

Results and conclusions. We identified a total of 38 families of natural enemies: 25 predators and 13 parasitoids. These families belong to six orders of Insecta and one of Arachnida. The most diverse order in terms of number of families entomophagous referred was Hymenoptera-parasitic with 33% and followed by Araneae to 28%. It is noteworthy to mention that of all families of natural enemies recorded, 7 is not present at the orchard that used insecticides: Histeridae, Lampyridae, Lycidae, Vespidae, Chalcididae, Eupelmidae and Figitidae, while in the orchard was not sprayed, only 2 families were not represented: Carabidae and Nabidae. Similarly, of the 88 morphospecies of natural enemies recorded, 39 were absent in the orchard that used insecticides, while in the agro-ecological management, only 11 were not represented. This could be evidence of the harmful effect of insecticides. This is the first work focused on the search for natural enemies on orchards in mango Ataulfo in the Soconusco, Chiapas, which could be relevant at the Biological Control.

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Adsorption/Desorption of Carbamazepine to Biosolids Amended Agricultural Soil

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Sewage sludge, a byproduct of the wastewater treatment process (WWTP), conforming to certain restrictions (biosolids) can be applied to agricultural fields as a beneficial soil amendment. Contaminants that are not removed during the treatment process can also be applied in tandem. Little is known about the fate and transport of many emerging contaminants such as pharmaceutical and personal care products (PPCPs) often detected in biosolids. One emerging contaminant surviving the WWTP, detected in environmental waters, and biosolids amendments is Carbamazepine (CBZ), a widely used anticonvulsant, mood stabilizing medication. Although sorption of CBZ onto sediment surfaces has been investigated, the persistence of the compound necessitates investigation regarding its mobility through the soil column when biosolids are applied. An agricultural soil, a silty clay with a pH of 4.4, was amended with two class B biosolids. The biosolids differed in pH, treatment processes and percentage solids and organic matter. Samples were prepared in triplicate using OECD batch equilibrium sorption guidelines and CBZ was analyzed using liquid chromatography tandem mass spectrometry. Results indicate that adsorption of CBZ on the unamended soil was strong, with a distribution coefficient (K_d) of 18.0 L kg⁻¹. The desorption distribution coefficient of 33.7 L kg⁻¹ indicated a low leaching potential for CBZ, predicting poor mobility through the soil column. The K_d increased with biosolids amendment as a result of increased organic matter content. pH increase due to amendment was the dominant influence over sorption.

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Physiochemical Study of Eutectic Mixture of Tolbutamide and Nicotinamide Using Physical Mixture Method

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Both low solubility and bioavailability of drugs are the primary challenges of product development in the Pharmaceutical industries worldwide. Improvement of the solubility of drugs may be achieved by using a suitable excipient, and reducing particle size. The main objective of this study is to enhance the dissolution rate of Tolbutamide using a hydrophilic excipient. Eutectic mixtures of the sulfonylurea oral hypoglycemic drug Tolbutamide and the excipient Nicotinamide were prepared by the physical mixture method in order to enhance the solubility of this poorly water soluble drug. X-ray powder diffraction (XRPD) was used to analyze the drug alone and its eutectic mixture. The X-ray result of eutectic mixture confirmed that the drug alone and its eutectic mixture are found predominantly in crystalline form. Differential Scanning Calorimetry (DSC) was used to characterize the composition phase diagram of the constituents at different ratios. The Fourier Transform infrared spectroscopy (FT-IR) studies of Tolbutamide and its eutectic mixture indicated that no interaction occurred with physical mixing of the components. In vitro dissolution studies of the drug and its eutectic mixture were carried out in a pH 7.4 phosphate buffer. The eutectic mixture showed considerable increase in dissolution rate when compared to the drug alone.

Independent Generation of DNA Radicals Resulting From Low-Energy Electrons

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Radiotherapy uses ionizing radiation to target deoxyribonucleic acids (DNA) among other biological molecules for cancer treatment. As a result genotoxic, mutagenic and recombinogenic lesions can be formed. It has been established that when ionizing radiation deposits its energy in a cell one of the results is the formation of secondary low energy electrons (LEE, 0–20 eV). LEE can be added to all components of DNA leading to the formation of a transient anion species in which an extra electron localizes in the unfilled P=O π^* orbital on the phosphodiester bond in the DNA. This transient anion can undergo dissociation by a process called dissociative electron attachment (DEA) initiating single and double strand breaks in the DNA. The postulated mechanism under investigation that could explain this cleavage includes two pathways; one pathway involving scission of the C-O bond giving carbon-centered radicals (C3' or C5' radicals) with phosphate anions as the opposing termini, whereas the other pathway is the scission of the P-O bond resulting in the formation of alkoxyl anions and phosphoryl radicals as the associated termini. It is believed that the process primarily occurs via C-O bond cleavage. To elucidate this mechanism our laboratory is investigating one of the proposed intermediates the 3'-deoxy-C3'- thymidinyl radical. The synthesis of 3'-deoxy-3'-(phenylseleno) thymidine as a precursor of the 3'-deoxy-C3'- thymidinyl radical has been completed. Kinetic studies regarding the estimation of the rate constant for trapping of the C3'-radical are currently in progress. Reversed DNA will be used to incorporate the radical precursor into oligonucleotides. The radical of interest will be generated photolytically using ultraviolet light ≥ 320 nm and the products formed will be characterized using high performance liquid chromatography (HPLC) and mass spectrometry (MS). Through these efforts a link will be established between the products of LEE and the deleterious effects of radiation in cancer chemotherapy.

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**Expression, Purification, and Biochemical Analysis of the Circadian CLOCK
Acetyltransferase Protein**

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Circadian control of behavioral and physiological processes other than sleep cycles is only beginning to be understood. Although much research has been done in the past several years regarding this curious involvement, we are still mostly in the dark as to how circadian rhythms actually function at a biochemical level. To help shed light on circadian function mysteries, the goal of this project is to clone, overexpress, and analyze the acetyltransferase domain of the CLOCK protein, an important component of the circadian oscillator in mammals, which is vital for maintaining the twenty-four hour circadian rhythm. By analyzing and understanding this function, novel drug therapies for circadian disorders can potentially be developed.

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Thermoelectric Property of CdS Thin Film*

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Cadmium sulfide has the optical band gap of 2.42 eV or 514.5 nm (in wavelength units), which is sensitive to visible light. Thin films of CdS have found applications as detectors of light and window materials for solar cells. There is little work on the thermoelectricity of CdS. Recently, we have demonstrated that CdS thin films are very sensitive to heat. The change of surface temperature of this material results in significant increase in electrical conductivity. In this study, we focus on the heat sensitivity of CdS thin films. CdS thin film in the thickness of about 5~10 nm was prepared by thermal evaporation at 300⁰C. A three-electrode system was used for linear sweep voltammetry measurement. The three electrodes are connected with a CHI 400A electrochemical quartz microbalance to conduct data acquisition. The three electrodes are the reference electrode, the work electrode (cathode), and the counter electrode (anode). The width of the specimens is 25 mm, and the distance between the counter electrode and the work electrode is also 25 mm. The potentials were changed in a triangle waveform. It was found that at room temperature of 20⁰C, the measured electric resistance is about $2.5 \times 10^9 \Omega$ as can be calculated from the results shown in Figure 1 (the blue data line). When a temperature field was applied, and the specimens were heated up to 24⁰C, the electrical conductivity of the material increased by 2 times as can be calculated from the results shown in Figure 1 (the red data line). Such a heat sensitive behavior reveals the thermoelectricity within the CdS thin film. More details in the relationship of temperature and resistance will be presented based on our on-going studies. Fundamental studies on how the temperature field causes the electron ejection are under the way.

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**The Effects of Ellagic Acid on Developmental Toxicity in Ethylmercury-exposed Zebrafish
(*Danio rerio*)**

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Ethylmercury, a preservative added to childhood vaccines during the 1990s, has been implicated as an environmental insult leading to neurodegenerative disorders such as autism. ⁽¹⁾ Ethylmercury is believed to cause neurodegenerative disorders because it causes oxidative stress during pivotal times in development. Ellagic acid is a strong antioxidant, meaning that it protects organisms from oxidative stress. These experiments will determine the effect of ellagic acid, an antioxidant found in some berries, on the development and behavior of zebrafish exposed to ethylmercury. This will be studied by exposing groups of zebrafish to concomitantly to ethylmercury and ellagic acid, then assessing the behavioral and developmental effects through testing and comparison with a control group exposed only to ethylmercury. Ergo, we expect that the concomitant administration of ellagic acid will reduce the oxidative stress experienced by the organism and therefore reduce the developmental and behavioral effects.

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Preparation and Characterization of Eudragit RL 100 Nanosuspensions for the Ocular Delivery of Sulfacetamide

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Sulfacetamide loaded polymeric nanosuspension (nanoparticle suspension) was prepared from inert polymer resins (Eudragit RL 100) with the aim of improving the availability of sulfacetamide at intraocular level and thereby reducing the frequency of dosing. Nanosuspensions were prepared by nanoprecipitation method using acetone and 1 % W/V pluronic F 108 solution. Characterization of NPs was performed by measuring particle size, zeta potential, Fourier Transform infrared spectra (FTIR), Differential Scanning Calorimetry (DSC), Powder X-Ray Diffraction (PXRD), drug entrapment efficiency, in vitro release. Spherical, uniform particles (size range between 112.4 nm to 398.1 nm) with polydispersity index (0.414 to 0.67) and positive zeta potential (range + 9.16 mV to + 24.1mV) were obtained. Positive surface charge can allow a longer residence time of nanoparticles on the cornea surface, with a consequence slower drug release and higher drug concentrations in the aqueous humor, compared to classical eye drop. In order to increase drug entrapment efficiency, selected batch was chosen to study the effect of changing polymer content, pH of external media and incorporation of polymethyl methacrylate (PMMA) on drug entrapment efficiency. Changing the external phase pH significantly increased entrapment efficiency. The results indicate that entrapment of Sulfacetamide in Eudragit RL 100 nanoparticles could be utilized as potential delivery system for treating ocular inflammation.

Preparation and characterization of microemulsions using pharmaceutically relevant components

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This study was designed to develop microemulsions using pharmaceutically relevant components and evaluate their antimicrobial effects. Microemulsions were prepared using a mixture of non-ionic surfactants such as Tween 40 and Span 80, isopropyl myristate, and deionized water. All formulations were prepared by the titration method and inspected for visual clarity. Compositions that formed an optically clear formulation were plotted in a pseudo-ternary phase diagram. Subsequently, several formulations were evaluated for optical birefringence, electrical conductivity, and rheological properties. Compositions that formed microemulsions did not exhibit optical birefringence when observed under polarized light. The electrical conductivity of formulations demonstrated composition dependent variations. Up to 5 % w/w water containing microemulsions possessed very low conductivity ($< 0.01 \mu\text{S}/\text{cm}$) indicating the formation a water-in-oil type system. The rheological properties were evaluated in a controlled stress/strain rheometer and formulations exhibited composition dependent changes in viscosity. All microemulsion samples showed Newtonian flow properties. Stable microemulsions were prepared using pharmaceutically relevant components. We are exploring potential applications for the developed formulations. An ongoing research in this regard involves characterization of antimicrobial properties of select preparations.

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Formulation and Characterization of Microemulsions Containing Diocetyl Sodium Sulfosuccinate and Ethyl Oleate

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Microemulsions are clear, thermodynamically stable solutions that contain at minimum water, oil and surfactant. They form almost spontaneously and exhibit Newtonian flow properties and low viscosity (1). Microemulsion droplet size is extremely small (10-100nm). Surfactants decrease the interfacial tension between the two phases to ultra-low levels allowing droplets of one phase to be evenly dispersed in the other phase. Microemulsions have the potential to be used in many different types of dosage forms. Oral and transdermal dosage forms are the most common. Increased absorption, improved clinical potency, and decreased drug toxicity are a few of the benefits of oral microemulsion formulations (2). Drugs delivered transdermally avoid hepatic first pass metabolism. Transdermal microemulsions also help improve the drug's percutaneous flux which results in higher plasma drug concentration during drug delivery (3). The present study investigates the use of diocetyl sodium sulfosuccinate (DOSS), an ionic surfactant, ethyl oleate, and water as a potential pharmaceutically relevant ternary microemulsion formulation.

Surfactant/oil mixtures were used in ratios of 1:5, 1:10 and 1:15, and water was added using the titration method to form microemulsions. A Gibb's triangle was prepared to identify the visually clear microemulsion forming compositions. The microemulsions were then characterized using polarized light microscopy, electrical conductivity, dynamic light scattering (DLS), and rheology measurements. The effect of buffers and pH on the amount of water held in the ethyl oleate microemulsion was also evaluated. All formulations were stable with no observable separation of phases throughout the period of study. Samples of microemulsions exhibited no birefringence when observed under polarized light. In conductivity studies, the samples in microemulsion forming region exhibited low conductivity indicating that the microemulsions were w/o. Large increases and fluctuations in conductivity between samples of increasing amounts of water indicated that the mixture was no longer a microemulsion, and water was becoming more of the continuous phase. DLS measurements indicated the presence of nanometer sized droplets in the microemulsions prepared with 1:10 DOSS/ethyl oleate. The smallest droplets were approximately 24 nm in size, and the largest droplets were approximately 40 nm. All microemulsions showed Newtonian flow properties when they were evaluated in a controlled stress-strain rheometer. Buffer studies indicated that the pH of the water added to DOSS/ethyl oleate microemulsions has an impact on the microemulsion forming region. Results from polarized light microscopy, conductivity, DLS, and rheological measurements are consistent with the formation of w/o microemulsions containing nanometer-sized droplets of water in oil. These microemulsions have been developed using pharmaceutically relevant components and may be potentially used in various drug delivery applications.

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Waste to Wonders: Studies on Ferrites Made with Maghemite

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The term “ferrite” is commonly used to describe a class of ceramic compounds of the formula AFe_2O_4 (where A is divalent Mg, Co, Ni, Cu, Zn or even Fe) that contain iron oxide as the principal component and are ferrimagnetic. Ferrimagnetic materials are like ferromagnets (such as iron, a permanent magnet) in that they hold a spontaneous magnetization below the Curie temperature and show no magnetic order (become paramagnetic) above this temperature. They possess unequal and opposing ionic magnetic moments that result in a net moment. Their applications range from credit and hotel room access cards to random access memory (RAM), RF transformers, inductors, magnetic cores of switched-mode power supply (SMPS) and satellite communication devices.

They are commercially made by the traditional ceramic route of solid-state reaction of hematite ($\alpha\text{-Fe}_2\text{O}_3$) with oxides of divalent metals. In order to tweak the magnetic properties, the A-site is frequently substituted with a host of cations.

In this work we elected to fabricate ferrites using maghemite ($\gamma\text{-Fe}_2\text{O}_3$) as the iron precursor instead. It is also ferromagnetic, isostructural to magnetite (Fe_3O_4) but chemically resembles hematite ($\alpha\text{-Fe}_2\text{O}_3$). Maghemite is formed by topotactic (structural rearrangement) of magnetite at low oxygen partial pressure: thus the name MAG(netite)HEM(at)ITE.

Interestingly, the maghemite used in this work was derived from Millscale - a skin waste of steel structures (annual production worldwide: ~ 20 million metric tons). Millscale is predominantly magnetite, and ~ 90% if it is currently land-fill destined. Mill-scale was successfully and quantitatively converted into maghemite by employing a simple proprietary technique. Some structural, microstructural aspects and the magnetic properties of maghemite-based nickel and zinc ferrites are presented. Current global market for ceramic magnets is worth \$5.4 billion/yr.

Trichloroethylene (TCE) Adsorption Using Sustainable Organic Mulch

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Soluble substrates (electron donors) have been commonly injected into chlorinated solvent contaminated plume to stimulate reductive dechlorination. Recently, different types of organic mulches have received much attention as new supporting materials with economic advantages and sustainable benefits for engineered biowall systems. Previous studies reported that mulch installed in biowall systems could provide long term sources of organic carbon and electron donors for chlorinated solvent bioremediation. However, sorption capacities of organic mulches for chlorinated solvents haven't been studied yet. In this study, the physicochemical properties of three commercially available mulches (hardwood, pine, cypress) were characterized and their sorption capacities were elucidated by single, binary and quaternary isotherm tests with trichloroethylene (TCE), tetrachloroethylene (PCE), trans-dichloroethylene (trans-DCE) and cis-dichloroethylene (cis-DCE). Among three mulches, pine showed better adsorption ability than hardwood and cypress.

Keywords: Trichloroethylene, Adsorption, Sustainable, Organic Mulch

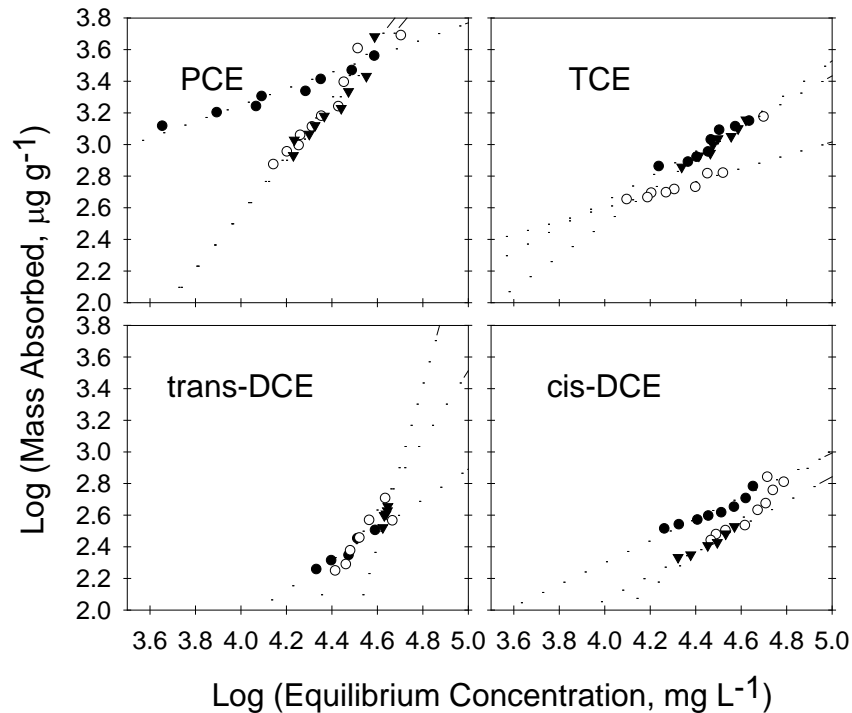


Figure 1 Log-Log Single Chemical Adsorption Isotherms for Different Mulch (●—Pine; ○—Hardwood; ▼—Cypress)