ACS Local Section
East Texas

April 2018

Next Section Meeting

Date:	Thursday, April 12
Place:	Berry Auditorium (C101) Glaske Center for Engineering Science and Technology LeTourneau University Longview, TX
Dinner:	On your own (refreshments will be provided)
Time:	Poster session beginning at 7:00 P.M.

Undergraduate Poster Session (abstracts received as of April 2)

Effect of Toxic Metal Ions on Photosensitized Singlet Oxygen Generation for Photodegradation of Polyaromatic Hydrocarbon Derivatives and Photoinactivation of *Escherichia coli*

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Inorganic toxic metals, polyaromatic hydrocarbons, and pathogens are common contaminants found in aquatic and terrestrial environments. Here we report an experimental study of the effect of toxic metal ions on photosensitized singlet oxygen generation for photodegradation of common polycyclic aromatic hydrocarbons derivatives (PAH derivatives) contaminants consisting of three benzenoid rings, such as Anthracene-9,10-dipropionic acid disodium salt (ADPA), and two benzenoid rings, such as 1,5-dihydroxynapthalene (DHN) by using water soluble cationic *meso*-tetra(N-methyl-4-pyridyl)porphine tetrachloride (TMPyP) as a singlet oxygen photosensitizer. In addition, we investigated the effect of toxic metal ions on singlet oxygen generation for photoinactivation of *E.coli* bacteria by using the same TMPyP singlet oxygen photosensitizer. The photodegradation of electron-rich ADPA and DHN by TMPyP-generated singlet oxygen ($^1O_2$) was examined and the rates of photodegradation of ADPA and

DHN were calculated to be $(1.50 \pm 0.26) \times 10^{-3}$ s^{-1} and $(6.62 \pm 0.50) \times 10^{-4}$ s^{-1}. The presence of s-block metals ions, such as Na^{+}, K^{+}, and Ca^{2+} showed no change of the rate of photodegradation of ADPA or DHN by TMPyP generated $^{1}O_2$. However, in the presence of heavy metals such as Cd^{2+}, Cu^{2+}, Hg^{2+}, Zn^{2+}, and Pb^{2+}, we observed a dramatic change in the photodegradation of ADPA and DHN. Interestingly, the photodegradation of electron-rich ADPA and DHN were observed to increase rapidly in the presence of heavy metal cadmium (II) ions (Cd^{2+}). The obtained photodegradation rate constants of ADPA and DHN in the presence of Cd^{2+} ions were $(3.91 \pm 0.20) \times 10^{-3}$ s^{-1} and $(7.18 \pm 0.35) \times 10^{-4}$ s^{-1}, respectively. Strikingly, the photodegradation of ADPA was moderately reduced in the presence of zinc ions (Zn^{2+}) and almost completely inhibited in the presence of mercury (II) ions (Hg^{2+}) and copper (II) ions. Similarly, DHN photodegradation was significantly slowed down in the presence of Hg^{2+} and Cu^{2+} ions. Finally, we tested the photoinactivation of *E.coli* by singlet oxygen from TMPyP in the presence of dissolved toxic metal ions such as Cd^{2+}, Cu^{2+}, Hg^{2+}, Zn^{2+}, and Pb^{2+} ions. A complete inhibition of growth of *E.coli* was observed when *E. coli* solutions were irradiated with TMPyP and heavy metal ions particularly, Cd^{2+}, Hg^{2+}, Zn^{2+}, and Pb^{2+} ions. Interestingly, toxic copper ions followed a similar trend as seen in photodegradation of DHN and ADPA. A significantly slow inhibition of *E.coli's* growth was observed in the presence of copper ions (Cu^{2+} ions) and TMPyP. A substantial dark toxicity for mercury ions and a complete dark toxicity for zinc ions against *E.coli* were observed in the presence of TMPyP. This result is demonstrating the fact that dissolved toxic metal ions except copper ions in the presence of TMPyP have a strong influence on generation of $^{1}O_2$ for photoinactivation of *E.coli* bacteria as well as killing *E. coli* under dark conditions.

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Study of Bacterial Species Present in La Nana Creek within Nacogdoches Area

Jennifer Hanes, Raven Turner*, Petra Kadakova, Michael A. Janusa, Beatrice Clack
Department of Chemistry and Biochemistry
Stephen F. Austin State University

This study focused on estimating the presence of bacterial species within La Nana Creek in proximity to Stephen F. Austin State University. The method used for this study involved the U.S. Environmental Protection Agency (USEPA) Method 1604: Total Coliforms and *Escherichia coli* in Water by Membrane Filtration Using a Simultaneous Detection. A 50 mL of freshwater sample was collected from four different sites along La Nana Creek and filtrated through a membrane filter via gravity filtration and rolled over a MI agar plate to determine a total coliforms and *E. coli* count within the site of collection. After colony count, some colonies were selected for sequencing to prove the presence of E coli or to determine the genus of colonies. The overall presence of *E. coli* in the water samples was very low (less than 3.5 colony per MI agar plate on average). Based on the sequencing data, all blue colored colonies were proven to be *E. coli* except for site I sample I. This colony appears to be a *Klebsiella pneumoniae*; however, that could be a result of contamination during colony PCR since the beige colored colony was growing in a proximity to the blue colony. The prevailing family of bacteria present within samples was *Enterobacteriaceae*, commonly found within intestines of animals as well as in soil and water. The only other family present was *Pseudomodaceae* which is found in all types of environment.

Determination of Selected Metals for La Nana Creek Water and Soil Samples within the Nacogdoches Area

Christine Villas*, JoAnn Harper*, Jennifer Hanes, Michael A. Janusa
Department of Chemistry and Biochemistry
Stephen F. Austin State University

La Nana Creek is one of two springs that surround Nacogdoches, TX. La Nana Creek starts southwest of Lake Naconiche, conjoining with several other bodies of water along its path, and becomes part of the Angelina River. This body of water eventually ends in the Gulf of Mexico which may contribute to the dead zone. La Nana Creek water and soil samples were studied for the determination of selected metals (Ag, Ba, Be, Bi, Cd, Co, Cr, Cs, Cu, Ga, In, Li, Mn, Mo, Ni, Pb, Rb, Sr, Tl, V, and Zn) from September 2016 through November 2017 (12 samples at each site). Sampling sites consisted of NE Stallings Drive, East College Street, Main St., and Martin Luther King Jr. Blvd. Samples were analyzed using the EPA protocol for digesting water and soil samples. Samples were acidified, digested (total recoverable), and filtered to remove residue. Results indicate that the water samples had Ba, Mn, Sr, and Zn at measurable amounts (greater than 10 ppb for majority of samples) while soil samples had these species at measurable amounts as well as Cr, Ni, Pb, Rb, and V. Soil samples have a much higher metal concentration than water samples except for Sr. Soil results tended to decrease from North to South in the creek for all metal concentrations due to soil variation while water samples tended to have similar results at all locations. All samples analyzed were found to have metal concentrations typical for creek water and soil type and well below WHO and EPA allowable values.

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Antimicrobial properties of S-benzofuran-2-yl ethanol produced by biotransformation

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Stephen F. Austin State University

All living organisms contain enzymes which carry out biological reactions which produce substances with a specific three dimensional shape. Enantiomers are two molecules that are mirror images of each other just as hands are mirror images of each other. It is well known in the pharmaceutical world that one of the enantiomers (one of the mirror-image molecules) has a positive biological effect while the other can be harmful or have no effect. Currently, any potential pharmaceutical that could exist as enantiomers must have each enantiomer tested for biological activity prior to FDA approval. In our laboratory, we have focused on one particular reaction in which enzymes in vegetables catalyze a reaction of benzofuranyl methyl ketone (BMK) to benzofuranylethanol (BMA). BMA can have two different three dimensional arrangements, so mirror image molecules are possible. The two enantiomers are designated S-BMA and R-BMA. Several vegetables have been utilized to determine which can catalyze this reaction, as well as to determine whether the various vegetables produce both enantiomers or only a single enantiomer. Several vegetables (carrot, parsnip, and celery) produce only one of the enantiomers, the S-isomer. However, potatoes and radishes produce a mixture of the R- and S-isomer, with the potato producing nearly equal amounts of both. Previous work in the laboratory has shown that the S-BMA produced from carrots has antimicrobial properties, inhibiting the growth of bacteria as well as yeast. Initial studies indicate the mixture of S- and R-BMA from potatoes has less potent antimicrobial activity than the pure S-BMA produced by carrots. Studies are underway to more fully assess the antimicrobial property of the mixture of the R-and S-isomer and compare to the antimicrobial property of the pure S-isomer produced by carrots.

An Efficient Procedure for the Synthesis of Sulfonamide Derivatives

Marisa R. Trosen* and Bruce A. Hathaway
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LeTourneau University

A method to efficiently produce sulfonamide derivatives from a variety of substituted benzaldehydes is reported. This method is a modification of a method reported by Helmuth Gilow (*J. Chem. Educ.*, **1979**, *56* (6), 419-420), which was unsuccessful in our hands. Sulfanilamide can be condensed with a number of substituted benzaldehydes in good yields by refluxing in 1-propanol for an hour. Reduction of the resulting imines with sodium borohydride worked well for most of the imines. We are currently investigating "one-pot" procedures to accomplish both steps without isolation of the imine intermediate. The substituted sulfonamides will be tested for antimicrobial activity. If all of the parts of the experiment can be optimized, this would be a nice interdisciplinary organic chemistry/microbiology project for our chemistry and biology students, which could illustrate the drug discovery process, as well as structure activity relationships of drugs.

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Examining Strategies for Improving Catalytic Activity of Enzymes Encapsulated in Virus-Like Particles

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[1]Department of Chemistry & Biochemistry, The University of Texas at Tyler
[2]Department of Chemistry, Indiana University

Encapsulation of enzymes into protein cage structures holds promise for developing catalytic nanomaterials and better understanding of enzyme function in cellular environments. This research presented evaluates the encapsulation of enzymes inside protein cage virus-like particles (VLPs) derived from bacteriophage P22 comparing a rapid *in vivo* encapsulation strategy with a temporally controlled expression strategy to improve the overall activity of enzymes encapsulated inside the P22 VLP. Results from the rapid *in vivo* encapsulation strategy showed greatly reduced kinetic activity in comparison with the temporally controlled strategy, suggesting that maturation of an enzyme before encapsulation is necessary.

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Developing the HK97 Virus-Like Particle as a Drug Delivery System

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Protein cages are ubiquitous in nature and present useful nanomaterials for applications ranging from drug delivery to the construction of nanoelectronics. Among protein cages, virus-like particles (VLPs), which are derived from the protein shell of viruses but lack pathogenic components, are particularly intriguing for constructing nanomaterials due to their stability and well-studied molecular assembly and structures. The VLP derived from the HK97 bacteriophage self assembles from a single coat protein to form a 55 nm particle which will not enter mammalian cells. This characteristic makes the HK97 VLP a potentially ideal platform for targeted drug delivery. The research presented will discuss the design and molecular modification of the HK97 VLP toward producing a drug delivery "smart bomb".

Encapsulation of Elastase inside the P22 Virus-like Particle

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The University of Texas at Tyler

Elastase is a protein that is secreted by the pathogen *Pseudomonas aeruginosa* that is responsible for tissue damage and infection by the pathogen in the human host. Elastase has been implicated in activation of the EGFR signaling pathway and there is an interest in understanding its involvement and mechanism of EGFR activation. The results presented here are for the encapsulation and characterization of Pseudomonas aeruginosa elastase enzyme in the P22 virus-like particle (VLP). By encapsulating the elastase enzyme inside the VLP biocontainer, preventing direct contact of the enzyme with the cell surface, but allowing free exchange of soluble substrates into the VLP through 2 nm pores in the protein wall, we seek to examine the mechanism for the activation of the EGFR pathway. In addition, the elastase-VLP holds potential for the development of a vaccine providing protection against *Pseudomonas aeruginosa*.

Upcoming Dates

August 19-23	ACS National Fall Meeting, Boston, MA
September	Career Fair, Eastman Chemical Company, Longview, TX
October/November	Michael McClendon, UT-Tyler, Tyler, TX
November 7-10	Southwest Regional Meeting, Little Rock, AR

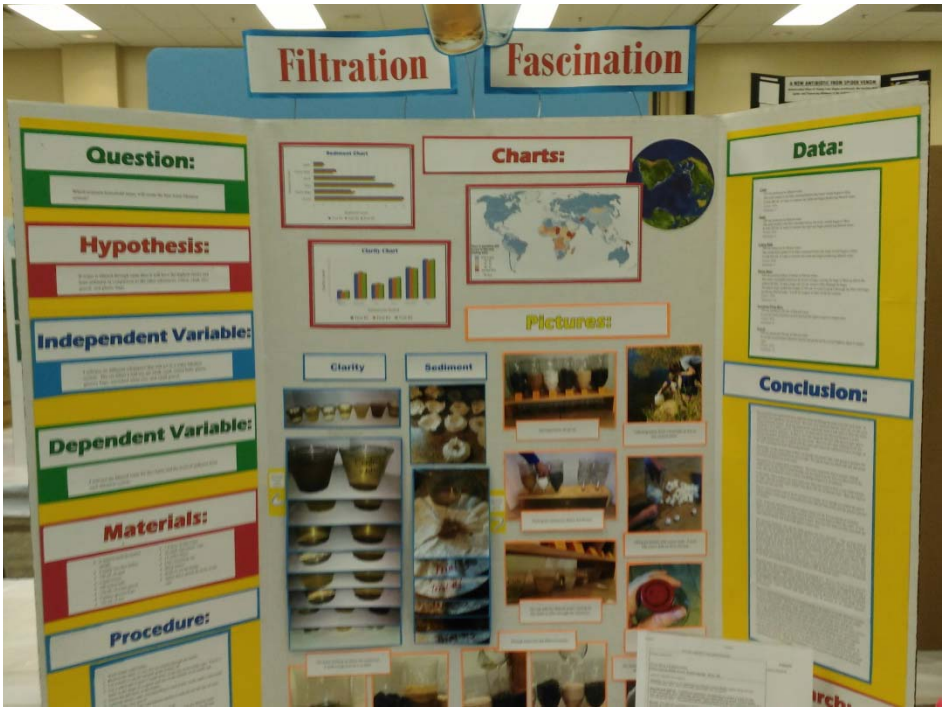
2018 Section Officers

Chair	Jerome Stavinoha	jstavinoha@gmail.com
Chair-elect	Ruth Hathaway	ruthhathaway@msn.com
Treasurer	Paul Zhang	pzhang@ana-lab.com
Secretary	Mike Sheets	mike.sheets@texarkanacollege.edu
Councilor	Philip Verhalen	philip.verhalen@gmail.com
Alt. Councilor	Mike Sheets	mike.sheets@texarkanacollege.edu

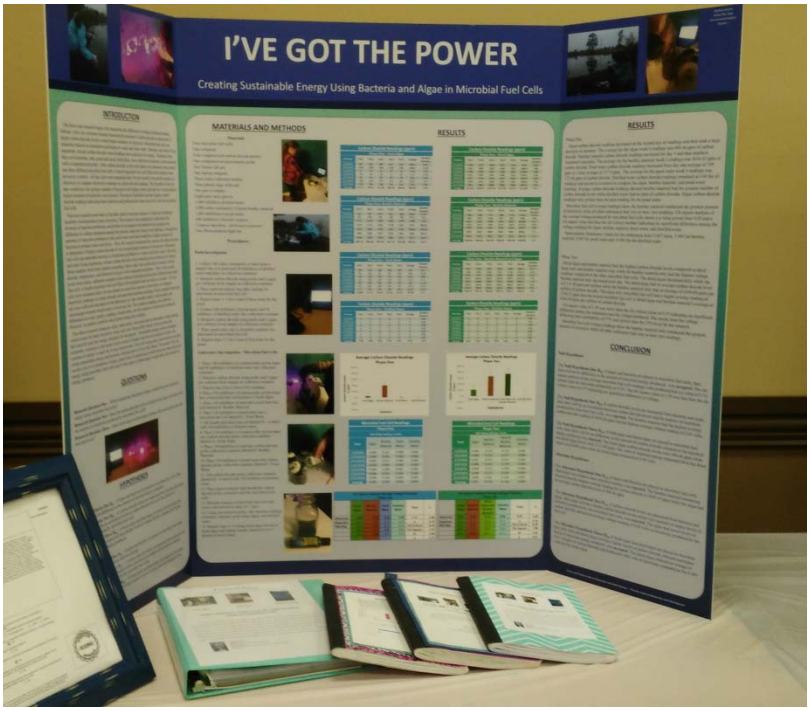
Section Website: **http://easttexasacs.sites.acs.org/**

2018 East Texas ACS Science Fair Winners

Junior Division



Connor Bailey and
Madison Bailey
Filtration Fascination
Sulphur Springs
Middle School



Madison Perkins
I've Got the Power
Gilmer Intermediate

Senior Division

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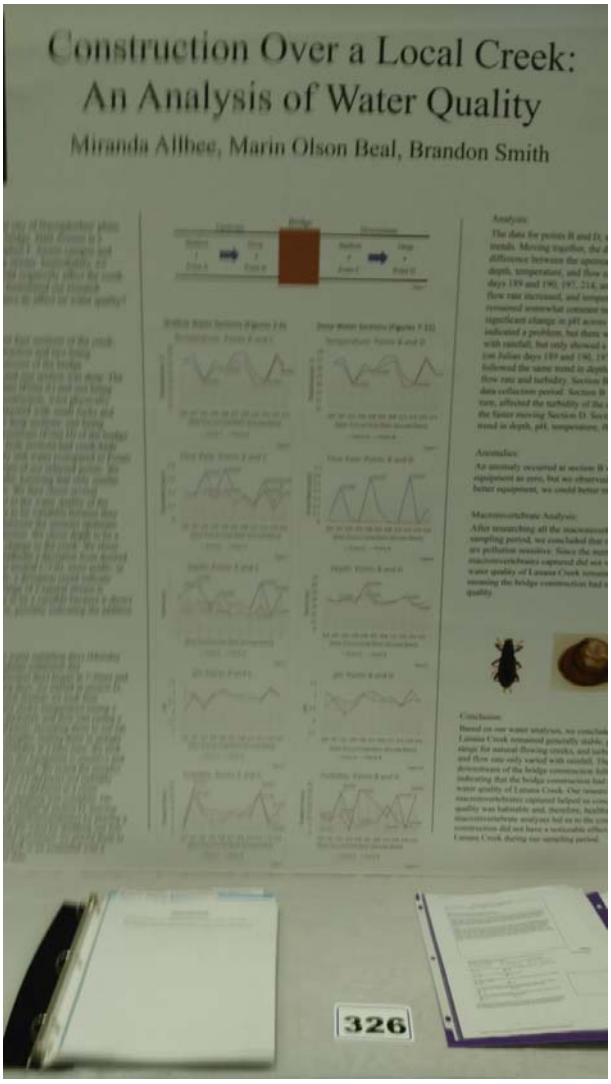
Brianna Parker
Effects of Water/Cement Ratio on the Strength of Concrete
Gilmer High School



Miranda Allbee, Marin Olson Beal and Brandon Smith
Construction over a Local Creek: An Analysis of Water Quality
Nacogdoches High School

About ACS Webinars™

ACS Webinars™ is a free, weekly online event serving to connect ACS members and scientific professionals with subject matter experts and global thought leaders in chemical sciences, management, and business. The ACS Webinars are divided into several series that address topics of interest to the chemical and scientific community; these series include careers, business and innovation, professional growth, joy of science, extreme chemistry, entrepreneurial initiative, green chemistry, and more. Each webinar is 60 minutes in length, comprising a short presentation followed by Q&A with the speaker. The live webinars are held on Thursdays from 2-3pm ET. Recordings of the webinars are available online and upcoming events are posted at http://acswebinars.org/.

Upcoming ACS Webinars

April 5

Creating New Models to Combat Neglected Disease Through, Industry, Government, and Public-Private Partnerships

https://www.acs.org/content/acs/en/acs-webinars/business-entrepreneurship/drug-partner.html

Neglected tropical diseases represent a mostly unprofitable area for drug discovery research. As a result, the drug industry doesn't usually approach this work solely using internal resources. Similarly, academic laboratories do not frequently have the depth and breadth of knowledge and experience in drug discovery. Join Michael Pollastri, Professor and Chair of Chemistry and Chemical Biology at Northeastern University and Félix Calderón of GlaxoSmithKline as they discuss a successful model of distributed neglected tropical disease drug discovery that involves collaborators in industry, government, and public-private partnerships.

April 12

NSF's Big Ideas: Understanding the Rules of Life and The Quantum Leap

https://www.acs.org/content/acs/en/acs-webinars/popular-chemistry/nsf-big-ideas.html

Recently the National Science Foundation unveiled a set of "Big Ideas" that are bold, long-term research and process ideas that all scientists should be aware of if they seek funding opportunities for their research. Join Angela Wilson of NSF, Cynthia Burrows of the University of Utah, Theodore Goodson of the University of Michigan, and Glenn Ruskin of ACS for an introduction to two of the most impactful "Big Ideas" as well as an overview of this innovative NSF program that will advance prosperity, security, health, and well-being in the United States.

May 3

Writing Competitive Research Proposals that Win Funding

https://www.acs.org/content/acs/en/acs-webinars/professional-development/write.html

One of the most pragmatic questions in scientific research is, "How will this research be funded?" The answer to this funding uncertainty often depends on how you present your research proposal just as much as having a good research idea. Fortunately, for researchers good presentation skills are an aptitude that can be learned by everyone. Join Nancy Jensen, a Program Manager of the Office of Research Grants at ACS, as she focuses on the basic skills and pointers for writing a competitive research proposal.

May 10

The Opioid Crisis and Quest for Superior Analgesics without Addiction

https://www.acs.org/content/acs/en/acs-webinars/popular-chemistry/crisis.html

Opioid-related drug overdoses are leading to approximately 150 deaths every day in the United States alone. Furthermore, present day statistics show that almost a third of the American population suffer from chronic pain and opioids continue to be our best choice for pain-relief. Join Ajay Yekkirala of Blue Therapeutics and Jane Aldrich of the University of Florida to discover how medicinal chemists are developing potent analgesics that are devoid of narcotic side effects to stop the cycle of pain-opioid abuse.

Parking lot to use

Glaske Hall – use the "back" entrance. Lobby is just inside the door and Karen's office is the first door on the right.

There is a stop light at the Mobberly/Green intersection. Turn right (assuming you are coming North from I-20 on Mobberly – this light is just past the post office). Take the first left which is Weller Dr. Parking lot will be on the left.