Schedule of Events

9:30-10:30  Registration, poster setup, and continental breakfast  
*Sponsored by Midland Scientific Inc.*

10:30-11:30  Research Talks (15 min/talk with 5 min for questions)  
*Session lists and abstracts found beginning on pg. 2*

11:30-12:30  Buffet lunch

12:30-2:00  Poster presentations  
*12:30-1:15 – poster presentations with an odd numbered abstract  
1:15-2:30 – poster presentations with an even numbered abstract  
Abstracts found beginning on pg. 8*

2:00-3:00  Keynote address  
**Expanding Research Frontiers: Food Questions for a New Millennium**  
Dr. Sunil Malapati, Clarke University  
*Abstract and biography found on pg. 19*

3:00-3:30  Recognition of students
Research Talks

Session A:

A1 Metabolic Diversity in Pancreatic Cancer Cell Lines: The Effect of Saracatinib  
Stephanie N. Lankford, Monmouth College

A2 Nanoscale Coordination Polymers for the Co-delivery of siRNAs and cisplatin for Treating Resistant Ovarian Cancer  
Kristine Ma, The University of Chicago

A3 The Effect of Psychosocial Stressors on Cancer Biology in a Spontaneous Model of Heterogeneous Breast Cancer  
Daniel Villalobos-Terrazas, The University of Chicago

Session B:

B1 A Molecular Dynamics Simulation of Aquaporin-0 Water Conduction Regulation by Calmodulin  
Thanh Bach, Coe College

B2 Sensory Evaluation and Instrumental Modeling: Applying Food Science  
Maxwell Holle, Monmouth College

B3 The Role of Maternal Care on the Development of Stereotypy in the Rat  
Samantha Lauby, Carroll University

Session C:

C1 Peptide Binding to Nanoparticles: Synthesis of Al₂O₃ Nanoparticles and Optimization of Primary Amine Quantitation  
Madeleine Meyer, University of Wisconsin-Madison

C2 The Aroma of Coffee: Analyzing 2-Furfurylthiol and Caffeine in Coffee Beans  
Sydney Oppelt and Gavin Parker, St. Ambrose University

C3 Stereoelectronics of Silyloxybenzoic Acid  
Paolo Suating, Northern Illinois University
Research Talk Abstracts

Abstract #A1

**Metabolic Diversity in Pancreatic Cancer Cell Lines: The Effect of Saracatinib**
Stephanie N. Lankford, Venugopal Gunda, Vinee Purohit, Jamie Abrego, and Pankaj K. Singh
Department of Chemistry, Monmouth College

Pancreatic cancer is among the most deadly cancers in the United States primarily due to the lack of known specific biomarkers, late stage diagnosis, poor therapeutic response, and frequent recurrence of disease. Recently, our group has standardized a method for metabolite detection using LC-MS/MS analysis. We employed this technique to identify the metabolic basis for saracatinib responsiveness in pancreatic ductal adenocarcinoma.

Abstract #A2

**Nanoscale Coordination Polymers for the Co-delivery of siRNAs and cisplatin for Treating Resistant Ovarian Cancer**
Kristine Ma, Chunbai He, Demin Liu, Xiaopin Duan, and Wenbin Lin
Department of Chemistry, The University of Chicago

One of the major limitations for successful cancer treatment is the developed resistivity to the chemotherapeutic agent, Cisplatin. The critical development of novel strategies to overcome intrinsic and acquired resistance to chemotherapy is important to effective treatment of ovarian cancer and other types of cancers. We have sought to re-sensitize resistant ovarian cancer cells to chemotherapy by co-delivering chemotherapeutics and pooled siRNAs targeting multi-drug resistance (MDR) genes using self-assembled nanoscale coordination polymers (NCPs). NCP-1 particles with trigger release properties were first constructed by linking cisplatin prodrug-based bisphosphonate bridging ligands with Zn2+ metal-connecting points and then coated with a cationic lipid layer, followed by the adsorption of pooled siRNAs targeting three MDR genes - including survivin, Bcl-2, and P-glycoprotein via electrostatic interactions. The NCP-1/siRNA particles promoted cellular uptake of cisplatin and siRNA, which enabled efficient endosomal escape in cisplatin-resistant ovarian cancer cells. By down-regulating the expression of MDR genes, NCP-1/siRNAs enhanced the chemotherapeutic efficacy as indicated by cell viability assay, DNA ladder, and flow cytometry. Local administration of NCP-1/siRNAs effectively reduced tumor sizes of cisplatin-resistant SKOV-3 subcutaneous xenografts. The NCP-1/siRNA platform shows a promising outlook in enhancing chemotherapeutic efficacy for the effective treatment of drug-resistant cancers.
Abstract #A3

The Effect of Psychosocial Stressors on Cancer Biology in a Spontaneous Model of Heterogeneous Breast Cancer

Daniel Villalobos, Marianna Johnson, Suzanne Conzen, Martha McClintock, and Matthew Brady
Department of Medicine, The University of Chicago

Chronic stressors are reported to have substantial influences on breast cancer proliferation and metastasis. A heightened stress response in a transgenic murine model of triple negative breast cancer is associated with increased expression of key metabolic genes and a divergent mammary adipose tissue secretome in the mammary gland preceding the development of invasive tumors (1, 2). Furthermore, the secretome of isolated mice has been found to be more proliferative on mouse mammary epithelial cells representative of ductal carcinoma in situ (1). In this study, Sprague-Dawley (SD) rats, a spontaneous and heterogeneous model of breast cancer, were raised in group or isolated housing conditions in order to investigate the underlying mechanisms whereby psychosocial stressors alter the mammary microenvironment prior to breast tumor formation. Contrary to previous findings, the mammary glands from isolated rats (16 weeks of age, 12 weeks of social isolation) are more metabolically active, but have lower protein concentrations in their MAT’s secretome. Consequently, human mammary epithelial cells proliferate at a more rapid rate with the group-housed rat CM than with CM from the isolated rats. These findings suggest that protein concentrations in the MAT secretome are pivotal antecedents of breast cancer metastasis in SD rats. Determining the specific protein composition of the respective conditioned media may offer a greater understanding of psychosocial stressors’ effects on breast cancer proliferation.

Abstract #B1

A Molecular Dynamics Simulation of Aquaporin-0 Water Conduction Regulation by Calmodulin

Thanh Bach, Ugur Akgun and Lucas Montgomery
Department of Chemistry and Department of Physics, Coe College

Aquaporin-0 (AQP0) contributes to the nurturing and cleaning of waste products from the eye lens. AQP0 is a tetrameric protein composed of four identical monomers, each of which has its own water pore. AQP0 water conduction is regulated by pH, Ca$^{2+}$ concentration, and the phosphorylation of Serine residues at the C-terminus. High cellular Ca$^{2+}$ concentration enhances the binding of Calmodulin (CaM), a Ca$^{2+}$ dependent protein, to AQP0 from the cytoplasm. Molecular Dynamics (MD) simulations performed to investigate the effects of two Calmodulin binding to AQP0 tetramer revealed free energy barriers up to 6 kcal/mol for water conduction. Steered MD simulations also exposed three distinct locations, where the water molecule’s pathway changes between the AQP0-CaM model versus the apo-AQP0 model.
Abstract #B2

Sensory Evaluation and Instrumental Modeling: Applying Food Science
Maxwell Holle,1 Jessie Usaga,2 and Olga I. Padilla-Zakour2
1Monmouth College and 2Department of Food Science, Cornell University

Reduction of Sodium in Ranch Dressing using NuTek 14510: Over consumption of sodium is known cause of hypertension which can lead to a multitude of health detriments. Potassium has been targeted for replacing sodium through substitution of KCl for NaCl. This is not a simple substitution because potassium chloride possesses a metallic bitter taste at certain concentrations. NuTek Salt Co. has developed a potassium chloride substitute (14510) in order to replace salt and/or MSG in ranch dressing. Ten formulations of varying sodium reduction were developed and evaluated while a sensory panel was performed using the best two (selected by NuTek). Sensory evaluations, a triangle and a forced paired preference test, were performed using a panel of 40 tasters between the ages of 20 and 60. The results indicated that there was no significant difference and no significant preference between a standard ranch dressing and the ranch dressing made with 14510. The 14510 can be used to reduce sodium and MSG in ranch dressing.

Evaluating Ascorbic Acid for Commercial UV Pasteurization Modeling: UV pasteurization has been of particular interest to small juice producers due to its cost, effectiveness, and minimal physical, chemical and nutritional changes in the product. The presence of UV absorbing chemicals interferes with the UV pasteurization. The UV absorbing chemical ascorbic acid is present in many juices. The absorption coefficients for varying ascorbic acid concentrations were determined as well as the correlating flow rate (determined using the UV CiderSure 3500). Using this relationship, pilot plant trials were conducted using 8 commercial juices of varying physiochemical characteristics in order to evaluate whether a juice’s flow rate could be predicted using its absorptivity. In order to determine the safety validation of the method commercial juices were inoculated with E. coli ATCC 25922 in order to determine the log reduction after UV treatment. The model was able to predict flow rate, but 5 out of the 8 juices tested were not in compliance with the 5 log reduction required by the Federal Juice HACCP Regulation.
Abstract #B3

The Role of Maternal Care on the Development of Stereotypy in the Rat
Samantha Lauby¹ and Patrick McGowan²
¹Carroll University and ²Department of Biological Sciences, University of Toronto

Stereotypies are of interest to researchers because of their implications in animal welfare. However, not much is known about how and why they develop in some animals and not others in the same conditions. In this experiment, we hypothesize that maternal care is a mediator that increases or decreases susceptibility to developing stereotypies. Higher amounts of maternal care should decrease risk of stereotypies in the offspring. Maternal behavior of female rats, which were either stressed or unstressed, and stereotypic behavior in the offspring were recorded and coded. Though there was not a negative correlation between maternal care and prevalence of stereotypic behavior, there was a interaction between gestational stress and sex. The implication of this exploratory study was to establish a protocol for measuring stereotypic behavior in rats. Further studies should look into individual care received and the prevalence of stereotypies.

Abstract #C1

Peptide Binding to Nanoparticles: Synthesis of Al₂O₃ Nanoparticles and Optimization of Primary Amine Quantitation
Madeleine Meyer, Marco Torelli, Thomas Kuech, Joel Pedersen, Robert Hamers
Department of Chemistry, University of Wisconsin- Madison

Aluminum has long been recognized as a potential neurotoxin. Though exposure to the general public generally occurs in the form of aluminum oxide (Al₂O₃) at the oxidized surface of solid aluminum, nanoparticulate Al₂O₃ is also found abundantly in many commercial products, such as sunscreen, cosmetics, polishing abrasives, and paint. Due to their very small size, Al₂O₃ nanoparticles could conceivably cause misfolding in proteins. The wide use and potential toxicity of Al₂O₃ nanoparticles highlights the importance of understanding how these particles might interact with biological systems. Specifically, we seek to study how nano-Al₂O₃ might interact with and disrupt protein conformation by studying particle interactions with model peptides. Required for this study are size controllable and well-characterized nano-Al₂O₃, as well as a means to measure peptide binding at low concentrations in situ.

To provide systematic study of nano-alumina, we synthesized Al₂O₃ nanoparticles at sub-30 nm sizes through a sol-gel method and characterized these particles by Fourier transform infrared spectroscopy, powdered X-ray diffraction, dynamic light scattering, and laser Doppler micro-electrophoresis. In addition, we demonstrate the importance of optimizing conditions to perform a quantitative primary amine detecting fluorescamine assay and provide a systematic means to do so, thereby lowering the obtainable detection limit. Subsequently, binding isotherms of peptide to nano-Al₂O₃ to peptide can be determined.
Abstract #C2

**The Aroma of Coffee: Analyzing 2-Furfurylthiol and Caffeine in Coffee Beans**

Allie Daniel, Sydney Oppelt, Gavin Parker, Kelly Gierlus, and Joshua Stratton  
Chemistry Department, St. Ambrose University

There are more than 1,000 volatile compounds contributing to coffee’s complex aroma. One of these compounds is 2-furfurylthiol (FFT), which is known to contribute to coffee’s roasty aroma. The goal of this study was to determine FFT and caffeine concentrations in coffee beans from three different blends. Both roasted and green, unroasted, coffee beans were collected from Ethiopian (Yirgacheffe), Colombian, and Sumatran blends. FFT and caffeine were isolated using solid-liquid extraction and analyzed using gas chromatography-mass spectrometry. Calculated average concentrations (±standard deviations) of FFT in roasted Yirgacheffe, Colombian, and Sumatran beans were 0.9 (±0.2), 1.0 (±0.5), and 0.9 (±0.1) mg L⁻¹, respectively. While, calculated average concentrations of FFT in green Yirgacheffe, Colombian, and Sumatran beans were 0.20 (±0.03), 0.16 (±0.04), and 0.3 (±0.2) mg L⁻¹, respectively. This study showed the concentrations of FFT in roasted Yirgacheffe and Sumatran beans were significantly different at a 95% confidence interval from their green beans, while Colombian were not significantly different. Average concentrations of caffeine in roasted Yirgacheffe, Colombian, and Sumatran beans were 24 (±8), 20 (±7), and 26 (±5) mg g⁻¹, respectively. While, average concentrations of caffeine in green Yirgacheffe, Colombian, and Sumatran beans were 14.0 (± 1), 15 (±2), and 21 (±3) mg g⁻¹, respectively. The caffeine in roasted and unroasted coffee beans were not significantly different at a 95% confidence interval. This study suggests that origin of the coffee did not significantly affect FFT concentrations.

Abstract #C3

**Stereoelectronics of Silyloxybenzoic Acids**

Sami E Varjosaari, Jeremy P Hess, Paolo Suating, John M Price, Thomas N Gilbert, and Marc J Adler  
Department of Chemistry and Biochemistry, Northern Illinois University

Alkyl silyl groups, such as the trimethyl, triethyl, tert-butyldimethyl, and others, are merely regarded as effective protecting groups for labile oxygen groups such as phenols. Because of the sheer size of the silicon atom and the bulk added on to it by the alkyl and aryl groups this could force the lone pairs of the phenolic oxygen to twist out of the plane of the aromatic ring which effectively reverses the role of the phenolic oxygen from an electron-donating to an electron-withdrawing group. This study focuses on the potential of some ortho- and para- substituted benzoic acid silyloxy ethers to catalyse the Friedel-Crafts reaction between indole and β-nitrostyrene, as this reaction is sensitive to stereoelectronic changes in the benzoic acid catalyst.
Poster Abstracts

Abstract #1

A Molecular Dynamics Simulation of Aquaporin-0 Water Conduction Regulation by Calmodulin
Thanh Bach, Ugur Akgun and Lucas Montgomery
Department of Chemistry and Department of Physics, Coe College

Aquaporin-0 (AQP0) contributes to the nurturing and cleaning of waste products from the eye lens. AQP0 is a tetrameric protein composed of four identical monomers, each of which has its own water pore. AQP0 water conduction is regulated by pH, Ca2+ concentration, and the phosphorylation of Serine residues at the C-terminus. High cellular Ca2+ concentration enhances the binding of Calmodulin (CaM), a Ca2+ dependent protein, to AQP0 from the cytoplasm. Molecular Dynamics (MD) simulations performed to investigate the effects of two Calmodulin binding to AQP0 tetramer revealed free energy barriers up to 6 kcal/mol for water conduction. Steered MD simulations also exposed three distinct locations, where the water molecule’s pathway changes between the AQP0-CaM model versus the apo-AQP0 model.

Abstract #2

Polystyrene Degradation: Optimal Photosensitization in the Presence of Benzophenone
Ty Balduf and Kelly Gierlus
Chemistry Department, St. Ambrose University

Polystyrene waste poses a serious dilemma due to the difficulty associated with treating the waste. Photodegradative processes using UV light and photosensitizers could be used to manage this growing problem. The photodegradation of polystyrene films has previously been tested with various photosensitizers to a fair degree of success. Specifically, Goi et al. studied the effect of irradiation time on the degradation of polystyrene photosensitized with benzophenone. The aim of this study is to investigate the effect of the benzophenone to polystyrene mass ratio on the extent of degradation at a constant irradiation time of 24 hrs. To pursue this objective, small modifications were made to existing methodology found in the chemical literature. Thin films of polystyrene and benzophenone were prepared by dissolving them in dichloromethane and spreading the mixture over a watch glass. Samples were then irradiated using a commercial nail dryer with a known UV-Vis emission spectra. These samples could then be examined using Attenuated Total Reflectance/Fourier Transform Infrared spectroscopy. The carbonyl (1842-1539 cm⁻¹) and hydroxyl (3635-3121 cm⁻¹) peak areas could serve as proxy for measuring photoproduc formation and thus degradation. By utilizing these techniques, samples of differing substrate to sensitizer ratios were compared. From the preliminary results thus far obtained, a ratio of benzophenone to polystyrene of 0.6 may be optimal.
Think-Tac-Toe is a grid-based logic puzzle similar to the computer game Minesweeper. The puzzle’s goal is to determine the location of Xs and Os in a grid, given a corresponding clue grid of numbers. The number in each cell of the clue grid represents the number of Xs in its “neighborhood.” A puzzle is considered solvable if a given clue grid corresponds to a unique configuration of Xs and Os. It is useful to know which puzzles are solvable, because it is difficult to check all the puzzles when mass-producing them. Previous research showed that rectangular grids with the neighborhood defined by edges, vertices, and self are always solvable for certain sizes (neither length nor width congruent to 2 modulo 3). Our current research extends this work to non-rectangular grids and alternative neighborhood definitions.

We used a combination of linear algebra and graph theory to find solvability patterns and prove them for specific grid geometries. When the determinant of the adjacency matrix of connected grid cells is nonzero, this indicates that the matrix is invertible, and any puzzle of that grid size is solvable. By calculating determinants for small puzzles, we identified patterns of solvability, which were extrapolated to conjecture theorems that hold for arbitrarily large grids. For triangular grids with edge-sharing self-excluding neighborhoods, we proved that no grid sizes can guarantee puzzle solvability. This work presents this proof, as well as other proofs and conjectures for this class of puzzles, and a summary of open problems and future work.
Abstract #4

A Comparison of Selected Green Methods in Silver Nanoparticle Synthesis
Kevin Campbell and Andrew Axup
Chemistry Department, St. Ambrose University

Silver nanoparticles were synthesized by reacting mole ratios of different reducing agents to silver ion in order to successfully produce silver nanoparticles. Significant work has been performed in determining more environmentally-friendly green chemical methodologies in nanoparticle synthesis, which have significant applications in the medical and electronics fields. The wavelengths of maximum absorbance, $\lambda_{\text{max}}$, of the nanoparticle suspensions were determined by UV-Vis spectroscopy following the step-wise addition of Darjeeling tea and found to range between 420 and 470 nm. $\lambda_{\text{max}}$'s between 413 and 438 nm were observed for sodium citrate, suggesting nanoparticles of smaller size, while wavelengths between 440 and 460 nm were found for sodium sulfite, suggesting approximately similar sized particles to that from tea. As larger concentrations of sodium citrate were added to a constant 5 micromoles of silver ion, $\lambda_{\text{max}}$ increased to a maximum of 438 nm and appeared to remain constant. Varied concentrations of sodium sulfite resulted in similar maximum wavelengths around 445 nm regardless of concentration. $\lambda_{\text{max}}$ appears dependent on the concentration used to induce nucleation in the case of tea and citrate, meaning that nanoparticle sizes are dependent on reducing and capping agent concentration. This does not appear to be the case for sulfite, which is only a reducing agent, yet similar nanoparticle sizes based on $\lambda_{\text{max}}$’s are obtained.

Abstract #5

Are the Levels of Brominated Vegetable Oil in Citrus Drinks a Health Threat?
Brian Didier, Jackie Hinderks, Alyssa Daniel, Kyle Krol, Kelly Gierlus, and Joshua Stratton
Chemistry Department, St. Ambrose University

Brominated vegetable oil (BVO) is a substance used in soft drinks to prevent the settling of citrus residues on top of the beverage. Many lab studies about the effects of BVO consumption have been published. The toxicity of BVO has caused it to be banned in Europe. According to the FDA drinks containing BVO should be consumed on an interim basis and not exceed 15 ppm. A previous study found that orange colored sodas contained more BVO than other colored sodas. It was predicted that the brand name soda’s would have higher levels of BVO than the generic brand and that Mountain Dew Live Wire would have the highest level of BVO among Mountain Dew flavors. The Ion Chromatography Dionex ICS-1000 was used to measure the bromide ion levels in four soft drinks (Mountain Dew, Mountain Dew Voltage, Mountain Dew Livewire, and Heee Haw). The BVO was extracted using diethyl ether and then converted to bromide by reacting with zinc dust. Although BVO is listed as an ingredient on the soda cans, bromide ion levels in all samples were below the limit of detection for the method (LOD = 0.01 ppm). These BVO levels were below those previously reported.
Abstract #6

**Comparative Structural Studies of A₂BTeO₆ (A = Ca, Sr, or Ba; B = Ca or Cd) Double Perovskites**

Ashley V. Flores,¹ Hailey M. Albert,¹ Amanda J. Stiner,¹ Travis Mansur,¹ Paris W. Barnes,¹ and Allyson M. Fry²

¹Department of Chemistry, Millikin University and ²Department of Chemistry and Department of Physics and Astronomy, John Hopkins University

Tellurium (VI)-containing compounds have the potential to be useful as capacitor materials for applications utilizing microwave dielectrics. However, the synthesis and crystallography of double perovskites containing Te (VI) has not been extensively discussed in the chemical literature. We prepared six A₂BTeO₆ double perovskites, where A is one of the heavier divalent alkaline earth metal cations (Ca, Sr, or Ba) and B is either Ca (II) or Cd (II). Their crystal structures were determined by Rietveld refinement of X-ray powder diffraction data. This poster will focus on comparing the crystal structures of the six closely related double perovskites.

Abstract #7

**Iron Levels in Relation to Cacao Concentrations in Dark Chocolate**

Aubrey Graham, Jordan Lester, Hannah McAfoos, Amy Marszalek, Joshua Stratton, and Kelly Gierlus

Chemistry Department, St. Ambrose University

Chocolate has been increasingly marketed as a food beneficial to one’s health despite its traditional reputation as “junk food.” Iron is essential to human life due to its role in hemoglobin and myoglobin production. The recommended daily value is 18 mg based on a 2,000 calorie diet. Chocolate samples of Ghirardelli and Lindt containing varying levels of cacao were ashed and dissolved in 1M nitric acid. The iron content was measured using flame atomic absorption spectroscopy. It was determined that to meet the recommended daily value, one must consume between 160 g and 880 g of dark chocolate (between 4 and 22 servings) depending on the percent cacao in the sample. In the Ghirardelli brand of chocolate, higher cacao concentrations coincided with increasing levels of iron, while the Lindt brand did not exhibit this trend. Future research should include an iron recovery study to further investigate why the iron values measured in the Ghirardelli chocolate were consistently lower than the values listed on the nutritional labels. Additional studies may determine why the Lindt brand of chocolate did not follow the expected pattern and investigate the sources of cacao and other sources of iron in the ingredients.
Abstract #8

**Investigating the Mechanism of Furfural Inhibition in E. coli**

Keri Hannie, Skyler Johnson, Maxwell Holle, Laura Moore, and Audra Sostarecz
Chemistry Department, Monmouth College

A current challenge in the production of biofuels from cellulosic biomass is to develop strains of E. coli that can be grown in the presence of toxins that are found in the biomass. Furfural is a cellulosic breakdown product that is found in processed biomass that is known to inhibit growth of E. coli. It has been suggested that furfural causes single-stranded DNA breaks in E. coli, membrane disruption of the cell, as well as an intracellular pH drop that all lead to cell death. In this study, we describe the isolation of genes from metagenomic libraries that appear to give tolerance to furfural using an enrichment cycle and a plate selection method. In addition, furfural interaction with a model cell membrane system was examined using Langmuir Blodgett technique. Genes isolated from the metagenomic library to this date all contained aminoglycoside 3’-phosphotransferase, an enzyme that provides kanamycin resistance in the plasmid and not to furfural. Early studies suggest furfural does not affect the properties of the model cell membrane. Both experiments help gain understanding of developing strains of E. coli for biofuel production.

Abstract #9

**An Investigation of the Physical Properties of Spirulina pacifica C-Phycocyanin**

Andrew Kendell and Mark Sinton
Department of Natural and Applied Sciences, University of Dubuque

C-phycocyanin (CPC) is a photosynthetic protein found in many species of blue-green algae. The function of CPC is to transfer light energy to a chlorophyll reaction center as part of the photosynthetic light harvesting photosynthetic complex. While CPC has been isolated and extensively studied from a variety of blue-green algae, little is known about the physical properties of CPC from Spirulina pacifica, even though it has been suggested that S. pacifica is the best source from which to isolate the protein. Following the isolation procedure of Patel (Patel, Mishra, Pawar, & Ghosh, 2004), CPC was isolated from S. pacifica, and its physical properties investigated. The mass of S. pacifica CPC was about 17 kD as determined by gel electrophoresis, and is similar to the masses reported for other blue-green algae. However, while CPC from other species is composed of multiple α and β subunits that have different masses, our electrophoretic analysis indicated that S. pacifica CPC is composed of only one subunit, or in the alternative, two subunits that have the same mass. Further, intrinsic fluorescence studies of S. pacifica CPC indicate that the protein resists denaturation over a wide range of sodium chloride concentrations and pH values.
Abstract #10

The Oxidation of a-Crystallin Len Protein Resulting from Xanthurenic Acid Radical

Chris Knutson, Carley Folluo, and Brad Sturgeon
Department of Chemistry, Monmouth College

The concentration of the tryptophan metabolite xanthurenic acid (xan) increases in the eye with age. The photo-excitation of xan in the presence of the a-crystallin lens protein has been shown to result in the polymerization of the a-crystallin, hence a possible mechanism for the formation of cataracts. An alternative mechanism for the role of xan, in the formation of cataracts, is the 1-electron oxidation leading to the xan radical. This poster will present ESR data showing the detection of xan radical formed from peroxidase/H₂O₂. Additionally the detection of peroxidase-associated polymerization of a-crystallin will be presented.

Abstract #11

Concentration of Vitamin E in Various Oils

Lauren McDonough, Izzy Hoffman, and Karen Glover
Chemistry Department, Clarke University

The goal of this experiment was to find a method of analysis of vitamin E, scientifically known as tocopherol, using the HPLC (high performance liquid chromatography) instrument. This instrument separates a sample by its attraction to a solid support inside a steel column, while a solution moves the samples along. The time it takes is measured and compared to known compounds to determine its identity. Vitamin E is a hydrocarbon product of photosynthetic organisms such as plants. The type of vitamin E that was analyzed is alpha-tocopherol which is only one type; others include: gamma-, beta-, and sigma-tocopherol. The method was tested to determine the amount of vitamin E in various oils and spreads, and the results were compared with the FDA (food and drug administration) for accuracy. A standard curve was made using synthetic alpha-tocopherol to find the concentrations of vitamin E in the samples. Olive oil and Sunflower oil had the highest concentrations of vitamin E.
Abstract #12

**Site Specific N-Methylation of Arginine Residues within Arginine and Tryptophan Rich Peptides**
Drake Mellott, Paris Barnes, and Anne Rammelsberg
Chemistry Department, Millikin University

Peptides rich in arginine and tryptophan residues exhibit potent anticancer and antimicrobial activities. Furthermore, many peptides rich in arginine and tryptophan are known cell-penetrating peptides (CPPs) and exhibit a high potential for cell entry. Arginine methylation of various proteins can control cell proliferation, migration, apoptosis, and disturbances in cellular homeostasis. Modification of known antimicrobial and anticancer peptides via site-specific methylation may prove fruitful in the search for novel peptide based drugs. Arginine and tryptophan rich peptides synthesized via Fmoc/t-Bu chemistry included RR(Me), WR(Me)W, RWR(Me). Different methodologies for site-specific arginine methylation were explored, including o-NBS methylation and N-trifluoroacetamide selective on-resin N-methylation.

Abstract #13

**Peptide Binding to Nanoparticles: Synthesis of Al₂O₃ Nanoparticles and Optimization of Primary Amine Quantitation**
Madeleine Meyer, Marco Torelli, Thomas Kuech, Joel Pedersen and Robert Hamers
Department of Chemistry, University of Wisconsin- Madison

Aluminum has long been recognized as a potential neurotoxin. Though exposure to the general public generally occurs in the form of aluminum oxide (Al₂O₃) at the oxidized surface of solid aluminum, nanoparticulate Al₂O₃ is also found abundantly in many commercial products, such as sunscreen, cosmetics, polishing abrasives, and paint. Due to their very small size, Al₂O₃ nanoparticles could conceivably cause misfolding in proteins. The wide use and potential toxicity of Al₂O₃ nanoparticles highlights the importance of understanding how these particles might interact with biological systems. Specifically, we seek to study how nano-Al₂O₃ might interact with and disrupt protein conformation by studying particle interactions with model peptides. Required for this study are size controllable and well-characterized nano-Al₂O₃, as well as a means to measure peptide binding at low concentrations in situ.

To provide systematic study of nano-alumina, we synthesized Al₂O₃ nanoparticles at sub-30 nm sizes through a sol-gel method and characterized these particles by Fourier transform infrared spectroscopy, powdered X-ray diffraction, dynamic light scattering, and laser Doppler micro-electrophoresis. In addition, we demonstrate the importance of optimizing conditions to perform a quantitative primary amine detecting fluorescamine assay and provide a systematic means to do so, thereby lowering the obtainable detection limit. Subsequently, binding isotherms of peptide to nano-Al₂O₃ to peptide can be determined.
Abstract #14

**Comparison of Protein Carriers of the CA-19-9 Antigen in Biological Fluids from Pancreatic Cancer vs. Controls**

Kaitlyn A. Miller,¹ Jana M. Rocker,² and Lewis K. Pannell²

¹Monmouth College and ²Mitchell Cancer Institute, University of South Alabama

Known for a survival rate less than 5%, once metastasized, pancreatic cancer is amongst the deadliest cancers in the world. There has been no significant improvement in disease prognosis in the past 20 years. Early diagnosis is the best approach to improve patient survival. However, over 80% are diagnosed only after the cancer has metastasized and the tumor becomes inoperable. New and better detection of this disease is needed. One procedure that is currently being implemented to improve early detection is the proteomic analyses. Proteomics attempts to find suitable biomarkers to identify proteins present in the early stages of cancer. The most successful biomarker to date has been cancer antigen CA-19-9. CA-19-9 has been found to have the highest sensitivity and specificity, ranging between 69-98.5%. To achieve a biomarker that has much better sensitivity and specificity rating, supplementary methods are need to be found. Rather than analyzing all proteins in a sample, this research aims to only analyze bowel fluids for proteins carrying the CA19-9 antigen. This research may drastically improve the early detection rating.

Abstract #15

**Phragmatopoma lapidosa cDNA Library Construction and Biocement Protein Exploration**

Ashley Rackow, Kasey Lierz, Caleb Miller, Austin Ciesielski, Marissa Franke, Grant Cooling and Maria A. Dean

Chemistry Department, Coe College

Phragmatopoma lapidosa is a polychaete worm that lives in the intertidal zone along the eastern Atlantic coast that secretes a biocement to adhere grains of sand, forming a protective tube. The biocement of P. lapidosa was specifically chosen for this study because of its unique ability to harden and endure in seawater. The goal of the project was to isolate and sequence genes responsible for composing the biocement. Strongly skewed amino acid compositions enriched with glycine (G), tyrosine (Y), and serine (S) were found in repeating peptide motifs (GAGY, SRSR, and SSGYG). Through the construction and analysis of a cDNA library seven new biocement proteins and 65 other proteins were discovered.
Abstract #16

Analysis of Levels of Caffeine in Pre-workout Supplements by Gas Chromatography-Mass Spectrometry
Jessica Richter, Kory Schmidt, Ziyad Thaljd, Tori Zlomie, Kelly Gierlus, and Joshua Stratton
Chemistry Department, St. Ambrose University

Caffeine is a nitrogenous, organic compound that occurs naturally and is found in many consumable products such as pre-workout supplements. Caffeine is said to be dangerous to human health if more than 100 mg per day are consumed. This study focused on the levels of caffeine present in powdered pre-workout supplements obtained from popular brands such as GNC and Cellucor. The pre-workout supplements were dissolved in 250 mL of deionized water, the recommended amount for one serving. The caffeine was then extracted with dichloromethane and analyzed using gas chromatography-mass spectrometry. Deuterated caffeine was used as an internal standard. Results show that the powdered pre-workout supplements tested have a caffeine content ranging from 91.7 mg to 615 mg, supporting the hypothesis that nearly all brands of pre-workout supplements tested have elevated, unhealthy levels of caffeine (>100 mg per day) present.

Abstract #17

Pectinaria gouldii cDNA Library Construction and Bio cement Protein Exploration
Kayla Rohr, Ashley Rackow, Caleb Miller, and Maria Dean
Chemistry Department, Coe College

Pectinaria gouldii is a benthic sea worm, which produces a protein-based bio cement that allows a protective cone to be created by fusing grains of sand together. The goal of the project was to isolate and sequence genes responsible for composing the bio cement. In order to better understand the organism and its ability to make this cement-like proteins, we extracted total RNA from fresh tissue samples. This total mRNA was purified before being transformed into a cDNA pool. DNA fragments were then isolated and inserted into bacterial plasmids, which were used to transform E. coli to complete the cDNA library. The cDNA was then amplified and isolated before it was sent for DNA sequencing. Sequencing results were analyzed via bioinformatics software and published to GenBank. DNA primers from previously isolated bio cement sequences were used to probe the cDNA, and three novel bio-cement gene sequences were identified. The protein sequencing was useful in peak assignments for analysis of the bio cement using Raman Spectroscopy.
Abstract #18

**Crystal Structures of $A_2B\text{TeO}_6$ Materials Under Ambient Conditions**

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Tellurium-containing solids are of interest to the solid-state chemistry community for their potential charge storage applications. A recent review of the chemical literature revealed that the crystallography of $A_2B\text{TeO}_6$ solids has not been studied extensively. Accurate crystal structure determination for a given compound is essential to understanding important structure-property relationships. Tellurium-containing materials where $A = \text{Ca}^{2+}$, $\text{Sr}^{2+}$, or $\text{Ba}^{2+}$ and $B = \text{Co}^{2+}$ or $\text{Zn}^{2+}$ were synthesized by conventional solid-state methods. Preliminary crystal structures of these materials were determined from X-ray powder diffraction data. Three of the compositions – $\text{Sr}_2\text{CoTeO}_6$, $\text{Ca}_2\text{CoTeO}_6$, and $\text{Sr}_2\text{ZnTeO}_6$ – crystallize with the double perovskite structure. $\text{Ba}_2\text{CoTeO}_6$ and $\text{Ba}_2\text{ZnTeO}_6$ adopt the 6L-trigonal perovskite-like structure. This work describes the crystal structures of $\text{Ba}_2\text{ZnTeO}_6$ and $\text{Sr}_2\text{ZnTeO}_6$ for the first time.

Abstract #19

**Stereoelectronics of Silyloxybenzoic Acids**

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Alkyl silyl groups, such as the trimethyl, triethyl, tert-butyldimethyl, and others, are merely regarded as effective protecting groups for labile oxygen groups such as phenols. Because of the sheer size of the silicon atom and the bulk added on to it by the alkyl and aryl groups this could force the lone pairs of the phenolic oxygen to twist out of the plane of the aromatic ring which effectively reverses the role of the phenolic oxygen from an electron-donating to an electron-withdrawing group. This study focuses on the potential of some *ortho-* and *para-* substituted benzoic acid silyloxy ethers to catalyse the Friedel-Crafts reaction between indole and β-nitrostyrene, as this reaction is sensitive to stereoelectronic changes in the benzoic acid catalyst.
Abstract #20

The Effect of Psychosocial Stressors on Cancer Biology in a Spontaneous Model of Heterogeneous Breast Cancer
Daniel Villalobos, Marianna Johnson, Suzanne Conzen, Martha McClintock, and Matthew Brady
Department of Medicine, The University of Chicago

Chronic stressors are reported to have substantial influences on breast cancer proliferation and metastasis. A heightened stress response in a transgenic murine model of triple negative breast cancer is associated with increased expression of key metabolic genes and a divergent mammary adipose tissue secretome in the mammary gland preceding the development of invasive tumors (1, 2). Furthermore, the secretome of isolated mice has been found to be more proliferative on mouse mammary epithelial cells representative of ductal carcinoma in situ (1). In this study, Sprague-Dawley (SD) rats, a spontaneous and heterogeneous model of breast cancer, were raised in group or isolated housing conditions in order to investigate the underlying mechanisms whereby psychosocial stressors alter the mammary microenvironment prior to breast tumor formation. Contrary to previous findings, the mammary glands from isolated rats (16 weeks of age, 12 weeks of social isolation) are more metabolically active, but have lower protein concentrations in their MAT’s secretome. Consequently, human mammary epithelial cells proliferate at a more rapid rate with the group-housed rat CM than with CM from the isolated rats. These findings suggest that protein concentrations in the MAT secretome are pivotal antecedents of breast cancer metastasis in SD rats. Determining the specific protein composition of the respective conditioned media may offer a greater understanding of psychosocial stressors’ effects on breast cancer proliferation.

Abstract #21

Photoredox biocatalysis via ruthenium polypyridyl artificial metalloenzymes
Chen Zhang, Andrew Ng, and Jared Lewis
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Visible light photoredox catalysis is an increasingly popular approach toward small molecule activation, an important goal of catalysis. A common class of photocatalysts are ruthenium polypyridyl complexes, which give stable, long-lived photoexcited states upon excitation by visible light. Though normally poor ground state oxidants/reductants, they exhibit potent single-electron transfer ability in the excited state. Recent work by Yoon, MacMillan, and Stephenson has spurred on renewed interest in photoredox catalysis. Our group is incorporating such photocatalysts into host protein scaffolds to create artificial metalloenzymes (ArMs), coupling the reactivity of the photocatalysts with the selectivity and adaptability of proteins. We are currently testing our biocatalytic system in aqueous environments for promotion of photocatalytic activity for reactions such as D/L-selective enone cyclization and photooxidative addition. Studies on the electron transfer mechanism within proteins are also being conducted.
Keynote Address

Expanding Research Frontiers: Food Questions for a New Millennium
Dr. Sunil Malapati, Clarke University

Abstract

The world of food poses unique challenges and opportunities for a chemist. There are “big” issues like ensuring adequate and safe supplies of food and water, sustainability practices to reduce waste, designing new foods and flavors to appeal to a modern consumer, and many others. On the smaller scale, chemists have to develop methods to detect adulterated foods or mislabeled foods, detect toxins or allergens that may be present in picogram quantities, etc. Some of our research projects at Clarke have involved detecting goat milk tampered with hydrogen peroxide and developing an analytical tool to detect adulteration of cranberry juice with beet juice or grape juice. In this talk, I will share some of the food scenarios that have inspired our projects and expand to some of the bigger issues.

Biography

Dr. Sunil Malapati, associate professor of biochemistry at Clarke, developed a fascination with food early on and cultivated an expertise during the past decade. In addition to conducting multiple cooking shows in Dubuque as a chef trained in South Indian cuisine, Sunil developed and continues to teach a course in food chemistry as a way to introduce science to non-science students. He conducts an annual NSF (National Science Foundation) sponsored week-long workshop on food chemistry for faculty from across the nation, and has done presentations and mini-workshops at national conferences. He is currently working on curriculum development for the Food Science degree at Clarke and food science summer camps for middle school students. His current research interests include food authentication and the science behind the development of cuisine, especially the influence of history and geography and the incorporation of new foods. Dr. Malapati has a Masters in Chemical Engineering from Indian Institute of Technology, Mumbai and a doctorate in Biology from Northwestern University, Evanston, IL. His thesis work was on signaling in the immune system. He currently teaches biochemistry, food chemistry and chemistry for health sciences. His educational pedagogy focus is on technology-enabled discovery-based learning in the classroom.

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