



# Abstracts

## Regional Undergraduate Poster Competition

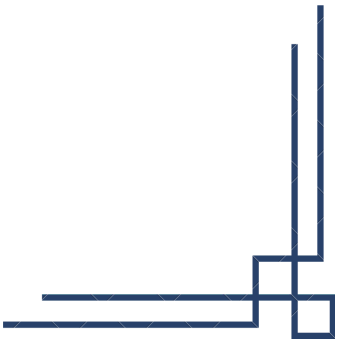
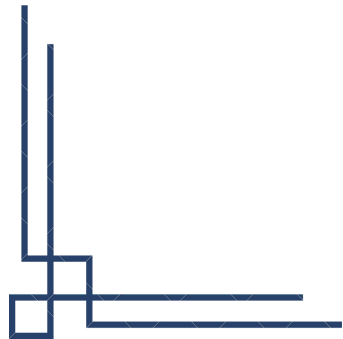
Jacobs Science Building

March 29, 2024

11:30am-4:00pm



University of Kentucky  
Department of Chemistry  
Lexington, KY 40508



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\*Group A presents from 12:00pm to 1:30pm

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# 1

## Generating Tools to Examine Energy Conserving Biochemical Reactions

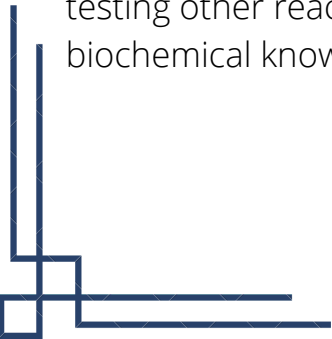
**Hena Kachroo, Junior, Chemistry, University of Kentucky**

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Anne-Frances Miller, Chemistry, University of Kentucky

### Abstract

The electron transport flavoprotein (ETF) found in mitochondria mediates transfer of electrons in respiration. However anaerobic bacteria such as *Acidaminococcus fermentans* possess a different type of ETF, which is able to execute electron transfer bifurcation. *A. fermentans* ETF (AfeETF) couples two electron transfer reactions, producing a more energetic product than the starting material. This is a newly recognized mechanism that naturally conserves energy at the level of electron flow. Thus, the ETF protein is a valuable source of insight for creating novel materials and devices to capture and store energy. The knowledge of how ETF conformational (open or closed) changes are coupled to the reactivity of its cofactor flavin is essential for understanding how to make the electron flow of such reactions more energy efficient. This project aims to test small extensions to the ETF proteins, that will act as steric doorstops, to hold the protein in its closed or open conformation. These extensions are small polypeptide chains that will be attached to the N terminus or C terminus subunit of the AfeETF. Failure of the new constructs to fold properly will be observed via diminished yield or protein fractionation into the insoluble phase after expression, via SDS PAGE. Integrity will be assessed via the stoichiometry of bound flavin and their optical spectra. Being able to hold the conformation in the open or closed state will in turn allow us to control ETF conformation while testing other reaction variables for energy efficiency. Thus, this project will provide key biochemical knowledge to harness biological reactions for sustainable energy solutions.



# Resoration of the Counterregulatory Response to Hypoglycemia by Avoiding Hypoglycemia

**Ashlee Marksbury, Junior, Chemistry, University of Kentucky**

Megan Music, Internal Medicine, University of Kentucky | Bansi Patel, Internal Medicine, University of Kentucky  
Lily Schoeder, Internal Medicine, University of Kentucky | Zachary Beckner, Internal Medicine, University of Kentucky  
Andrea Woodcox, Internal Medicine, University of Kentucky | Micah Devore, Internal Medicine, University of Kentucky  
Erica Macon, Internal Medicine, University of Kentucky | Simon Fisher, Internal Medicine, University of Kentucky

## Abstract

It is unclear whether the blunted counterregulatory response to hypoglycemia can be restored. The goal of this experiment was to determine if the blunted counterregulatory response to hypoglycemia (due to recurrent hypoglycemia) could be restored by avoiding hypoglycemia. Therefore, 10 week old Sprague -Dawley rats underwent a recurrent hypoglycemic conditioning protocol. The hypothesis is that over time, the avoidance of hypoglycemia would allow for the counterregulatory response to be similar to control animals. Animals were randomized into four groups: recurrent saline (RS, n=2), recurrent hypoglycemia (RH, n=3), 1-week post-RH (1wk, n=3), and 3 weeks post-RH (3wk, n=2). All rats underwent a hyperinsulinemic-hypoglycemic clamp. By experimental design, blood glucose during the clamp was similar between experimental groups. Glucose infusion rates for groups 1wk and 3wk were significantly greater than the RH group (p-values <0.0001 and 0.0065, respectively). The 3wk groups also showed an increase in peak epinephrine levels compared to the RS, RH, and 1 wk groups, however, there is not a high enough n value to determine significance. The mean basal epinephrine levels for RS, RH, 1wk, and 3wk were 296.6, 195.4, 434.3, and 261.1 pg/mL, respectively. The mean peak epinephrine levels for RS, RH, 1wk, and 3wk were 3274, 3430, 3032, and 9357 pg/mL respectively. In summary, data indicates that there may be some restoration to the counterregulatory response 3 weeks after RH based on peak epinephrine levels. However, there are not enough n values to achieve statistical significance. Additional experiment will need to be done in the future to fully analyze all data.

# Differentiating the Three Most Stable 2,2,3,3,3-pentafluoro-1-propanol Conformers using Matrix Isolation FTIR Spectroscopy

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Annalisa Duree, Chemistry, Rose-Hulman Institute of Technology

Caitlin Hriljac, Chemistry, Rose-Hulman Institute of Technology

## Abstract

As a part of 10-week research rotation course at Rose-Hulman Institute of Technology, the relative stabilities of the three most stable monomeric 2,2,3,3,3-pentafluoro-1-propanol (PFP) conformers were explored experimentally using matrix isolation FTIR spectroscopy based on the results of a previously reported microwave study. We have conducted theoretical study on these conformers not only to confirm the relative stabilities and abundances reported by Xu et al [1] but also to simulate corresponding FTIR spectra at the B3LYP/6-311+G(d,p) level of theory. The bulk of time in this project was used to optimize the experimental parameters (sample temperature and deposition time) involved in recording the matrix isolation FTIR spectrum in order to reduce the width of the vibrational bands to acceptable 2-5  $\text{cm}^{-1}$  range so that we can differentiate the peaks from different conformers. Once the optimal conditions were found, the recorded spectrum was compared with the theoretical spectra for conformers I, II, and III to determine if there was evidence indicating the presence of more than one of these conformers. The presence of peaks specific to conformers I and II were a testament of their presence meaning that at least two conformers could be observed. No significant evidence of conformer III was found.

## REFERENCES

1. Wu, B.; Seifert, N. A.; Insausti, A.; Ma, J.; Oswald, S.; Jäger, W.; Xu, Y. 2,2,3,3,3- Pentafluoro-1-Propanol and Its Dimer: Structural Diversity, Conformational Conversion, and Tunnelling Motion. *Phys. Chem. Chem. Phys.* 2022, 24 (24), 14975–14984. <https://doi.org/10.1039/D2CP01895K>.

# Investigation of the Emissive Properties of Low Dimensional Lead Free Hybrid Materials

**Chloe Shamel, Senior, Chemistry, University of Kentucky**

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Ali Costello, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky

## Abstract

Hybrid organic-inorganic metalates (HOIMs) are hybrid materials composed of organic cations and inorganic anions, designed to exploit properties of both ions while improving their overall stability in the solid state. It is important to tailor band alignment to the application by choosing a Halide Perovskite to pair with the organic semiconductor. There are two common types of HOIMs type I, used for light emission, and type II, used for charge separation. In inverse type I HOIMs the organic semiconductor band is smaller than the halide perovskite band and emits light. This experiment aimed for an inverse type I HOIM where our organic core will emit light. We hypothesized that the fluorescence quantum yield and lifetime of organic emitters based on 1,8-naphthalene imide would improve upon inclusion in ZnCl<sub>4</sub>-based HOIMs. To test this, 1,8-naphthalene imide-based cations were synthesized and characterized via NMR and UV-Vis. We then attempted to grow crystals and measured their fluorescence in solution and as thin films. From those findings we concluded that including the organic emitter in an HOIM with ZnCl<sub>4</sub> did not improve their emissive properties. Future work is focusing on different organic emitters and different inorganic metalates.

# Development of High-Porosity Polymers for Cysteine Capture

**Srija Badireddi, Sophomore, Chemistry, Centre College**

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Ward Alafef, Chemistry, Centre College

Mehak Mittal, Chemistry, Centre College

Andrew Hitron, Chemistry, Centre College

## Abstract

Oxidative stress triggers a variety of chronic and degenerative health conditions, ranging from cancer and rapid aging to diseases affecting cardiovascular, neurological, respiratory, and renal health (Pizzino et al., 2017). This research focuses on developing high-porosity, surface-functionalized polyacrylamide-based cryogels to capture cellular cysteine, an early indicator for oxidative stress. Cryogel beads with the desired structural results were prepared through the pre-freezing method described by Savina et al. [2] with a higher relative concentration of the cross-linker N,N'-methylene bisacrylamide to the acrylamide polymer. Current work involves functionalizing acrylamide polymer chains through a three-step reaction pathway that modifies amide ends to aldehydes, thiols, and activated disulfides successively.

## REFERENCES

1. Pizzino, G., Irrera, N., Cucinotta, M., Pallio, G., Mannino, F., Arcoraci, V., Squadrito, F., Altavilla, D., & Bitto, A. (2017). Oxidative Stress: Harms and Benefits for Human Health. *Oxidative medicine and cellular longevity*, 2017, 8416763. <https://doi.org/10.1155/2017/8416763>
2. Savina, I. N., Ingavle, G., Cundy, A. B., & Mikhalovsky, S. V. (2016). A simple method for the production of large volume 3D macroporous hydrogels for advanced biotechnological, medical and environmental applications. *Scientific Reports*, 6(1). <https://doi.org/10.1038/srep21154>

# Application of Diffraction Techniques for the Characterization of Transition Metal Oxide Nanomaterials

**Rachel Moscona, Senior, Chemistry, University of Kentucky**

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Beth Guiton, Chemistry, University of Kentucky

Manisha De Alwis Goonatilleke, Chemistry, University of Kentucky

Ireshika Wickramasuriya, Chemistry, University of Kentucky

## Abstract

As many technologies have decreased in size to the nanometer length scale, a concurrent increase in demand for these technologies has occurred. Nanotechnology approaches are popular in many industries for their use (for example) in green chemistry, and in health care treatments. A grand challenge, and also opportunity, researchers face in the development of nanoscale technologies are the changing characteristics of materials when scaled down to the nano-size. Determining the physical and chemical properties of materials on the nanometer length scale will aid in the mass production of nanotechnology. To characterize nanomaterials, researchers use a myriad of techniques, among them diffraction, using either electromagnetic radiation (e.g. optical microscopy, X-ray diffraction) or particle waves (e.g. transmission electron microscopy, neutron diffraction) as the illuminating source. The objective of this project is to apply diffraction techniques to characterize transition metal oxide nanomaterials. The diffraction techniques used for this work were powder X-ray diffraction (XRD), and Fast Fourier Transformation (FFT) analysis of high-resolution transmission electron microscopy (HRTEM) data. XRD patterns provided crystalline phase identification, and FFTs extracted from HRTEM data were used to determine the structure, phase, and growth direction of the nanomaterials. The discussion herein focuses on the signal production for XRD and HRTEM FFTs and methods by which researchers interpret the data. Analysis of the XRD data showed phase differentiation of two iron oxide samples and determined them to be Akaganeite ( $\beta$ -FeOOH) and Maghemite ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>). The HRTEM FFTs determined the growth direction and crystal structure of a Au catalyst-pure SnO<sub>2</sub> nanowire composite. The characterization of iron oxide nanomaterials and SnO<sub>2</sub> nanowires will contribute to the development of nanotechnologies for applications such as cancer therapeutics and solar cells.



# Fabrication and Theoretical Analysis of 2D Materials: Graphene and CrI<sub>3</sub>

**Eisen Wang, Junior, Material Science, University of Kentucky**

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Beth Guiton, Chemistry, University of Kentucky  
Douglas Strachan, Physics, University of Kentucky  
Kathryn Pitton, Chemistry, University of Kentucky

## Abstract

In our study, we present the fabrication process and theoretical analysis of two-dimensional (2D) materials, focusing on graphene and chromium triiodide (CrI<sub>3</sub>). The fabrication process involved the utilization of mechanical exfoliation technique, a reliable method for obtaining mono- and few-layered flakes of 2D materials. Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, and CrI<sub>3</sub>, a layered material with intriguing magnetic properties, were both successfully exfoliated to mono- and bi-layered flakes.

In the field of condensed matter physics, there is a burgeoning interest, particularly in the analysis of 2D materials. Building upon the extensive prior research, our study seeks to trace the footsteps of past investigations to gain a comprehensive understanding of this kind of materials. Our research involves to use Scotch tape to peel off the thin layer graphene and apply the stamping process by micromanipulator to fabricate the specimen, then employing theoretical analyses to unveil their structural, electronic, and magnetic characteristics (although those were discovered quite a long time).

Consistent with established findings, Utilizing Density Functional Theory (DFT) calculations, we delve into the electronic band structures, density of states, and magnetic properties of both graphene and CrI<sub>3</sub>. We saw the remarkable electronic properties of graphene, characterized by its distinctive Dirac cone-shaped band structure and high electron mobility. Additionally, we analyzed the electronic bandgap and magnetic behavior of mono- and bi-layered CrI<sub>3</sub>, demonstrating the emergence of ferromagnetic ordering in the bi-layered configuration due to interlayer magnetic coupling.

Moreover, we conduct a relatively comprehensive analysis of bilayer twisted graphene, tBLG, systematically varying the twist angle between the layers. Our theoretical calculations unveil the formation of Van Hove singularities in the electronic density of states, indicative of the presence of flat bands near the Fermi level at specific twist angles, consistent with prior research. Furthermore, our investigation extends to investigate the electronic and magnetic properties of tBLG across various twist angles, giving insights to us into its potential applications in unconventional superconductivity and correlated electron systems.

Overall, our study provides valuable insights for us into the fabrication techniques and theoretical analysis of 2D materials, shedding light on their unique properties and potential applications in future nanoelectronic devices.

# Presentation Elucidating Amiloride-based Small Molecule Recognition of SARS-CoV-2 Regulatory Structures

**Kanika Chopra, Senior, Chemistry, Transylvania University**

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TinTin Luu, Chemistry, Duke University

Martina Zafferani, Chemistry, Duke University

Shinya Suzuki, Chemistry, Duke University

Amanda Hargrove, Chemistry and Biochemistry, Duke University

## Abstract

The COVID-19 pandemic demonstrated the imperative need for novel antivirals to prevent any future coronavirus outbreaks. SARS-CoV-2, a positive-sense single-stranded RNA virus, is the causative agent of COVID-19. The 5' untranslated region (UTR) of this RNA is evolutionarily conserved and previously determined to be implicated in viral replication. Recently, small molecules featuring an amiloride-based scaffold have been found to inhibit SARS-CoV-2 viral replication by targeting this region. However, the mechanism of action of these small molecules with SARS-CoV-2 5' UTR secondary structures still requires further investigation. In this study, we evaluated the binding activity of novel amiloride small molecules with stem loop (SL) 1 and 5A of the 5' UTR. SL1 and SL5A were both previously determined to have bulges and apical loops, structural characteristics amilorides have preferential affinity for. As a result, SL1 and SL5A are attractive targets for small-molecule targeting of SARS-CoV-2 RNA. Through fluorescent indicator displacement assays (IDA), our findings demonstrated preliminary structure-activity relationship trends specifically at the C6, C5, and newly accessible C3 positions on the pyrazine core. Our findings will advance the expansion and tuning of our current amiloride library. We anticipate these amilorides to be chemical probes to further understand SARS-CoV-2 RNA biology and small-molecule targeting of viral RNA motifs.

# Synthesizing a Copper-Atom Catalyst for Use in Clean Energy Conversion Technologies

**Jenna Rector, Senior, Chemistry, University of Kentucky**

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Prakhar Sharma, Chemistry, University of Kentucky

Doo Young Kim, Chemistry, University of Kentucky

## Abstract

The electrocatalyst is pivotal in determining the cost and efficiency of clean energy conversion technologies. Current noble-metal catalysts have certain limitations preventing them from being implemented on a global scale. First, these catalysts are not cost effective due to low metal utilization. Second, they involve a large wastage of metal due to the oxidation and dissolving of bulk metal during electrolysis. Third, the surface-level attachment of metal to the carbon support is unstable shown by the removal of the metal during electrolysis. We proposed to combat these limitations by synthesizing a single-atom catalyst (SAC) using a common transition metal to replace noble- and bulk-metal catalysts. In our experiment, we used bottom-up synthesis and heat stabilization techniques to synthesize a copper-atom catalyst from a citric acid precursor. After confirming the SAC structure, we immobilized it onto a carbon backbone using a layer-by-layer technique. This technique allowed us to create a stable electrode with our SAC to undergo carbon dioxide reduction (CO<sub>2</sub>RR). Preliminary data shows evidence of an effective and economically viable catalyst to be used in a variety of clean energy conversion technologies.

# Design and Implementation of Parametric Amplifier for Transform-limited Ultrafast Laser Spectroscopy

**Jamoson Green, Senior, Chemistry, University of Kentucky**

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Shahnawaz Rather, Chemistry, University of Kentucky

## Abstract

A clear understanding of the mechanisms and dynamics of processes initiated by light in energy molecules and materials is crucial to developing their more efficient versions for next-generation photovoltaics, light-emitting diodes, photocatalysts, quantum gates sensors, etc. Typically, a light absorption event places energy into a system, and then depending on the properties of the system, that energy can be dissipated in many shapes and forms. The field of ultrafast laser spectroscopy has been at the forefront of studying photoinduced dynamical processes in molecules, materials, nanostructures, etc. This field encompasses many techniques that typically use a sequence of ultrashort laser pulses to resolve dynamics spectrally and temporally, thereby providing a comprehensive layout of the energy dissipation pathways. A big challenge in these techniques is the generation of ultrashort laser pulses. When we say, ultrashort laser pulses, we are speaking of less than 10-femtosecond (10<sup>-14</sup> sec) pulse widths. This extreme time resolution allows us to track excited state events as they unfold in real-time upon the absorption of a photon. Towards this goal, my task in the Rather lab has been to design and implement the technique of parametric amplification in a non-collinear setting to generate laser pulses with bandwidths that cover a large spectrum of white light. The advantage of a large spectral bandwidth is that it can be Fourier-transformed to a much smaller temporal width, by exploiting Heisenberg's uncertainty relation. My progress so far has been in the design and layout of all the optical components necessary for the non-collinear parametric amplifier (NOPA). In the next month, I plan to route the high-energy laser pulses from a laser amplifier into the NOPA for generation of spectrally broad laser pulses. Then, we will proceed towards temporally compressing these laser pulses to less than 10-femtoseconds.

# Effect of Anion Size in Electrochemical Doping Process on Thermoelectric Properties of Conjugated Polymer Materials

Carter Pryor, Junior, Chemistry, University of Kentucky

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Kenneth Graham, Chemistry, University of Kentucky

Augustine Yusuf, Chemistry, University of Kentucky

Kyle Baustert, Chemistry, University of Kentucky

## Abstract

Semiconductor technology is the backbone of the digital age. Semiconductors are the key components in the diodes and transistors that enable compact devices, in scientific instrumentation like X-ray detectors and Peltier coolers, and in energy technologies like solar cells. However, though traditional inorganic semiconductors are well-studied, they are expensive, structurally rigid, and made from rare elements like Germanium and Gallium. Novel organic semiconductors made from conjugated polymers have potential to generate semiconductors that are cheap, flexible, and not reliant on rare materials, but there is still much that is not understood about these materials. One important parameter for conjugated polymer semiconductors is the *counterion* used. Doping a conjugated polymer results in a net charge on the polymer backbone which must be balanced by a counterion entering the film. Existing literature is split on the effect of the counterion on the electronic properties of the film; some sources suggest that it has no effect, while others suggest that there is an influence. Understanding this discrepancy is further confounded by typical doping approaches, which use chemical doping, making quantifying the number of charge carriers in a polymer material difficult. To better understand the effect of the counterion, we investigated the spectroelectrochemistry of the conjugated polymers Blue-3 and PDPP4T by electrochemical doping using two electrolytes of different sizes – LiBF<sub>4</sub> and NaBARF. We then characterize the films by UV-VIS-NIR absorbance spectroscopy. The relative energies of peaks in the electronic spectra indicate that a larger counterion is associated with lower energy charges on the polymer backbone. Further characterization of Blue-3 by EPR Spectroscopy and measurement of its thermoelectric properties (conductivity, Seebeck coefficient) also indicated that counterion size plays a significant role in determining these properties, and that a lower energy charge is more delocalized along the polymer backbone. Our results demonstrate that counterion size is important for the electronic properties of conjugated polymer materials.

# Synthesis and Characterization of Novel Au(I) Complexes with a bis(diphenylphosphino)carborane Chelator as Anti-cancer Agents

**Emma Groetecke, Senior, Chemistry, University of Kentucky**

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Charles Grief, Chemistry, University of Kentucky

Samuel Awuah, Chemistry, University of Kentucky

## Abstract

Metallodrugs are attractive compounds for drug development due to their unique structures and efficacy as antineoplastic agents. However, due to limited target specificity and high toxicity, they often have side effects. Many approaches, including dual-targeting and smart delivery, have been employed to prepare novel metallodrugs with maximum efficacy and reduced systemic toxicity.

This research aims to synthesize a class of novel gold(I) complexes featuring a carborane chelator, an electron-delocalized molecular cluster that is easily functionalized at the carbon atoms. Previous findings have identified boron compounds as efficacious and tumor-selective radiotherapeutics, while gold(I) complexes exhibit potential in the treatment of various cancers. However, the clinical applications of gold-containing boron compounds remain largely unexplored. The addition of gold(I) to a closed-cage carborane framework can enable the anti-cancer potential of gold and boron to be simultaneously exploited while providing enhanced molecular tunability.

# An Attempted Synthesis of a Tetracene Based Dimer for the Study of Singlet Fission

**Mason Reeves, Senior, Chemistry, University of Kentucky**

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John Anthony, Chemistry, University of Kentucky

Karl Thorley, Chemistry, University of Kentucky

## Abstract

Beginning with TIPS-Bromo-pentacene and diphenyldiboronic acid, a palladium catalyzed Suzuki coupling was attempted in order to synthesize a dimer composed of two TIPS-pentacenes bound together by a diphenyl bridge, which in turn would be used for research on singlet fission. Singlet fission is the as of yet still mysterious process by which some molecules are capable of producing 2 triplet excitons per each photon absorbed. TIPS-pentacene has already demonstrated the capacity for performing singlet fission. Covalently linked dimers made up of 2 chromophores as a class of chemicals have as well. By synthesizing a covalently linked dimer composed of two TIPS-pentacenes, we are given the opportunity to observe singlet fission in a new molecule and further investigate its mechanism. By elucidating the mysteries behind what occurs in singlet fission and the ways it is affected by molecular structure, there is potential not only to further scientific understanding of the process but also hope of future industrial applications. Singlet fission presents the possibility of essentially doubling the efficiency of organic light emitting diodes as well as photovoltaic cells. In a future that continues to demand ever more energy to be generated and used, improving both power generation from solar as well as increasing the output from OLEDs holds obvious benefits for humanity. Results from MALDI and proton NMR suggest that the desired product was produced, but at no point was it successfully isolated. A pathway was determined that may lead to successful isolation in the future, but until such isolation is successfully performed, it can not be said for certain if the product was in fact produced.