# POSTER PRESENTATIONS

** Graduate Student    ** Undergraduate Student*

# Azide and Difluorocarbene: In Situ Generation of Azidodifluoromethide (N3CF2$^-$) and Addition to Electrophiles

**Colby Barrett,*** *Presenter*
**G.K. Surya Prakash,** *Principal Investigator*
**Department of Chemistry and Loker Hydrocarbon Research Institute,**
**University of Southern California**

**Abstract:** An essential component of biorthogonal click chemistry, of recent Nobel acclaim, is organic azide. Incorporation of fluorine atoms into these organic azides is quite rare in the literature, despite the well-established value of fluorinated moieties in biological contexts. We have thus developed a simple protocol for the in situ generation of N3CF2$^-$ and subsequent addition to aldehyde electrophiles, providing azidodifluoromethyl alcohols and silyl ethers. The scope of substrates and further reactions of the product azides will be discussed.

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# Poly(succinimide) and its Derivatives as Biodegradable Alternatives to Poly(acrylamide) in Hydraulic Fracturing

**Mason Cooper,**** *Presenter*
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**Department of Chemistry & Biochemistry,**
**University of California, Los Angeles**

**Abstract:** During hydraulic fracturing, non-biodegradable friction reducers such as poly(acrylamide) (PAM) are employed to reduce the friction built up between the pipe walls and the fracturing proppant (typically a sand and water mixture) in order to attenuate the wear that high flow rates inflict on these pipes. PAM remains in the wastewater produced from the proppant and it can degrade into its toxic monomer under typical hydraulic fracturing conditions; its monomer, acrylamide, is a neurotoxin and a carcinogen. This poses a threat to aquatic ecosystems and drinking water resources as wastewater can end up in waterways. The derivatized polymers of poly(succinimide) (PSI) have the potential to behave rheologically and tribologically similar to PAM and be more readily degradable than PAM due to the presence of amide groups in the polymer backbones. I modified PSI's structure to produce water-soluble polymers via ring-opening reactions with primary amine-containing reagents. The two PSI derivatives that I have studied are polyasparagine, derivatized with $NH_4OH$, and poly[(2-hydroxyethyl)-DL-aspartamide], derivatized with ethanolamine. Our rheology measurements show PAM can maintain a viscosity greater than 2 cP at high shear rates and these PSI derivatives can both maintain viscosities greater than 1 cP at high shear rates. This is a necessary property because proppants in wellbore pipes travel at high flow rates and the polymers need to maintain high viscosities to coat the inner wall of the pipes. Currently, the PSI derivatives are being tested in a friction flow loop system to gauge their tribological properties.

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# Quantitative Analysis of Alkenes in Alternative Fuels via Comprehensive Two-Dimensional Gas Chromatography

**Genesis Barzallo,* Hung Gieng,*** *Presenters*
**Petr Vozka,** *Principal Investigator*
**Department of Chemistry and Biochemistr,**
**California State University, Los Angeles**

**Abstract:** Over the previous several decades, there has been a substantial buildup of plastic waste in landfills and the environment, amounting to over 6 billion tons. Alternative fuels made from plastic waste can be produced using conversion techniques like pyrolysis and hydrothermal processing. The alkene (olefin) component of these fuels may vary from a few ppm to tenths of a wt. %. However, particularly at these high concentrations, there are presently no methods for the detailed quantitation of olefins. In this study, a derivatization process employing DMDS, and comprehensive two-dimensional gas chromatography (GC×GC) was employed for the characterization and quantitation of olefins in alternative fuels. This method was tested with olefin standards ranging from C6 to C24, as well as fuels made from plastic waste pyrolysis.

# Aqueous Base Promoted O-Difluoromethylation of Carboxylic Acids with $TMSCF_2Br$: Bench-Top Access to Difluoromethyl Esters

**Authors: Matthew Coe,*** *Presenter*
**G. K. Surya Prakash,** *Principal Investigator*
**Department of Chemistry and Loker Hydrocarbon Research Institute,**
**University of Southern California**

**Abstract:** A method for the synthesis of difluoromethyl esters from carboxylic acids is disclosed. This benchtop reaction uses $TMSCF_2Br$ as a difluorocarbene source and is air stable with mild conditions. The method was applied to aliphatic and aromatic substrates and showed compatibility with a variety of functional groups. Furthermore, difluoromethyl esters of pharmaceutically relevant molecules and APIs were successfully synthesized, demonstrating the potential for late-stage functionalization.

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# Simple Synthesis of a Ni–TiO2 Nanocomposite as an Enzyme–less, Amperometric Sensor for the Electrooxidation of Glucose

**Juan Pablo de los Rios,*** *Presenter,* **Vicente Galvan,**
**G. K. Surya Prakash,** *Corresponding Author Principal Investigator*
**Loker Hydrocarbon Research Institute, Department of Chemistry,**
**University of Southern California**

**Abstract:** The simple synthesis of a Ni–TiO2 nanocomposite supported on Vulcan carbon (XC–72R) for the electrochemical oxidation of glucose is reported. The binary catalysts, with varied Ni: TiO2 weight ratios, were characterized by X–ray diffraction (XRD), inductively coupled plasma optical emission spectroscopy (ICP–OES), X–ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and energy dispersive X–ray spectroscopy (EDS). Cyclic voltammetry studies in 0.1 M NaOH demonstrate that the four metal catalysts can effectively oxidize 1 mM glucose, with the 3:1 (60%) Ni to Ti nanocomposite yielding the highest current density. The 60% Ni–TiO2/XC72R catalyst was used to construct an enzyme–less, chronoamperometric sensor for glucose detection and monitoring in an alkaline medium. Using 50 μM aliquots of glucose at a potential of +0.7V (vs Hg/HgO), the sensor responded rapidly (< 3 s), provided a sensitivity of 3300 μA mM-1 cm-2, detection limits of 144 nM (S/N = 3), and excellent selectivity and reproducibility. The glucose aliquot concentrations were then increased to 1 mM to mimic physiological blood conditions of 1–20 mM. At a potential of +0.7V (vs Hg/HgO), the sensor continued to respond rapidly (< 1 s), showed a sensitivity of 273.7 μA mM-1 cm-2, detection limits of 3.13 μM (S/N = 3), and excellent selectivity and reproducibility. The catalyst also exhibited an ideal anti–poisoning capability to free chloride ions and negligible signals towards interfering species of 0.1 M ascorbic acid, uric acid, and lactic acid.

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# Visible-light Photoredox-catalyzed C(sp2)–H Difluoromethoxylation of (Hetero)arenes Utilizing a Shelf-stable Pyridinium Reagent

**Daniel Lin,*** *Presenter*
**G.K. Surya Prakash,** *Principal Investigator*
**Department of Chemistry and Loker Hydrocarbon Research Institute,**
**University of Southern California**

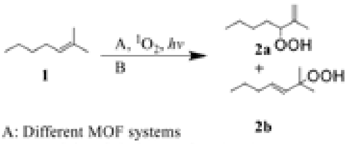
**Abstract:** Difluoromethoxyarene moieties have been demonstrated to impart desirable physio-chemical properties to organic molecules. Presented herein is a shelfstable radical difluoromethoxylating reagent that enables facile and direct C(sp2)–H difluoromethoxylation of (hetero)arenes under blue light photoredox catalysis. 4-cyano-1-(difluoromethoxy)pyridin-1-ium trifluoromethanesulfonate is prepared in one simple step from the parent pyridine N-oxide. The current protocol tolerates a variety of synthetically and pharmacologically relevant functional groups. Applicability towards the late-stage functionalization of API's and drug-like molecules is also demonstrated.

# Regiochemistry of the Singlet Oxygen Ene Reaction in Metal-Organic Frameworks

**Raymond Lo,**** *Presenter,* **Jin Hyeok Yoon**
**Matthias Selke,** *Principal Investigator*
**Department of Chemistry and Biochemistry, California State University, Los Angeles**

**Abstract:** Photooxidation of olefins leading to allylic hydroperoxides is a versatile reaction with various synthetic applications. However, when carried out in homogenous media, this reaction's potential is limited due to formation of different regioisomeric products. Studies in heterogenous media such as zeolites have previously been shown to lead to improved regioselectivity. In this work, the regiochemistry of singlet oxygen ene reaction was studied in metal-organic frameworks (MOFs). As catalysts, MOFs can both generate singlet oxygen and function as the active sites to influence the regioselective outcomes of the singlet oxygen ene reaction. We have utilized the photooxidation of 2-methyl-2-heptene to investigate the singlet oxygen ene reaction in MOFs. Product regioselectivity and yields have been studied for a variety of solvents systems and MOFs with different pore sizes.

Scheme 1. Singlet oxygen ene reaction carried out in MOF.



A: Different MOF systems
B: Aprotic/Protic/Mixture of Both solvents

# Does a Non-Phthalate Plasticizer Contain Phthalate?

**Yolanda McDow,**** *Presenter*
**Barbara Belmont,** *Principal Investigator*
**Department of Chemistry and Biochemistry,**
**California State University, Dominguez Hills**

**Abstract:** The plastic we use is naturally very stiff and brittle, so the modifying agents we use make plastics flexible and soft. The most common used plasticizers for these jobs were part of the phthalate compounds, but due to their link to endocrine disruption and possible fertility issues, these compounds have been banned in most of the consumer products used today. There are several alternatives to non-phthalate plasticizers available in the market, but DINCH comes at a particular interest. DINCH is composed of 1,2-Cyclohexane dicarboxylic acid diisononyl ester and isomers and is produced through catalytic hydrogenation of di-isononyl phthalate (DINP). The question arises as to whether DINCH contains detectible amounts of DINP, and if it does, are the levels significant to the toxicological regulations. A GC-MS method was used to separate the components of DINCH and a selected-ion-monitoring technique was used to determine to analyze the components for evidence of DINP. These components were compared to existing technical reports and regulations to determine whether the DINCH compound can be stated with statistical certainty that it does or does not contain toxicologically significant amounts of DINP.

# Analyzing Sand for Hydrocarbon Presence after Huntington Beach Oil Spill Using Solid-Phase Microextraction Gas Chromatography-Mass Spectrometry (SPME-GC-MS)

**Elena Mosham,* Kelly Nguyen,**** *Presenters*
**Petr Vozka,** *Principal Investigator*
**California State University, Los Angeles**

**Abstract:** On October 2, 2021, a pipeline connecting Long Beach and Elly drilling platform burst, and crude oil entered Huntington Beach, resulting in a ten-day beach closure. The public was skeptical after city officials stated that toxic compounds were not detected in ocean water ten days after the spill. This project aims to determine how hydrocarbon compounds in the Huntington Beach sand change monthly for a year using solid-phase microextraction (SPME) with a combination of gas chromatography-mass spectrometry (GC-MS). An Agilent 59778 GC/MSD was used to separate and detect compounds in each sand sample. A divinylbenzene/polydimethylsiloxane SPME fiber, capable of adsorbing volatile, amine, and nitroaromatic compounds, was found to be compatible with adsorbing the compounds of interest. The preliminary data shows that the number of compounds fluctuated as the year progressed. Notable hydrocarbon presence includes 2-methylindene (detected in October 2021), hexadecane, heptadecane, and octadecane (detected in December 2021), dodecane, tetradecane, pentadecane, hexadecane, and heptadecane (detected in January 2022), and 9-octadecene (detected in June 2022). The next step of this research is determining how the quantitation of the hydrocarbons detected changed throughout the year.

# Optimization of Thermo-Responsive Nanocarrier Drug Delivery System Under Simulated Blood Flow Conditions

**Victoria Sarkisian,**** *Presenter*
**Kasha Slowinska,** *Principal Investigator*
**California State University, Long Beach**

**Abstract:** Current cancer treatments include chemotherapy and systemic combination therapies. Unfortunately, these methods often lead to adverse side effects and exhibit non-selective toxicity to all tissues. This project seeks to eliminate these systemic effects by applying a thermo-responsive drug delivery system based on a peptide folding mechanism. The short peptide nanocarrier adopts inactive coil conformation (unfolded) at HIGH (37°C) temperature and a helix conformation (folded) at LOW temperature. Peptides in helix conformation can penetrate cell membranes and deliver cargo; here, a fluorescent tag (Fluorescein, FITC). Thus, inducing highly localized hypothermia in a targeted (tumor) area allows for activation of the helix conformation, administering the cargo to cancer cells only, and vastly reducing systemic side effects. We present a kinetic approach that mimics blood flow conditions in tumor proximity. We have exposed 3T3 Swiss mice fibroblast cells (model) to a range of flow rates, mimicking that of the blood flow rate in capillary veins. Temperature is monitored using an IR camera, and the delivery of cargo (FITC) is determined by fluorescent microscopy in tandem with flow cytometry. Static results have confirmed temperature specificity of peptide cargo delivery to cells. Preliminary kinetic data indicates that with a properly established temperature gradient, we can effectively demonstrate that the rate at which the peptide reaches active helix conformation is faster than the blood flow rate of capillary veins. Therefore, our method is a promising candidate for selective drug-delivery applications.

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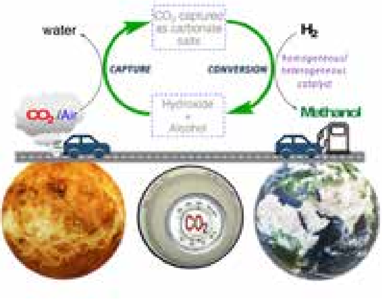
# Green Methanol for the Blue Planet:
# Novel Catalysis for Conversion of CO2 from Air

**Raktim Sen,*** *Presenter,* **Alain Goeppert,**
**G. K. Surya Prakash,** *Principal Investigator*
**Department of Chemistry and Loker Hydrocarbon Research Institute,**
**University of Southern California**

**Abstract:** With the objective of achieving carbon neutrality and a circular economy, recent years have witnessed the emergence of CO2 capture and recycling or utilization models (CCR or CCU), wherein CO2 released from various anthropogenic sources is captured and directed downstream as a C-1 building block for the production of a multitude of value-added chemicals and materials including methanol. Methanol, the simplest alcohol, is already used on a large scale (> 100 billion liters annually) with numerous key applications as an alternate fuel, fuel additive, hydrogen storage media, and a valuable carbon feedstock to produce various chemicals and polymers. Lately, there has been an increasing demand for methanol in several countries as fuel substitute (M100) and additive (M15, M85 in gasoline) in cars, buses, ships as well as a boiler and cooking fuel.

In the direction of chemical recycling of CO2, we have achieved the integration of the two steps: a) direct air capture of CO2 and b) conversion of CO2 to methanol, an emerging avenue in the field of Carbon Capture and Utilization/Recycling (CCU or CCR). We demonstrated that CO2 can be captured efficiently using alkali hydroxides under ambient conditions (room temperature and atmospheric pressure) from air. Notably, direct air capture (DAC) of CO2 is challenging, as ambient air contains only 0.042 % of CO2 (420 ppm CO2). The carbonate and bicarbonate capture products, without any purification and separation, were directly subjected to hydrogenative conditions in presence of catalysts to synthesize methanol, bypassing the energy intensive steps of desorption and compression of CO2 required in existing processes. Overall, such integrated systems synergize well with emerging DAC ecosystems and are promising pathways for renewable and carbon-neutral technologies.



# N-Bromosuccinmide-Methanesulfonic Acid, a Safe, Efficient, and Powerful Electrophilic Bromination System for Arenes

**Antonio Vasquez,*** *Presenter*
**G. K. Surya Prakash,** *Principal Investigator*
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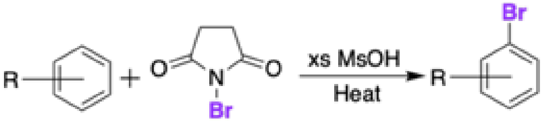
**University of Southern California**

**Abstract:** Electrophilic halogenation of arenes has been well studied. Given the myriad of applications for haloarenes, there still exists the need for an efficient method that allows for the safe and convenient halogenation of deactivated arenes. Methanesulfonic acid (MsOH) has been found to be an excellent Bronsted acid catalyst for this transformation. In conjunction with N-bromosuccinimide (NBS), activated and deactivated arenes were shown to undergo bromination in the presence of MsOH. Additionally, MsOH is safe, commercially available, and exhibits an impressive tolerance to many functional groups compared to other acid catalysts invoked for this transformation. The details of this study will be presented.



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# Lipidomic Analysis of Ceramide Synthases in Human Glioblastoma Multiforme Cells Resistant and Non-Resistant to Temozolomide Treatment

**Xiaohui Weng,* California State University, Fullerton,** *Presenter*
**Simone da Silva Rosa, University of Manitoba,** *Collaborator*
**Saeid Ghavami, University of Manitoba,** *Collaborator*
**Stevan Pecic, California State University, Fullerton,** *Principal Investigator*

**Abstract:** Glioblastoma multiforme (GBM) is a type of primary brain cancer with a low median survival of 15 months. Currently, the only FDA-approved chemotherapeutic agent for GBM is temozolomide (TMZ), an alkylating agent that initiates apoptosis. Our long-term goal is to understand how the regulation of ceramide synthases correlates with the development of chemoresistance as a result of TMZ-induced autophagy. Lipidomic analysis was used to compare the lipid distribution between TMZ-resistant and non-resistant U251 cells. A total of 30 lipids from 5 ceramide lipid subfamilies with various chain lengths were analyzed using ANOVA, heatmap, volcano plot, and VIP score. These analyses help visualize and identify the lipids that are up or downregulated in TMZ-resistant and non-resistant cells. The heatmap showed that 8 out of 30 lipids were downregulated, and 22 were upregulated in the resistant cells. Pair-wise comparisons from ANOVA identified at least one lipid from each ceramide subfamily that shows a statistically significant change between the cells. The volcano plot identified 4 lipids that are upregulated in the resistant cells. The results indicate that some ceramide synthases are up or downregulated in the GBM cells suggesting their involvement in the mechanism of TMZ resistance. Therefore, intervention in their synthesis pathways could provide therapeutic benefits. This study's results are significant because they provide insights into the lipid profiling of TMZ-resistant GBM cells. Furthermore, specific lipids are presented as potential drug targets for combination therapy to enhance the efficacy of TMZ treatment and therefore prolong the survival time of patients.

# Expansion Microscopy for Dual Imaging of Protein and RNA

**Jihyun Youn,**[*,1,2] **Wellesley College,** *Presenter*
**Chi Zhang,**[1]
**Edward S. Boyden,**[1,3,4,5,6,7,8] *Principal Investigator*

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**Abstract:** Expansion microscopy (ExM) enables nanoimaging with conventional optical microscopes by overcoming the diffraction limit through physical expansion. ExM works by anchoring biomolecules, such as proteins and RNAs, to a swellable hydrogel synthesized throughout cells and tissues, followed by mechanical softening of the specimen and isotropic hydrogel expansion to physically separate and decrowd biomolecules for better labeling and enhanced imaging resolution (Chen et al., 2015). However, current ExM variants (Wassie et al., 2019) do not allow imaging of multiple proteins and RNAs in the same specimen: the high-temperature alkaline treatments for protein ExM damage RNAs (Sarkar et al., 2022), while the strong proteinase treatments for RNA ExM destroy protein epitopes (Alon et al., 2021).

Here we optimized a range of biomolecule anchoring and sample softening conditions to enable multiplexed nanoimaging of proteins and RNAs in the same specimen. Specifically, we show that commercial epoxide and aldehyde-based reagents can anchor both proteins and RNAs to the hydrogel, followed by mild mechanical softening (e.g., site-specific enzyme digestion), allowing staining of proteins with antibodies and RNAs with fluorescence in situ hybridization probes, in RNA-protein complexes such as stress granule, which are involved in various biochemical processes and neuropathologies. We envision that this optimized protein-RNA dual imaging ExM will help to reveal nanoscale organizations of proteins and RNAs in diverse biological processes.

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