Abstracts

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MWRM 2026 MW28, MW101

***De novo* mini-protein binders for TREM2 associated with Alzheimer's disease**

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Alzheimer's disease (AD) is a neurodegenerative disorder characterized by the accumulation of amyloid-β (Aβ) plaques in the brain. Triggering receptor expressed on myeloid cells 2 (TREM2) is a microglial surface receptor essential for driving their ability to cluster around Aβ plaques and facilitate the clearing of these plaques. Apolipoprotein E (APOE) binds to the low-density lipoprotein receptor (LDLR) to facilitate the uptake of ApoE-lipoprotein particles. Several studies have shown that the binding of ApoE to TREM2 initiates a downstream intracellular signaling cascade that changes microglia to a highly neuroprotective phenotype known as disease-associated microglia (DAM), which drives microglia towards early Aβ deposits. However, TREM2 mutations can impair this clearance process, exacerbating AD progression. Consequently, TREM2 has emerged as a promising therapeutic target. Despite its clinical importance, a high-resolution molecular understanding of the complex remains elusive. We are developing de novo mini-protein binders targeting TREM2 utilizing AI-based design platforms, such as BindCraft and ODesign. These AI-driven platforms leverage deep-learning architectures to perform scaffold-based design and sequence optimization, allowing for the generation of high-affinity proteins that are computationally pre-validated for folding stability and target complementarity. We selected a few designs and synthesized them using solid-phase peptide synthesis (SPPS) and native chemical ligation (NCL). Following synthesis, we evaluated binding affinities via Microscale Thermophoresis (MST) and employed Circular Dichroism (CD) spectroscopy to analyze the secondary structure of each mini-protein, correlating structural integrity with binding capabilities. These de novo mini-proteins show binding to the hydrophobic tip of the TREM2 ectodomain, which is the same binding pocket for ApoE3 identified by intra- and inter-protein cross-links using chemical cross-linking mass spectrometry (XL-MS) analysis of

the ApoE3/TREM2ECD complex. These results establish a robust framework for developing mini-protein based TREM2 agonists.

MWRM 2026 MW405

In silico modeling of bispecific dual-affinity re-targeting (DART) molecules targeting PD-1 and LAG-3 for solid tumor and hematologic cancers immunotherapy

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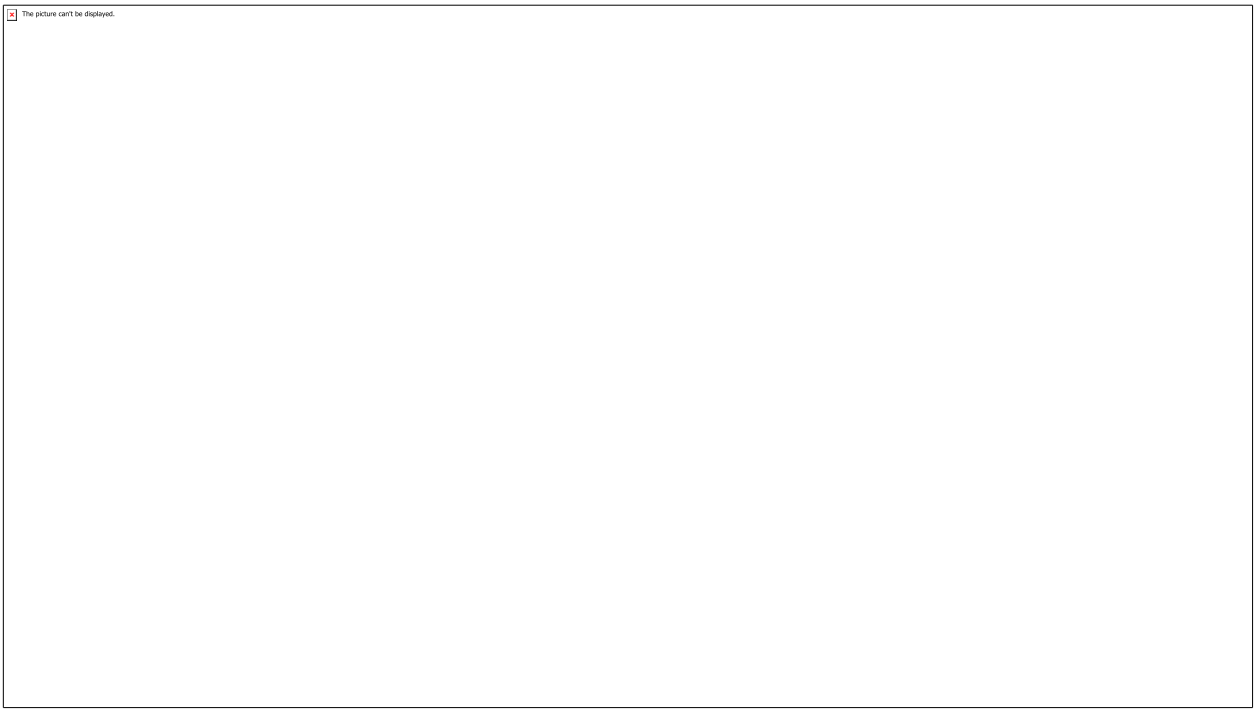
Solid tumors represent approximately 90% of adult human cancers and arise from the uncontrolled growth of cells in specific tissues or organs. Recently, immunotherapy that boosts the immune system's ability to fight cancer has gained significant attention. A promising therapeutic approach is the Dual-Affinity Re-Targeting (DART) molecule, which simultaneously targets two distinct immune checkpoint receptors to overcome immunosuppressive signaling and enhance immune system activation. DART can bind to two separate targets and simultaneously eliminate their inhibitory effects on the immune system. LAG-3 and PD-1 receptors are expressed on the surface of T cells, suppressing immune surveillance and thereby inhibiting their ability to recognize and attack tumors. We hypothesize that scFv 1p4i binds strongly to the LAG3 and 6uy3 PD-1 receptors, forming a bispecific DART that simultaneously increases immune activation in T cells. The receptors were modeled using the UniProt and AlphaFold 3 web servers. At the same time, 15 humanized single-chain variable fragments (scFv) were selected from the SAbPred web server and downloaded from the Protein Data Bank. In the next step, multiple configurations of the interactions between the receptors (LAG-3 and PD-1) and the scFv were computed and analyzed by the HDOCK and PLIP web servers. The receptor-scFv binding affinity was calculated to identify the most effective binding combinations (8dy1 and 6uy3) based on interaction strength and stability. Further mutational analysis was performed to enhance the binding energy of the selected candidate, and the results were subsequently validated through molecular dynamics simulations. Targeting inhibitory immune checkpoint proteins enables the efficient eradication of solid tumors and the rapid activation of an immune response against cancer cells, thereby paving the way for dual-targeted strategies that enhance therapeutic efficacy.

MWRM 2026 MW367

S. cerevisiae and *L. plantarum* co-fermentation improves fig wine quality: Identification of key aroma compounds via molecular docking and dynamics simulation

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Co-fermentation of Saccharomyces cerevisiae and lactic acid bacteria to improve fig wine quality and screen key aroma compounds. A co-inoculation strategy using S. cerevisiae and Lactobacillus plantarum at three ratios (1:1, 1:50, and 1:100) was employed. The physicochemical properties, color, volatile aroma profile, and sensory quality of the co-fermented fig wines were determined, and key aroma compounds were screened by integrating machine learning, network pharmacology, and molecular docking. Different inoculation ratios significantly affected the organic acid composition—including malic, lactic, citric, and succinic acids—and the overall color parameters of fig wine. The 1:50 ratio sample exhibited more thorough malic acid degradation, the highest lactic acid content, the lowest succinic acid content, superior overall color, and better mouthfeel with a more youthful color profile. Volatile compound analysis of the three wine samples revealed that increasing the L. plantarum inoculation proportion significantly increased the contents of esters, terpenes, and certain varietal aroma compounds, enhancing the aromatic complexity of fig wine. Twenty-nine key volatile aroma compounds were screened via PLS-DA, and six compounds—trans-β-ionone, phenethyl acetate, α-terpineol, terpinen-4-ol, D-limonene, and benzoic acid—were further identified through network pharmacology and molecular docking as major contributors to the pleasant aroma of fig wine. These compounds may participate in the formation of the pleasant sensory experience of fig wine through hydrogen bonding and hydrophobic interactions with olfactory receptors as well as dopamine- and serotonin-related receptors.



MWRM 2026 MW222

3-D printing as a responsive tool to pedagogical and laboratory needs

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Historically, if chemists need a demonstration model, a test-tube rack, a lab jack, or a pipette stand for micropipettes the paradigm has been to find one online and purchase it. The advent of 3D printing and accessible design software has created a new option: in some situations a temporary or even permanent solution to a problem can be generated in a day or less, obviating large costs and long shipping times, order approvals, and more. This work focuses on discussing a few problems, potential stumbling points, and some solutions generated to solve problems in both industry and academic settings. It also endeavors to raise awareness for a solution that is often cost- and time-effective.

MWRM 2026 MW347

Acetylcholine electrochemical assay derived from biohybrid cyclophane-based organic semiconductor frameworks for point-of-care testing to aid Alzheimer's disease diagnosis

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Acetylcholine (ACh) is a vital neurotransmitter involved in numerous physiological processes, and deficiencies in ACh have been associated with neurodegenerative disorders such as Alzheimer's disease. Current state-of-the-art detection methods primarily quantify ACh indirectly through the measurement of acetylcholine receptor antibodies or enzyme activity. Although electromyography (EMG) studies are effective, they are time-consuming and require highly specialized personnel to be performed. Therefore, a direct, rapid, and straightforward detection method is needed. Here, we utilize electrochemical impedance spectroscopy, cyclic voltammetry, and UV-visible spectroscopy to establish an electrochemical sensing platform using conductive polymers embedded with biocompatible cyclophanes which selectively bind ACh via non-covalent interactions with high sensitivity. The sensing platform demonstrated a sensitivity of 0.402° mM^{-1} for ACh detection while providing a rapid, point-of-care electrochemical readout. These findings establish an effective electrochemical sensing platform for the direct detection of acetylcholine and provide a foundation for the development of rapid, point-of-care diagnostic tools to aid in the early detection and diagnosis of Alzheimer's disease.

MWRM 2026 MW118

Acid-catalyzed non-reductive deoxygenation of biocrude

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Hydrothermal Liquefaction (HTL) is a promising thermochemical approach for converting wet biomass into energy-dense biocrude. However, the high oxygen content inherent to biomass feedstocks yields an unstable product, necessitating efficient deoxygenation mechanisms. While non-reductive pathways (dehydration, decarboxylation, and decarbonylation) bypass the need for external hydrogen and expensive metal catalysts, finding a solvent system that is chemically stable under the high temperatures (200-370°C) and pressures (5-25 MPa) required for HTL remains a major challenge, as the choice of stable solvents is extremely limited.
In this work, we investigated the use of trifluoroacetic acid (TFA) acting simultaneously as both the reaction solvent and the acid catalyst. Because of the highly corrosive and demanding nature of this strongly acidic, high-temperature environment, a novel experimental setup was custom-designed to safely and reliably carry out the HTL reactions. Preliminary spectroscopic evaluations demonstrated highly promising deoxygenation results; post-reaction analysis revealed a significant reduction in the -OH infrared absorption peak, while the characteristic C=O peak completely disappeared. These results indicate accelerated dehydration and decarbonylation/decarboxylation pathways facilitated by the TFA matrix. This study offers a new technical framework for executing harsh, acid-catalyzed HTL processes and highlights a viable solvent-catalyst strategy for upgrading heavy biocrude.

MWRM 2026 MW285

Activation energies and activation volumes for water dynamics in cryoprotectant solutions

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Cryoprotectant agents have been extensively studied to understand their role in freezing human and animal cells at cryogenic temperatures and recovering them with appropriate functionality. While significant gaps remain in understanding their behavior, their ability to alter water properties through hydrogen bonding is of particular interest. Hence, we consider a series of cryoprotectant candidates with varying properties, including dimethyl sulfoxide and glycerol, and examine water dynamics as a function of cryoprotectant concentration. The focus is on elucidating the underlying thermodynamic driving forces for the dynamics, with water diffusion as a key example. The activation energies for diffusion were calculated using the fluctuation theory for dynamics (FTD) approach, which determines the analytical temperature derivative of any rate constant

or timescale from single temperature simulations. In addition, the pressure dependence of the dynamical property was obtained by calculating activation volumes using FTD from the same simulations. To accelerate convergence of the calculated quantities, connections between the microcanonical and isothermal-isobaric dynamics were exploited.

MWRM 2026 MW284

Activation energies from single-temperature simulations: Insights into water dynamics

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Understanding how molecular dynamics respond to thermodynamic conditions is central to connecting microscopic behavior with macroscopic properties. We recently improved upon a general framework for computing activation energies from single-temperature simulations, overcoming the need for conventional Arrhenius analysis over temperature ranges. By leveraging energetic fluctuations and their connection to dynamical properties, this approach provides direct, efficient access to activation energies associated with rate processes such as diffusion. In application to neat, ambient liquid water, we demonstrated that the method robustly captures activation energies and non-Arrhenius effects for diffusion.
We extend this framework to supercooled water to probe the driving forces of the proposed liquid-liquid phase transition between high-density (HDL) and low-density (LDL) liquid states. Near ambient pressure, crossing the Widom line is expected to shift the system between predominantly HDL-like and LDL-like regimes. Using activation energies for diffusion and hydrogen-bond jump times, we identify changes in temperature-dependent dynamics that reflect the underlying behavior of the hydrogen-bond network.

MWRM 2026 MW63

Adapting organic reactions to flow chemistry: Synthesis of salen and octyl 3-phenylpropanoate

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Continuous flow chemistry has emerged as an attractive alternative to conventional batch synthesis by improving reaction efficiency, safety, and sustainability. In this research, two representative organic reactions, the synthesis of the classic Schiff-base, Salen and the ester, octyl 3-phenylpropanoate were successfully adapted from batch to flow conditions. Flow reactions were performed using syringe pumps and a tubular reactor under optimized operating conditions to achieve efficient mixing and controlled residence times. The synthesized products were characterized by FT-IR and proton and

^{1}H and ^{13}C NMR spectroscopy to identify their structures and purities. The flow method product yields were comparable to those obtained through conventional batch synthesis while offering improved reaction control and reproducibility. In addition, the flow method reduced reaction times, minimized manual handling of hazardous reagents, and enhanced heat and mass transfer throughout the reaction process. Furthermore, the use of continuous flow technology decreased solvent usage and chemical waste, demonstrating its alignment with the principles of green chemistry. Therefore, this study shows the potential of continuous flow chemistry as an effective and environmentally important for organic synthesis in educational, research laboratories and industrial applications.



MWRM 2026 MW34

Addressing heparin contamination risks: Exploring bovine-derived alternatives through collagenase-assisted extractions

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In recent years, there has been a need to re-evaluate methods for extracting heparin from alternative sources due to ongoing contamination issues in the Chinese production of porcine-derived heparin and projected increase in demand due to the aging population. While bovine and ovine heparins have been discussed as possible alternatives, their extraction processes have not been optimized, and many researchers remain uncertain about their safety for human use. Heparin, a sulfate glycosaminoglycan widely used as an anticoagulant, is typically extracted using hydrolase enzymes such as trypsin or alcalase. However, its association with collagen-rich extracellular matrices suggests that collagenase may improve extraction efficiency by disrupting connective tissue structures. This study will investigate the feasibility of enhancing heparin extraction from bovine intestinal mucosa through the incorporation of collagenase, an enzyme not traditionally used in heparin isolation.
This research will compare porcine and bovine heparin extraction across three enzymatic conditions: hydrolase, hydrolase and collagenase, and collagenase. Extracted products are analyzed using infrared (IR) spectroscopy, an assay for anticoagulant activity, and agarose gel electrophoresis to confirm chemical identity and purity. It is hypothesized that the inclusion of collagenase will increase heparin yield by facilitating the release of collagen-associated heparin without compromising structural

characteristics. If bovine and porcine heparin products are comparable, this would support the potential reintroduction of bovine-derived heparin as a viable alternative.

MWRM 2026 MW394

Adsorption models of superheavy elements and their chemical homologs

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Gas-surface chromatography on pristine, stable surfaces, usually gold or amorphous silica, is among the very few methods that provide access to the chemical signatures of these elements in the form of interaction energies between single superheavy atoms and these surfaces. The calibration of the experimental setup rests on chemical homology: the idea that the properties of an SHE resemble those of the lighter element directly above it in the respective group, e.g., mercury (Hg, Z = 80) is homologous to copernicium (Cn, Z = 112). This approach faces two fundamental challenges. First, extreme relativistic effects in SHEs can disrupt the chemical trends homology presumes. Second, experimental and theoretical data on the chemical behavior of the sixth-period homologs are surprisingly scarce and inconsistent. Nihonium (Nh, Z = 113) and livermorium (Lv, Z = 116) are the next targets for chemical study, which increases the demand for detailed information about their respective homologs, thallium (Tl, Z = 81) and polonium (Po, Z = 84), and the re-examination of the notion of chemical homology.
To resolve these inconsistencies, we develop a realistic model of the adsorption of single SHE species and their lighter homologs on an amorphous silica surface. This model includes large silica clusters to represent various adsorption sites, including those with defects such as an under-coordinated Si atom or a non-bonding O. To model the electronic structure of the adsorption complexes, we utilize high-quality relativistic pseudopotentials for heavy atoms in combination with in-house basis sets and a reliable relativistic density functional theory approach based on the non-empirical PBE0 functional. We investigate the adsorption behavior of Nh, its formal homolog Tl, and its potential non-intuitive homolog At. We find that, unlike previously reported results, a defect-free surface only allows for physisorption with an energy around 40 kJ/mol for all single atoms tested. With a non-bonding O, At (205 kJ/mol), and not Tl (396 kJ/mol), behaves as a chemical homolog to Nh (204 kJ/mol). With an undercoordinated Si atom, however, neither Tl (219 kJ/mol) nor At (251 kJ/mol) displays chemical homology with Nh (135 kJ/mol). These findings challenge the concept of chemical homology and warrant further investigation into the theoretical interpretation of the behavior of Tl, At, and Nh in gas-solid chromatography on a silica surface.

MWRM 2026 MW419

Advances in catalytic acylations and fragmentative generation of [$ArCF_2^-$] synthons from accessible precursors

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The development of synthetic methods from readily accessible precursors can reduce reliance on highly prefunctionalized reagents while enabling divergent and mechanistically distinct reaction pathways. This presentation will describe two complementary research directions from our laboratory involving the controlled activation of carboxylic acids and the use of isolable fluoroalkyl hemiaminals as masked synthons for nucleophilic fluoroalkylation chemistry.

In the first area, carboxylic acids are activated through acyloxyphosphonium intermediates to enable selective acyl-transfer reactions. Copper-catalyzed coupling with organozinc reagents provides direct access to ketones, including fluorinated ketones, without requiring the prior isolation of an acyl electrophile. Mechanochemical variants of this chemistry produce divergent reaction outcomes. Changes in milling parameters, including ball size and the number of milling balls, shift the selectivity toward either N-acylsuccinimides or carboxylic anhydrides under otherwise identical conditions. These findings demonstrate that a common activation manifold can be directed toward distinct product classes through control of both the reaction partner and the mechanochemical environment.

The second area focuses on the generation of aryldifluoromethyl nucleophiles from isolable fluorinated hemiaminals prepared without the use of ozone-depleting substances. Base-promoted formation of the corresponding hemiaminolate induces C–C bond fragmentation, regenerates the imide carbonyl group, and releases a transient [$ArCF_2^-$] equivalent. Protonation of this intermediate furnishes difluoromethyl arenes, ($ArCF_2H$). Precursor structure, N-substitution, aryl electronics, and reaction conditions can be varied to modulate fragmentation and subsequent electrophilic trapping. These findings establish fluorinated hemiaminals as tunable, masked [$ArCF_2^-$] synthons and provide a foundation for ongoing efforts to intercept the released nucleophile with carbon- and heteroatom-based electrophiles.

Together, these studies illustrate how catalytic activation, mechanochemical control, and programmed fragmentation can unlock divergent synthetic reactivity from readily accessible precursors.

MWRM 2026 MW210

AI-driven peptide prediction integrated with molecular dynamics simulations for mechanistic insights into membrane selectivity

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AI-driven approaches and molecular simulations provide complementary strategies for studying membrane-active peptides; however, these methods are rarely integrated into a unified mechanistic framework. Cell-penetrating peptides (CPPs) and antimicrobial peptides (AMPs) exhibit selective membrane interactions governed by sequence-dependent physicochemical features that remain challenging to predict and interpret. Recent advances in protein language models (pLMs) enable extraction of contextual sequence representations that capture evolutionary and physicochemical information directly from peptide sequences.

In this work, we integrated pLM-based deep learning with all-atom molecular dynamics (MD) simulations to connect sequence-derived representations with atomistic mechanisms of membrane interaction. Building on our recent work, we developed pLM4CPPs, a convolutional neural network framework utilizing embeddings generated from pretrained protein language models, including ESM-2, ProtT5, SeqVec, and BEPLER. Benchmarking analyses demonstrated improved predictive performance and robust generalization relative to existing CPP prediction methods.

To mechanistically interpret these sequence-derived features, we performed long-timescale all-atom MD simulations of the antimicrobial peptide Snakin-Z in membrane models representing bacterial, fungal, and mammalian systems. The simulations revealed that membrane selectivity is driven by persistent electrostatic anchoring and amphipathic insertion mechanisms. Residue-level analyses identified Arg- and Lys-rich regions as dominant anchoring sites that formed persistent interactions with anionic lipid headgroups in microbial membranes. Relative to mammalian membranes, microbial membranes exhibited stronger peptide association, deeper insertion, enhanced hydrogen-bond occupancy, membrane thinning, and increased lipid disordering, whereas cholesterol-rich mammalian membranes resisted peptide insertion and perturbation.

These findings establish a direct connection between sequence-derived representations captured by protein language models and the molecular mechanisms governing membrane selectivity, providing a scalable framework for AI-guided design of membrane-active peptides.

MWRM 2026 MW49

AI-guided design of AshPhos-P3 ligand: A predictively engineered ligand for Pd-catalyzed amination of hindered primary amines

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Among catalytic transformations, the palladium-catalyzed carbon–nitrogen (C-N) cross-coupling reaction is one of the most powerful and widely applied reactions for constructing key intermediates in pharmaceuticals, fine chemicals, and functional materials. Despite tremendous progress, the animation of hindered α-tertiary primary amines and strongly coordinating heteroaryl electrophiles remains particularly challenging. To address this, we integrated DFT-derived insights with ML-guided ligand optimization to decode how structural and electronic factors influence catalytic efficiency.
Herein, we developed a two-stage random forest (RF) model to correlate ligand structure, reaction descriptors, and catalytic yield. This ML-guided framework enabled the rational design of AshPhos-P3, a ligand that achieves the ideal steric-electronic balance for efficient palladium-catalyzed C-N bond formation with hindered primary amines and heteroaryl electrophiles. The model successfully predicted reaction yields for new substrate-ligand combinations and showed strong agreement with experimental outcomes. This work demonstrates that AI-guided approaches can provide actionable insights into catalyst design and have the potential to accelerate chemical discovery.

MWRM 2026 MW409

AI-guided optimization and structure-based virtual screening identify novel dual-state KRAS G12D candidate binders

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KRAS G12D is one of the most prevalent oncogenic drivers in pancreatic and colorectal cancers and remains a challenging therapeutic target because of its high affinity for GTP and the absence of a reactive residue for covalent inhibition. Identifying non-covalent inhibitors capable of targeting multiple conformational states may provide an effective strategy to overcome these limitations. Methods: An open-source computational workflow integrating high-throughput virtual screening, molecular docking, AI-guided ligand optimization using DeepFrag, and ADMET prediction was employed to identify and optimize potential dual-state predicted KRAS G12D candidate binders. FDA- and internationally approved compounds from the ZINC World-approved library were screened against the inactive (7RPZ) and active (7T47) KRAS G12D crystal structures. Promising candidates were structurally optimized and subsequently

evaluated for binding affinity, binding interactions, and predicted pharmacokinetic properties. Results: Virtual screening identified split1062 as a promising dual-state scaffold suitable for AI-guided optimization. Three derivatives were generated, among opt3 retained favorable predicted docking scores against both conformational states while improving its predicted drug-like properties. Interaction analysis revealed conserved hydrogen bonding with the mutant Asp12 residue in both conformational states. ADMET profiling indicated that opt3 satisfied Lipinski's Rule of Five, exhibited high predicted gastrointestinal absorption, lacked PAINS and Brenk alerts, and eliminated the predicted blood-brain barrier permeability observed for the parent compound while maintaining favorable drug-like properties. Conclusion: This study suggest that integrating AI-guided ligand optimization with virtual screening can optimize the pharmacokinetic properties while retaining favorable predicted binding and pharmacokinetic properties of repurposed predicted KRAS G12D candidate binders. The optimized compound opt3 displayed favorable dual-state binding characteristics together with a modestly improved predicted drug-likeness profile, supporting its prioritization for molecular dynamics simulations and experimental validation.

MWRM 2026 MW163

Alkyl radical addition to activated vinyl imines

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Functionalization of 3-formylchromone provides an efficient strategy for accessing structurally complex, biologically relevant heterocyclic compounds. In this study, the synthesis and reactivity of imines derived from 3-formylchromone were investigated through condensation reactions with aromatic amines, followed by radical addition to the activated alkene adjacent to the chromone oxygen. 2-aminopyrimidine and aniline imines were used to further study the radical addition reactions. Various alkyl radical additions using triethylborane as the radical initiator and zinc trifluoromethanesulfonate as a Lewis acid were done to understand the reactivity of the vinyl imines. The aniline-derived imine had better results after the radical addition step, having higher yields of the radical-functionalized products that were characterized by IR and H NMR. These findings demonstrate a versatile approach for the synthesis of highly functionalized chromone imines bearing diverse alkyl substituents, providing valuable intermediates for the development of structurally diverse molecules with potential applications in medicinal chemistry and heterocyclic synthesis.

MWRM 2026 MW359

Alpha-synuclein interaction with gedunin

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Parkinson's disease (PD) and other synucleinopathies develop when α-synuclein misfolds and aggregates into toxic amyloids. While existing treatments for PD are primarily focused on managing its symptoms, a viable solution for slowing disease progression involves targeting the toxic α-synuclein amyloids.Gedunin, a natural inhibitor of heat shock protein 90 (Hsp90), has demonstrated significant antimalarial activity.. Also, recent research studies have shed light on its potential beyond malaria therapy, indicating that Gedunin may offer a possible therapeutic strategy for treating a variety of neurodegenerative diseases. Using plate-based assays, we examined how Gedunin influences α-synuclein fibrillation and its impact on the pathophysiology of Parkinson's. The findings reveal Gedunin modulates α-synuclein fibrillation in a dose-dependent manner, reducing the buildup of toxic oligomers while increasing their susceptibility to proteolytic breakdown. Gedunin decreases α-synuclein amyloid toxicity by binding to the hydrophobic parts of α-synuclein oligomers. This suggests that oligomerization may be crucial for α-synuclein to manifest its neurotoxic effects. These findings provide strong evidence of Gedunin's neuroprotective potential in PD by targeting protein misfolding and aggregation, while also suggesting a path forward for treatments that modify the disease course.

MWRM 2026 MW116

Altering the physicochemical properties of benzoxazol derivatives through co-crystallization

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The therapeutic potential of many biologically active molecules is limited by unfavorable physicochemical properties, particularly poor aqueous solubility. Benzoxazole derivatives have demonstrated anticancer activity through mechanisms including modulation of signaling pathways, enzyme inhibition, and DNA intercalation; however, their limited solubility may restrict their pharmaceutical utility. Co-crystallization offers a promising strategy for modifying the physicochemical properties of molecular solids without altering the covalent structure of the active compound. This study examines the propensity of a series of acylated bromoaminobenzoxazole derivatives to form co-crystals with aromatic carboxylic acids and explores relationships between molecular structure and co-crystal formation. Five benzoxazole derivatives—N-(6-bromobenzo[d]oxazol-2-yl)acetamide, N-(6-bromobenzo[d]oxazol-2-yl)propionamide, N-(6-bromobenzo[d]oxazol-2-yl)butyramide, N-(6-bromobenzo[d]oxazol-2-yl)hexanamide, and N-(6-bromobenzo[d]oxazol-2-yl)heptanamide—were screened against 13 aromatic acid co-formers spanning a broad range of acidities using liquid-assisted grinding with methanol in a 1:1 molar ratio. The resulting solids were characterized by infrared spectroscopy and differential scanning calorimetry, and promising combinations were subsequently subjected to slow-evaporation crystallization from methanol. Single-crystal

X-ray diffraction was used to determine the structures of successfully crystallized products. The results reveal a high incidence of co-crystal formation and several unusual solid-state architectures, providing insight into the intermolecular interactions governing assembly within this family of benzoxazole derivatives and offering a basis for identifying structural trends in their co-crystallization behavior.

MWRM 2026 MW288

Alternating ADMET as a platform for precision polymer design

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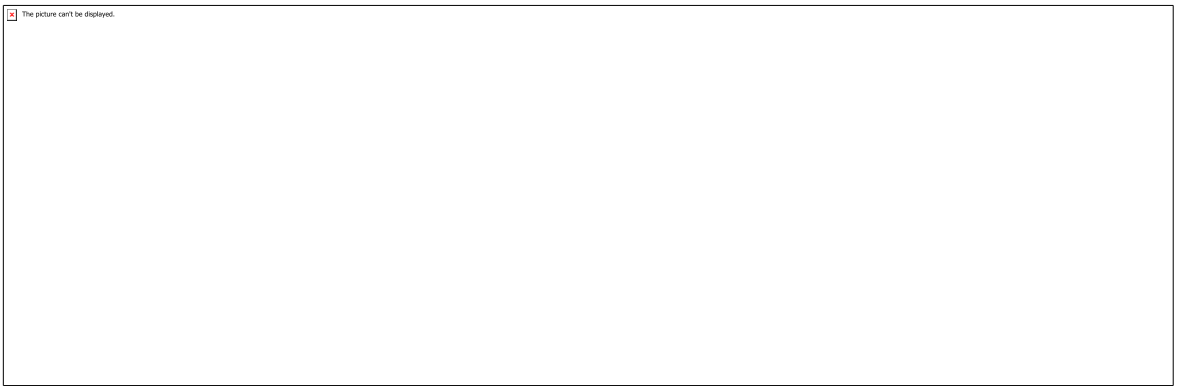
Controlling polymer sequence and functional-group placement with high precision is crucial for developing materials with predictable and adjustable properties. Here, we report a modular alternating acyclic diene metathesis (ADMET) polymerization approach for synthesizing precision unsaturated aliphatic polyesters. Commercially available α,ω-dienes and diacrylates with varying chain lengths were polymerized using the second-generation Hoveyda-Grubbs catalyst. Careful optimization of the reaction conditions produced highly alternating copolymers with high monomer conversion, excellent sequence selectivity, and number-average molecular weights >10 kg mol -1. Evaluation of different monomer combinations demonstrated the broad applicability of this strategy, while the use of an AB-type monomer provided precise control over the spacing of unsaturated units throughout the polymer backbone.
The resulting polymers, which contain conjugated α,β-unsaturated ester groups, were efficiently functionalized through thiol–Michael addition under mild conditions, allowing a variety of side-chain functionalities to be introduced. Quantitative hydrogenation of the polymer backbone was also achieved. Thermal characterization revealed that the spacer lengths of both the diene and diacrylate monomers, together with post-polymerization modification, strongly affect the thermal stability and crystallization behavior of the polymers. These findings demonstrate a clear connection between precisely controlled molecular structure and bulk material properties. Overall, this work presents a versatile and synthetically accessible method for constructing precision macromolecular architectures and establishes a useful platform for investigating structure–property relationships in sequence-controlled functional polyesters.

MWRM 2026 MW91

Alternative solvents to dichloromethane for ring closing metathesis of azamacrocycles

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Azamacrocyles can be synthesized via ring-closing metathesis (RCM) with dichloromethane as the solvent. Compliance with OSHA Standard 1910.1052 requires monitoring of dichloromethane exposure, which can make its use cost prohibitive. This research focuses on exploring different solvents, catalyst loading via increasing or incremental loading, and through heating or sonication, to allow for a similar or better reaction yield. Thin-layer chromatography (TLC) and proton nuclear magnetic resonance spectroscopy (^{1}H NMR) indicate that 1,2-dichloroethane is a promising substitute and with modified reaction conditions it showed catalytic conversion rates of 67%. Future work will investigate a variety of different aprotic solvents under different reaction conditions.



MWRM 2026 MW410

Analysis of a novel decoupled relaxation method for estimating condensed-phase water dipoles

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Analyzing trends in the dipole moments of water monomers provides insight into the structural and electrostatic changes bulk water undergoes in different environmental conditions. We employ a novel single-point quantum mechanical (QM) decoupled relaxation method in combination with molecular dynamics (MD) simulations to model condensed-phase liquid and crystalline water systems. This approach estimates the dipole moments of individual water molecules by isolating clusters surrounding a central molecule, defined by the radial distribution function. The resulting dipoles were used to were used to examine how environmental conditions influence water polarization, producing qualitative trends consistent with previous ab initio molecular dynamics (AIMD) simulations across a range of thermodynamic conditions. We observe an inverse correlation between water polarization and temperature, and a direct correlation with pressure. Density also displays a direct correlation with structural variation between clusters. Although our method reproduces the average dipole moments reported by

AIMD simulations, it does not yet capture the full distribution of monomer dipoles. Furthermore, it is not currently transferable to crystalline ice, as it does not replicate the increased polarization relative to liquid water reported in the literature. However, incorporating hydrogen-bond orientations and angular information into the model represents a promising strategy for improving its predictive capability and extending applicability.

MWRM 2026 MW422

Analyzing the role of microplastic size, surface area and chemical composition on PFAS sorption in sanitary water samples: A case study of the Galesburg area

***Lumala Nelum Naullage**, lnperera@knox.edu. Knox College Department of Chemistry, Galesburg, Illinois, United States*

Persistent environmental contaminants are a growing global concern due to their longevity and potential impacts on ecosystems and human health. One such persistent chemical, perfluoroalkyl substances (PFAS), is known to adsorb onto another widely distributed environmental contaminant, microplastics (MPs) and nanaoplastics (NPs). The coexistence of PFAS and MPs poses an increased risk due to the ability of MPs to enter into animal and human body through multiple pathways. While there is a gap in understanding the interactions between MPs and PFAS, there are concerns about the exposure to elevated PFAS levels in certain areas in the US. One such area is Galesburg, IL.
Even the drinking water of the Galesburg area is estimated to exceed the new federal and state maximum contaminant level (MCL) of 4 ppt PFAS. Perfluorooctanoid acid is the most abundant PFAS in the Galesburg water. No study has been done on levels of MPs and NPs contamination in the area and their interactions with PFAS. In our study, the water samples were subjected to acoustofluidcs to separate the MPs based on their size and type. PFAS was extracted from plastic with solid-phase extraction methods and analyzed. We will present our findings on the levels of MPs, NPs, and PFAS in treated waste water samples collected from the sanitary district of Galesburg. We will discuss the levels of PFAS adsorbed onto MPs and NPs. The relationship between the types of MPs and their surface area to volume ratio in relation to PFAS adsorption will also be discussed. Our findings on the interaction between plastics and PFAS are the first environmentally relevant study in the US that also is actually relevant to the communities in the area. We anticipate that our findings will broaden understanding of how the interplay of these contaminants potentially affect human health in areas where actual risks are evident.

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MWRM 2026 MW401

Anatomy of vapor-liquid interfacial structure formed by pentafluoroethane (HFC-125) using molecular dynamics simulations

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The vapor-liquid interfacial structure directly influences phase equilibria, interfacial mass transport, surface tension, and evaporation kinetics, all of which are important in materials science, physical chemistry, and separation applications. The capillary-wave broadening of liquid–vapor interfaces was first formulated theoretically by Buff, who demonstrated that thermal fluctuations of the interfacial height contribute to the observed interfacial width. Later scattering experiments, validated the predicted interfacial roughness at mesoscopic length scales, while molecular simulations have directly resolved instantaneous interface fluctuations and distinguished capillary-wave broadening from the intrinsic molecular structure. Although classical fixed-charge force fields (FF) have successfully reproduced the vapor and liquid properties of fluorocarbon-

containing systems, including liquid and vapor densities over a wide temperature range, accurately describing the interfacial structure and surface tension remains more challenging. The highly polar carbon–fluorine bond induces strong local electric fields and anisotropic intermolecular interactions, making molecular polarizability an important factor governing molecular packing and orientation at the interface.

In the present work, we developed the Drude polarizable FF model to investigate the vapor-liquid interfacial structure of pentafluoroethane (HFC-125), a widely used hydrofluorocarbon (HFC) refrigerant in modern heating and ventilation systems. Starting from the initial setup of a vacuum on both sides of the liquid, we successfully reproduced vapor–liquid coexistence over a range of temperatures, with excellent agreement for both the liquid and vapor phase densities and, more importantly, the interfacial tension. Taking advantage of the polarizable FF, we computed the dipole moments in the gas and liquid regions of HFC-125. We found that both permanent and induced dipoles influence the interfacial structure. From the decomposition of dipole moments in the z direction, we found that the induced and permanent dipole moments act in opposite directions, and the contribution to the total dipole moment is more by the permanent dipole of the HFC-125 molecules. These findings suggest that complex interfacial structures form in HFC-125 due to dipole moment restructuring and provide valuable insights that can help improve separation technology, enable energy-efficient recovery, and reduce environmental impacts.

MWRM 2026 MW304

Antibacterial testing of hyaluronic acid derivatives

Hannah Warner, Derek Ross, Alessandro Francisco Martins, ***Charles J. Neef****, cneef@pittstate.edu. Pittsburg State University, Pittsburg, Kansas, United States*

Hyaluronic acid (HA) is an important biomolecule found in skin, eyes, and joints. HA is a very hydrophilic material and able to absorb large amounts of water. This property gives rise to applications such as eye drops to prevent drying, moisturizers to reduce the appearance of wrinkles or age spots, or as injections into joints for osteoarthritis to help with lubrication and decrease joint pain. The inherent biocompatibility and biodegradability of HA along with its antibacterial properties facilitates HA’s use in tissue regeneration and wound healing. HA hydrogels have also been shown to significantly accelerate common wound healing as well as diabetic wound healing. In addition, HA hydrogels have been studied for tissue regeneration by transporting cells for tissue repair or simply as a biological glue to aid scaffolding materials for tissue engineering.

HA was modified by the addition of various epoxides (glycidyl phenyl ether, ethyl glycidyl ether, or glycidol) to the carboxylic acid of HA. Upon addition of the epoxide, the resulting polymers showed greater solubility in water and the solutions exhibited a significant decrease in viscosity compared to HA solutions. FTIR and H-NMR spectra were consistent with the structure of the polymers. Antibacterial testing of the modified HA polymers will also be reported.

MWRM 2026 MW388

Antioxidant cannabinoids and polycannabinoids enable low temperature additive manufacturing of oxidation-free copper

*Michael Sotzing, **Alex Chortos**, achortos@purdue.edu. Mechanical Engineering, Purdue University, West Lafayette, Indiana, United States*

Additive manufacturing has been gaining traction as low-capital method to produce products with value-added geometries. In the additive manufacturing of metals, functional properties such as electrical conductivity and mechanical strength are strongly impacted by the presence of oxides. In this work, we show that the natural antioxidant cannabidiol (CBD) and polymers made of CBD (pCBD) can reduce copper oxides and have numerous other benefits in the synthesis and processing of copper inks for printed electronics. During synthesis, CBD coatings promote the stability of copper microparticles, allowing low-cost synthesis in water. CBD coatings show higher corrosion inhibitor efficiencies than common covalent ligands such as PVP despite having no covalent interactions with the copper surface. After printing, CBD and pCBD reduce the sintering temperature of copper traces from ~190 C to <140 C, potentially due to redox reactions that enhance the mobility of copper atoms to promote neck formation between particles. Furthermore, both CBD and pCBD reduce oxides on the copper particle surface, as revealed by in-situ XRD measurements. The occurrence of redox reactions are confirmed by HPLC measurements showing the conversion of CBD after thermally-induced reduction with copper oxide. Due to this oxide reduction capacity, the printed copper traces retain high conductivity during thermal aging at 200 C, ensuring compatibility with subsequent manufacturing steps. Ultimately, CBD/pCBD-coated copper particles have high stability, can be processed at low temperature, and remain oxidation resistant after processing. While questions remain about the mechanism for depressed sintering temperatures, the oxide reduction reactions are supported by direct measurements. This work demonstrates the potential of polymerized cannabinoids as potent reducing agents to reverse oxidation of metals. This finding could be widely applied within the field of additively manufactured metals.



MWRM 2026 MW55

Applied machine learning for green catalysis

***Kevin C. Leonard**, kcleonard@ku.edu. The University of Kansas, Lawrence, Kansas, United States*

Artificial intelligence has enormous potential to accelerate catalyst discovery, but its adoption in green chemistry requires trustworthy data, interpretable models, practical experimental guidance, and sustainable computational workflows. This presentation introduces a framework that addresses these challenges through the integration of automated literature mining, large language models, open-access computational databases, and interpretable machine learning.

MWRM 2026 MW280

Aqueous electrolytes in nanoscale slit pores: Structure, dynamics, and ion-pairing thermodynamics

***Saswata Dasgupta**, saswata@ksu.edu. Chemistry, Kansas State University, Manhattan, Kansas, United States*

Understanding how ion–ion association changes under nanoscale confinement is a central challenge in physical chemistry, with implications for nanofluidics, energy storage, and selective separations. When aqueous electrolytes are confined within nanoscale slit pores, restricted solvent organization and altered interfacial environments modify hydration, dielectric screening, and the balance between ion association and dissociation. These effects become particularly important near chemically active interfaces, where direct ion–surface interactions can compete with ion hydration and ion pairing. Experimental characterization of these molecular-scale processes remains difficult, whereas conventional simulations often lack either the electronic-structure accuracy or computational efficiency required for a reliable description.

Here, we develop a graph neural network machine-learned potential trained on DC-SCAN electronic-structure data to achieve near-chemical accuracy at experimentally relevant length and time scales. An active-learning framework efficiently samples configurations spanning bulk aqueous solutions and nanoscale slit pores formed by graphene and hexagonal boron nitride (hBN), enabling direct comparison between bulk behavior, chemically inert confinement, and chemically active interfaces. Using lithium halide electrolytes as representative systems, we determine how confinement modifies hydration structure, solvent reorganization, and the equilibrium among contact, solvent-shared, and solvent-separated ion pairs. Relative to bulk solution, slit-pore confinement produces anisotropic hydration environments, shifts ion-pair free-energy landscapes, and promotes preferential interfacial localization. Comparisons between graphene and hBN further reveal that site-specific ion–surface interactions at the chemically active hBN interface can either reinforce or compete with confinement-induced ion association,

leading to behavior that cannot be explained by geometric restriction alone.

These results establish how nanoscale confinement and interfacial chemical activity jointly govern electrolyte structure and ion-pairing thermodynamics. More broadly, this work provides a molecular framework for predicting aqueous electrolyte behavior in chemically heterogeneous slit-pore environments.

MWRM 2026 MW123

Arene-bridged polyvalent triazolium salts with antiseptic properties

***Matthieu E. Carter**, matthieucarter@creighton.edu, James T. Fletcher. Chemistry and Biochemistry, Creighton University, Omaha, Nebraska, United States*

Emerging resistance in bacteria and yeast requires the development of new antiseptic molecules. Our lab has recently shown that 1,2,3-triazolium salts exhibit antiseptic properties that vary significantly with their structure and overall charge. The goal of this project was to compare monovalent, divalent, and trivalent analogs of triazolium salts to identify how overall charge and hydrophobicity impact antiseptic properties across different microbial classes. The bridge of the molecules consists of ethynylbenzene, 1,3-diethynylbenzene, or 1,3,5-triethynylbenzene. Consequently, either 3-*tert*-butylphenyl azide or 3,5-*tert*-butylphenyl azide was added through base-catalyzed click synthesis. Subsequent alkylation with benzyl bromide or para-*tert*-butylbenzyl bromide at the N3 nitrogen of the triazole ring resulted in trisubstituted 1,2,3-triazolium salts. Reaction success was verified by ^{1}H-NMR before minimum inhibitory concentration (MIC) assays against Gram-positive bacteria (S. epidermidis and B. subtilis), Gram-negative bacteria (E. coli and K. aerogenes), and yeast (C. albicans and S. cerevisiae) were performed to determine antiseptic potency. The presence of para-*tert*-butylbenzyl bromide or benzyl bromide significantly affected the effectiveness of the compounds. These results identify an upper size limit for 1,2,3-triazolium salt activity and indicate that higher formal charges do not inherently increase antiseptic potency against all organisms. In conclusion, these studies demonstrate how variations in size, charge, and functional groups dictate the ability of these molecules to serve as antiseptics.

MWRM 2026 MW408

Assessing the impact of AlphaFold3-derived structures on molecular docking accuracy

***Hadiza Elhadji Oumarou Harouna**, hadizae25@gmail.com, Xinqiu Yao. Chemistry, University of Nebraska Omaha, Omaha, Nebraska, United States*

Molecular docking has been a crucial computational tool to investigate receptor-ligand interactions efficiently and cost-effectively. Traditional docking calculations rely heavily on available experimental structures, which may not represent the optimal receptor conformation for accommodating a specific ligand in the active site. Recent advances in

deep-learning based structural modeling, particularly with AlphaFold3 (AF3), have enabled high-accuracy prediction of protein-ligand complex structures. Accurate complex modeling not only extends the applicability of docking to virtually any receptor-ligand pair, but also generates refined binding-site conformations that may enhance docking performance and prediction accuracy. In this study, we sought to systematically assess whether AF3-derived complex structures can improve docking accuracy relative to conventional approaches. We integrate AF3 with docking software, such as Autodock Vina, to evaluate the binding affinities of over 200 pairs of receptors and ligands derived from the Directory of Useful Decoys, Enhanced (DUD-E) dataset. Specifically, we address the following research questions: 1) Can AF3 identify the binding site correctly? 2) Can AF3 predict a receptor structure more ready for a specific ligand to bind? 3) Can AF3 help distinguish between active ligands (high binding affinity) and decoys (nonbinding molecules) better? 4) Can AF3-derived complex structures help improve docking accuracy in terms of correlation with experimental affinity data? Our findings offer practical guidance for optimizing docking-based virtual screening campaigns in drug discovery.

MWRM 2026 MW223

Assessment of an open-source stopped flow system

***Finley Hall**, finley.hall@drake.edu, Ryan Sturms. Chemistry and Physics, Drake University, Des Moines, Iowa, United States*

Stopped-flow spectroscopy is an important technique that enables the measurement of rapid biochemical reactions that occur on the millisecond timescale. It is widely used to characterize enzyme kinetics and ligand binding. Although UV-Vis spectrophotometry is commonly used to observe reaction kinetics, conventional instruments often have dead times that are too long to capture the earliest stages of fast reactions. The dead time is the interval between mixing reactants and the first measurable data point. Minimizing dead time enables observation of very fast reactions and their initial burst phase. Commercial stopped-flow instruments are expensive, which makes them particularly hard to obtain and use in undergraduate academic settings. An open-source alternative was designed to provide greater access to a stopped-flow in educational settings. The instrument consists of a motor-driven syringe pump that rapidly delivers two reactants into a mixing junction, followed by a flow cell positioned within a spectrophotometer and a receiving syringe. Mixing, timing, and data acquisition are controlled by custom electronics and software.

Although the open-source stopped-flow instrument has been successfully designed and assembled, its ability to accurately measure rapid reaction kinetics has not yet been evaluated. In particular, the instrument’s dead time must be characterized and optimized to ensure that fast kinetic events can be measured. Without comparison against a commercial stopped-flow system, the accuracy and reliability of kinetic parameters obtained using the homemade instrument remain uncertain. The purpose of this study is to evaluate the performance of the open-source stopped-flow apparatus

using the reaction of sodium azide binding to ferric horse heart myoglobin (Mb) as a model system. Here we report the optimized dead time and a direct comparison of the reaction between Mb and azide measured by the homemade instrument and a commercially available instrument.

MWRM 2026 MW256

Atropdiastereomerism in metacyclophane macrocycles

***Junqi Li**, junqili@iastate.edu. Department of Chemistry, Iowa State University of Science and Technology, Ames, Iowa, United States*

Metacyclophane macrocycles consist of an arene connected through the bridging chain attached at the 1,3-positions of the arene. This substitution pattern frequently occurs in pharmaceutically relevant macrocycles and can contain several stereochemical elements arising from atropisomerism. In this talk, we describe the design, synthesis, and structural verification of metacyclophane macrocycles that display atropdiastereomerism. We show how this simple system led us to design lasso molecules containing a tail that threads through the macrocycle. Our modular synthesis towards these complex macrocycles enabled us to systematically determine the structural factors that stabilize the threaded structure in these molecules.

MWRM 2026 MW396

At-scale data-driven exploration of high-voltage cathode materials for sodium batteries

***Suchona Akter**, sad8b@umkc.edu, Mohammadreza Momenitaheri. Division of Energy, Matter, and Systems, University of Missouri-Kansas City, Kansas City, Missouri, United States*

Sodium-ion batteries (SIBs) share similar electrochemistry with Li batteries but offer several advantages, including sodium's high abundance in nature, low cost, and favorable ion transport properties. However, the development of high-voltage, high-energy-density cathode-active materials (CAMs) remains a critical bottleneck, particularly across the vast and chemically diverse materials space. In this work, we present a scalable, data-driven framework for discovering robust SIB cathodes. Using desodiated charged-only data from the Materials Project battery dataset, we have benchmarked voltage predictions from various classical descriptor-based models, neural network (NN) models for composition-only features, and graph NN (GNN) models. Chemical extrapolation was studied using leave-one-cluster-out (LOCO) cross-validation. Our results demonstrate the promise of data-driven voltage predictions from charged-only structures and uncover important chemical and structural trends. Finally, a subset of top-ranked candidates from our large-scale curated database (>800k materials) is validated using first-principles calculations to confirm our model

performances. Our work establishes a scalable and transferable framework for accelerating the discovery of stable, high-voltage CAMs for SIBs and beyond.

MWRM 2026 MW440

Autonomous movement of Belousov-Zhabotinsky droplets enclosed by diverse surfactants

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The biochemistry of biological systems is organized in compartments such as cells and organelles. The interior of these compartments consists of various nonlinear chemical reactions, such as the Krebs cycle, and is separated from the external environment by a membrane. Interactions between the membrane, the enclosed chemical mixture, and the external environment influence the resultant behavior of the compartment. In this work, we used oscillatory chemical systems—specifically the Belousov-Zhabotinsky (BZ) reaction—to model the behavior of such compartments.
The BZ reaction is an autocatalytic oscillatory reaction that consists of bromate, bromide, organic substrate, sulfuric acid, and metal catalyst reagents that undergo a cyclic reduction-oxidation reaction. Periodic oscillations between an oxidized and reduced form are accompanied by changes in solution color, voltage, and hydrophobicity. Previous studies have shown that when BZ solution is enclosed in a millimeter-scale droplet in a surrounding oil medium, the oscillation of propagating waves between an oxidized and reduced state enables autonomous and self-directed motion of said droplet. In this study, we investigated how the concentration and properties of surfactants alter the dynamics of the BZ reaction and consequent autonomous motion of BZ droplets. We have used surfactants with diverse properties and varied concentrations of each surfactant over three orders of magnitude. Velocity and mean squared displacement of droplets were used to characterize droplet behavior. Preliminary analyses show characteristic differences in droplet behavior as a function of surfactant type and concentration. These findings carry implications for understanding cellular movement and for the potential design of autonomous synthetic microswimmers.

MWRM 2026 MW301

Backbone editing via the Beckmann rearrangement

***Peace Adelowokan**, padelowokan@ku.edu, Aaron Teator. Chemistry, The University of Kansas, Lawrence, Kansas, United States*

Editing the polymer backbone by introducing functionality into the main chain is an emergent strategy for maximizing polymer lifetimes and enabling re/upcycling and degradation or depolymerization. Current approaches for introducing functionality via nitrogen insertion into polyethylene-like backbones typically require access to

polyketones through ethylene–carbon monoxide (E-CO) copolymerization or C-H oxidation of polyethylene. These methods often suffer from low degrees of functionalization, harsh reaction conditions, significant side reactions, chain scission, and severe solubility challenges. An example of a strategy for producing tunable, unsaturated poly(keto-co-amides) by accessing polyketones through controlled ring-opening metathesis polymerization (ROMP) of seven- and eight-membered cyclic ketones, followed by post-polymer modification via the Beckmann rearrangement, is reported. Primary molecular characterization confirms the selective conversion of ketone functionalities to amide linkages. This strategy establishes a new approach to polymer backbone editing, expanding the scope of polyamide chemistry, increasing functional diversity, and introducing a pathway for designing polymers with emergent properties

MWRM 2026 MW413

Balancing divalent ions–functional group interactions for condensed phase simulation in the polarizable Drude force field

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Molecular dynamics (MD) simulations provide atomistic insight into biomolecular systems, but their predictive power critically depends on the accuracy of the underlying force field. Divalent ion–carboxylate interactions play essential roles in numerous biological processes, yet accurately modeling these interactions remains challenging due to the strong electrostatic, polarization, and hydration effects associated with ions such as Mg and Ca. Although recent advances in the CHARMM Drude polarizable force field have substantially improved the description of monovalent ion–biomolecule interactions, these parameterization strategies are not directly transferable to divalent ions.
Here, Mg–acetate and Ca–acetate are employed as representative model systems to develop a transferable parameterization protocol for divalent ion–functional group interactions. Rather than modifying individual ion, ligand, or water parameters, the protocol refines atom-pair-specific Lennard-Jones interactions (NBFIX) together with through-space Thole dipole screening (NBTHOLE) terms to achieve an improved balance of ion–ligand interactions while preserving the transferability of the underlying force field. Parameters were systematically optimized by minimizing differences between molecular mechanics (MM) and quantum mechanical (QM) potential energy surfaces (PES) for explicitly solvated ion–acetate clusters spanning multiple binding geometries, including bisector, 120°, 180°, perpendicular, and trimer configurations. Our results show that explicitly solvated, multi-body cluster geometries are essential for accurately reproducing both the depth and shape of the interaction PES, highlighting the limitations of conventional gas-phase dimer-based parameterization approaches. The optimized Mg–acetate parameters were validated using experimental osmotic pressures over a range of concentrations. Although demonstrated using acetate as a model carboxylate, the proposed protocol is broadly applicable to the development of

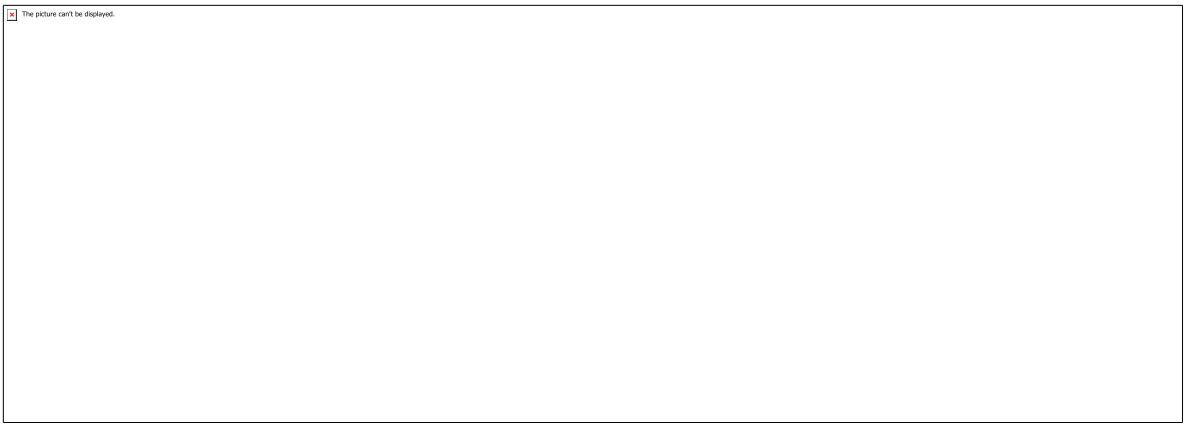
transferable polarizable force field parameters for biologically relevant functional groups, enabling more reliable simulations of ion-mediated interactions in proteins, nucleic acids, and other complex biomolecular systems.

MWRM 2026 MW300

Benzimidazolum salts from renewable sources for antibacterial applications

Kinsey Baldwin, Alessandro Francisco Martins, ***Charles J. Neef****, cneef@pittstate.edu. Pittsburg State University, Pittsburg, Kansas, United States*

Bacterial infections and bacterial contamination of food is a growing concern with the rise of antibiotic resistance bacteria. Several approaches such as antimicrobial peptides, silver nanoparticles, or carbohydrate polymers have shown promise in combating bacteria. Another approach which has received considerable attention is the use of imidazolium salts. Imidazolium salts are known to disrupt the cell wall of the bacteria causing death.
Here, we report the synthesis of benzimidazolium salts from epoxidized soybean oil (ESBO) as a potential antibacterial agent. ESBO is made from a renewable resource, in addition to being inexpensive and readily available. The synthesis of these materials was a straightforward two-step process. (see figure below) ESBO was reacted with benzimidazole in refluxing IPA overnight. The resulting benzimidazole containing ESBO was then reacted with an alkyl halide (pentyl, octyl, or undecyl). These benzimidazolium containing materials were characterized by IR and H-NMR spectroscopy. Subsequent research with these materials will include antibacterial properties with gram-positive and gram-negative bacteria and use as a plasticizer.



MWRM 2026 MW281

Beyond benzenoid aromatics' comfort zones

***Mikhail V. Barybin**, mbarybin@ku.edu. Chemistry, The University of Kansas, Lawrence, Kansas, United States*

Azulene is a polar nonbenzenoid aromatic hydrocarbon composed of edge-sharing 5- and 7-membered carbon rings. Its intrinsically polarized π-electron system gives rise to electronic behavior beyond the comfort zone of conventional benzenoid aromatics while enabling versatile electronic tuning through molecular functionalization. This overview presentation will highlight our recent advances in exploiting linearly functionalized azulenic and 6,6′-biazulenic π-frameworks as molecular platforms for probing long-range electronic communication and establishing quantitative linear free-energy relationships relevant to the design and optimization of π-conjugated functional materials. In particular, we will introduce complementary electrochemical and ^{13}C NMR spectroscopic strategies for inverse Hammett analysis, allowing determination of effective Hammett substituent constants (s_{eff}) for electronically unconventional (i.e., “designer”) substituents that are inaccessible through traditional empirical approaches. Our experimentally derived s_{eff} values are quantitatively anchored to the conventional Hammett parameter scale, thereby extending this classical framework beyond benzenoid aromatic systems. The unusual electronic polarizability of azulenic π-systems amplifies resonance interactions to facilitate unambiguous differentiation of strongly π-donating functional groups that have remained challenging to evaluate experimentally and computationally. The [–NCCr$(CO)_5$] moiety serves as a remarkably sensitive ancillary ^{13}C NMR reporter for quantifying long-range electronic communication and independently validating Hammett correlations across azulenic and 6,6′-biazulenic π-frameworks.

MWRM 2026 MW201

Beyond the weighted average: Non-linear structure-property relationships in grafted polysaccharides

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Copolymerization is a versatile strategy for tuning materials properties. In many synthetic systems, copolymer behavior follows near-linear structure-property relationships, with macroscopic properties tracking backbone composition as a weighted average of the constituent monomers and their sequence. These assumptions break down for natural building blocks whose properties emerge from complex, multiscale self-assembly.
Polysaccharides (e.g., cellulose, chitin, and their derivatives) are the most abundant and industrially relevant biomass-derived polymers. Unlike most synthetic polymers, many

have semi-rigid, intrinsically chiral backbones that drive hierarchical organization, from long-range order in solution to crystallization in the solid state. This self-assembly enables properties difficult to achieve synthetically, but it also complicates predictive copolymer design.
In this talk, I will show how grafting copolymers onto a chitosan backbone harnesses self-assembly to unlock property gains governed by non-linear structure-property relationships. I will first present chitosan-*g*-poly(hydroxybutyrate) (PHB), in which bottlebrush-like architectures dictate solution behavior, nanoscale assembly into filaments, and new crystalline phases. Single-chain imaging resolves this organization directly, complementing ensemble scattering measurements. In bulk, films show distinctive crystallinity, improved phase homogeneity, and thermal stability exceeding both parent polymers.
I will then extend these principles to other chitosan- and cellulose-based architectures, where side chains introduce plasticizing effects that unlock elastomeric behavior or mixed ionic-electronic conduction enabling emergent charge transport. Together, these results establish an architectural framework for expanding the property space of natural polymers and highlight grafted polysaccharides as sustainable platforms for next-generation functional materials.

MWRM 2026 MW56

Biocatalytic Oxa-Pictet-Spengler reactions

***David C. Miller**, dcmiller1126@gmail.com. Oklahoma State University, Stillwater, Oklahoma, United States*

Chiral oxacycles are prevalent pharmacophores with a broad range of biological activities. For dihydropyran-fused heterocycles, the asymmetric oxa-Pictet-Spengler (OPS) reaction is a leading technology for the enantioselective formation of these motifs. State-of-the-art methodologies report high yields and enantioselectivities using catalyst classes such as thioureas, phosphoric acids, and imidodiphosphates. While powerful, these catalysts are deployed with high loadings (typically 10 mol%): this is exacerbated by the fact that these catalysts are expensive if commercially available, require lengthy synthetic sequences to access, and are not reported to be recycled after each reaction. Access to inexpensive, highly active catalysts would expand the impact of these powerful reactions. Building upon these pioneering studies, this presentation describes new-to-nature enzymatic OPS reactions to generate chiral tetrahydropyranoindoles (THPIs). Directed evolution is used to furnish biocatalysts which catalyze OPS reactions with high activities (>2000 turnovers) and selectivities (up to 99:1 er) for these reactions, and the scope of our evolved biocatalyst is explored. MD simulations are used to interrogate mechanistic subtleties about this new-to-nature activity, including mechanistic origins of how mutations discovered via directed evolution improve enzyme activity. These findings can be extended to new classes of heterocycles which are challenging for contemporary asymmetric catalysis due to challenging stereoinduction or incompatibility with strongly acidic organocatalysts used for these transformations. These examples demonstrate the promise of biocatalysis to

expedite access to chiral heterocyclic cores for the synthesis of bioactive small molecules.

MWRM 2026 MW58

Biorenewable strategy for the synthesis of vinyl ethers via cobalt/photoredox decarboxylative eliminations

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Vinyl ethers are a synthetically powerful motif which, despite their structural simplicity, remain difficult to synthesize in an efficient manner. Traditionally, these products necessitate multistep synthesis of vinyl halide or vinyl boronate cross-coupling partners, commonly derived from petroleum-based feedstock. Ultimately, this increases the chemical industry's reliance on petroleum, to produce starting materials which are notorious for their short shelf-lives. The work that will be described obviates these unsustainable reagents in leu of biorenewable ketones via a two-step alkylation-decarboxylative elimination approach. Using this method we have synthesized a series of vinyl ethers from biorenewable reactants utilizing a cobalt-photoredox dual-catalyzed decarboxylative elimination. This strategy has opened access to vinyl ethers which have previously been inaccessible through traditional cross-coupling approaches, and has facilitated the synthesis of deuterium labeled products, while using readily available, benchtop-stable biorenewable starting materials.



MWRM 2026 MW418

Boron triiodide: A new reducing agent

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While historically used to cleave ethers or to perform electrophilic aromatic borylation, our lab has recently found that boron triiodide (BI_3) can act as a reductant, and that it

reduces a variety of nitroarenes, aldehydes and ketones. In this talk, I will discuss these reactions in addition to the capability of BI_3 to reduce acenes while investigating the mechanism of this new reduction.
Long chain acenes, like tetracene and pentacene, have seen increased use in organic field-effect transistors; however, their increased length contributes to decreased solubility and stability. Partially reduced acenes are better behaved, making partial reduction a common strategy for the handling of extended acenes, followed by oxidation on the device surface.
Most current methods to reduce acenes involve variations of the Birch reduction, but there have been a few reports of using boron as a reductant (BF_3-THF and HBPin). In our investigations, boron triiodide was able to reduce a number of acenes with varying substitution patterns. Mechanistic evidence supports a radical propagation pathway initiated by a super acid water adduct, BI_3-OH_2.



MWRM 2026 MW59

Brocazine family of natural products: From total synthesis efforts to targeted chemical screening library construction

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Natural products have been and continue to be one of the primary sources for discovery of pharmaceutically active compounds. Their total synthesis has given rise to multiple drugs that are the primary treatment for numerous diseases. Our lab has been focusing on the brocazine family of natural products isolated from an endophytic fungus derived from the marine mangrove plant Avicennia marina, named *Penicillium brocae* MA-231by Wang and co-workers. Seven different brocazines (A-G) were isolated, and of those, brocazine E showed the strongest activity against the human pancreatic cancer cell line SW1990 (IC_{50} of 2.1 μM), whereas Brocazine F was shown to possess the strongest activity against prostate cancer cell line DU145 (IC_{50} of 1.7 μM) and lung cancer cell line NCI-H460 ($IC_{50}$of 0.89 μM). Brocazine G showed strong activity against ovarian carcinoma cell line A2780 (IC_{50} of 0.664 μM), Cisplatin-resistant human ovarian cancer cells CisR A2780 (IC_{50} of 0.661 μM), and possesses strong and selective activity against human pathogen Staphylococcus aureus (MIC of 0.25 μg/mL). Other members possess different and interesting biological activities. All members of this family are

composed of two unique, but structurally comparable units. Our lab has developed multiple routes to access each of the discrete units of the brocazine family. Coupling these units furnishes the carbon framework of brocazine family members. We are currently in the final stages of installing the disulfide linkage to complete the first total synthesis of brocazine E, F, and G. These synthetic efforts will be presented. Furthermore, the route developed allows accessing new targeted small-molecule screening libraries. This can be achieved by derivatizing intermediates within the total synthesis route.

MWRM 2026 MW190

Can we predict photoreactivity?

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One of the largest challenges in organic photochemistry remains the lack of a consistent set of structural rules governing photoreactivity. While limited trends that largely remain observed phenomena exist, robust comprehension behind trends and application to wider scopes remains a mystery. In this work, we combine a theoretical foundation using state-mixing diagrams along with computational analysis using multireference methods to create a predictive model and compare those results to experimental rates of photoheterolysis in an aim to create a robust set of structural rules governing photoheterolysis reactivity. Trends examined include a variety of structural characteristics such as aromaticity, substituent effects, and hyperconjugation.
State correlation diagrams suggest that three factors lower the S_1 barrier for heterolysis of C-LG bonds: (1) The S_1 energy of the substrate; (2) the stability of the excited cation; (3) the degree of state mixing at the transition state between the initially-populated S_1 state—usually $^1(\pi,\pi^*)$—and the higher-energy excited state that correlates with the S_1 state of the cation—usually $^1(\pi,\sigma^*)$. Due to the multiconfigurational nature of singlet excited states, properties governing photoheterolytic bond cleavage were examined using CASSCF/CASPT2 methods.
Our results revealed often overlooked characteristics such as higher excited-state mixing and favored adiabaticity can be major factors when predicting experimental observations. Experimental rates of heterolysis and adiabaticity were confirmed using both femtosecond and nanosecond transient absorption spectroscopy in HFIP allowing for stabilization of the photogenerated carbocations. Finally, a predictive model was created by combining a S_1 hydride ion affinity (S_1 HIA) which encompassed both the substrate S_1 energy and excited-state carbocation stability, as well as estimates of state-mixing characterized by mixing of the S_1 substrate and the photoreactive state orbitals. This work provides a further understanding of the principles that govern photoreactivity and begins the curation of a set of structural rules for photoheterolysis.

MWRM 2026 MW387

Carboxamide-containing crosslinkers in soybean oil-based polyurethane adhesives

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The development of sustainable polyurethane (PU) adhesives with strong mechanical, thermal, and chemical performance is increasingly important for industrial applications. In this study, bio-based PU adhesives were synthesized using soybean oil polyol (SOP) and methylene diphenyl diisocyanate (MDI), with synthesized carboxamide bond-based crosslinkers (DEA and DPA) incorporated to improve mechanical performance. The influence of crosslinker type and concentration was systematically investigated by formulating adhesives with varying weight percentages (5–20 wt.% for DEA and 5–25 wt.% for DPA) and curing them at room temperature. Mechanical testing on oak wood substrates showed that tensile strength increased with crosslinker content up to an optimal level, followed by a decline at higher loadings due to possible over-crosslinking or network inhomogeneity. The maximum tensile strength for DEA-based adhesives was 6.77 MPa at 15 wt.%, decreasing to 4.1 MPa at 20 wt.%. Similarly, DPA-based adhesives exhibited a peak strength of 6.86 MPa at 20 wt.%, which decreased to 4.26 MPa at 25 wt.%. Curing at elevated temperature (90 °C) resulted in reduced tensile strength compared to room-temperature curing, suggesting changes in network structure and internal stress development. Thermal analysis using differential scanning calorimetry (DSC) indicated glass transition temperatures (Tg) in the range of 30–70 °C. Gel content and swelling studies further confirmed effective crosslinking within the polymer matrix. Overall, the results demonstrate that careful selection and optimization of crosslinkers to enhance the mechanical and thermal stability for bio-based adhesive.

MWRM 2026 MW110

Catalytic C–O bond formation in Heck reactions through terminal C–O reductive elimination pathways

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More than 85% of therapeutics approved by the U.S. Food and Drug Administration incorporate heterocyclic scaffolds, emphasizing their fundamental importance in modern drug design. Lactones and lactams represent particularly significant subclasses, as these motifs frequently occur in biologically active natural products and pharmaceutical compounds, where they contribute to molecular stability, target binding, and overall efficacy. A chemodivergent γ,δ-difunctionalization of homoallylamines has been established, providing controlled access to either δ-lactones or ζ-lactams through

deliberate adjustment of reaction parameters. The selectivity of this process is highly sensitive to the nature of the coupling partner employed. Ongoing mechanistic studies indicate that coordination effects likely suppress β-hydride elimination, thereby directing product formation. Conversely, the use of non-coordinating aryl halides results in conventional reactivity, yielding uninterrupted mono- or di-Heck arylation products from the homoallylamine substrates.

MWRM 2026 MW80

Cationic polycatechol polymer coatings for multifunctional cardiovascular implants

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Cardiovascular implants face significant challenges due to thrombosis, infection, and restenosis, and surface modification strategies cannot address these limitations simultaneously. Cationic polycatechol polymers have emerged as a promising platform for engineering multifunctional interfaces owing to their strong interfacial adhesion, versatile chemical functionality, and intrinsic biological activity. Among these materials, Tanfloc, an amino-functionalized polymer derived from condensed tannins of flavan-3-ol repeat units, has demonstrated potential for the construction of bioactive interfaces for cardiovascular implants.
Our previous studies demonstrated that Tanfloc-based nanostructures improve the biological performance by reducing platelet activation, promoting endothelialization, suppressing smooth muscle cell proliferation, and inhibiting bacterial adhesion and proliferation. These multifunctional properties arise from the synergistic combination of catechol and amine chemistry.
Despite these promising results, Tanfloc has intrinsic limitations stemming from its pH-dependent cationic character, which compromises electrostatic interactions with heparin under physiological conditions, leading to interface instability, polymer leaching, and reduced long-term biological performance. Furthermore, covalent immobilization strategies consume reactive amine groups, limiting subsequent functionalization and reducing interfacial bioactivity.
This presentation will discuss our efforts to develop a new generation of chemically defined cationic polyphenolic polymers that overcome these limitations by incorporating permanent cationic functionalities while preserving the adhesive and bioactive properties of catechol chemistry. Different synthetic approaches and surface engineering strategies, including covalent grafting and layer-by-layer assembly, will be presented to construct multifunctional coatings for cardiovascular implants with enhanced physicochemical stability. Particular emphasis will be placed on understanding how polymer chemistry and interfacial architecture regulate protein adsorption, platelet interactions, endothelialization, and antimicrobial activity. These studies establish cationic polyphenolic polymers as a versatile platform for designing multifunctional biointerfaces for advanced cardiovascular biomaterials.

MWRM 2026 MW235

Characterization of the oxidation of an Fe(II)-aqua complex via a hydrogen atom transfer reaction

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Lipoxygenases are a group of iron-containing enzymes that appear in a wide array of biological organisms. The first step in the lipoxygenase reaction pathway has been observed to be hydrogen atom abstraction. As there is currently little research modeling this reaction, our research hopes to fill this gap by modeling lipoxygenase as an iron-containing complex with a pentadentate amide-containing ligand to mimic the active site of lipoxygenase and replicate its reactivity. We aim to gain a better understanding of the first step of the lipoxygenase reaction pathway by utilizing the model complex [Fe(II)(OH)2(dpaq)](OTf) to conduct a series of hydrogen atom transfer (HAT) reactions. This work characterizes the oxidation of this Fe(II)-aqua complex into an Fe(III)-hydroxo complex through a HAT reaction performed in air-free conditions. These reactions are characterized by UV-vis and 1H NMR spectroscopy. This research contributes to the understanding of metalloenzyme oxidation reactions. Our research also has implications for the chemical industry, as iron complexes have potential for use as sustainable and economical industrial catalysts, and studying their reactivity is a key step in formulating new catalysts.

MWRM 2026 MW330

Characterizing microplastic pollution in Midwestern farmlands through farmer engagement

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Agricultural plastic products play a critical role in crop production and water management, however their weathering and incomplete recovery can introduce persistent microplastics (MPs) into agricultural soils. This study combines farmer engagement, field sampling, and advanced analytical techniques to characterize MP pollution in Midwestern agricultural systems. Soil samples were collected from 19 participating farms through a regional outreach effort in which farmers either submitted their soil samples, or hosted on-site sampling visits. Information on farm size, crop production, farming timeline, and the use of agricultural plastics (e.g., mulch films, geotextiles, irrigation components, greenhouse covers, plant containers, and polymer-coated fertilizers), was also collected. Soil samples were sieved and processed using Fe(II)-catalyzed wet peroxide oxidation, $ZnCl_2$ density separation, and vacuum filtration for extraction of MPs. for Polymer mass loadings were quantified using pyrolysis–gas

chromatography/mass spectrometry (Py-GC/MS), while optical microscopy and μ-FTIR spectroscopy were used to characterize MP morphology, size distribution, and polymer composition. Through Py-GC/MS analysis polyethylene (PE), polypropylene (PP), styrene-butadiene rubber (SBR), polymethyl methacrylate (PMMA), polystyrene (PS), and nylon-66 were detected. Analysis of the results from nine farms revealed that the total quantified polymer concentrations ranged from 51.94 to 8,434.05 μg kg^{-1} soil. PE was the dominant quantified polymer at five of the completed locations and reached 6,027.67 μg kg^{-1}, while maximum PP and SBR were 1,332.20 and 795.45 μg kg^{-1}, respectively. Complementary micro-FTIR analysis of MP>50 μm from six farms identified PE as the predominant polymer, with abundances ranging from 2 to 537 particles per 5 g of soil. Microscopy analysis revealed both fibers and fragments, with fiber lengths of 89–990 μm and fragment sizes of 17–654 μm. These preliminary findings demonstrate substantial spatial and polymer-specific variability in agricultural soils and highlight the value of combining chemical analysis with farmer-reported plastic-use information to identify potential sources and support practical agricultural-plastic management strategies. The analysis of samples from the remaining ten farms is ongoing and is expected to be completed by August 2026.

MWRM 2026 MW448

Characterizing piezoelectric motion for the construction of a micro Fabry-Pérot cavity

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Molecules at micromolar concentrations produce extremely weak Raman scattering signals, making them difficult to detect with conventional optical techniques, particularly within cellular environments. To address this challenge, we propose using a micro Fabry-Pérot cavity to enhance Raman scattering signals by several orders of magnitude. The cavity consists of two highly reflective mirrors separated by a few micrometers, forming an optical resonator. When the cavity length is tuned to an integer multiple of the scattered light wavelength, repeated reflections within the cavity produce constructive interference, increasing the optical intensity and strengthening the Raman signal.

In our experimental setup, one mirror is fixed while the other is mounted on a shear piezoelectric actuator, allowing precise control of the cavity length. By carefully adjusting the voltage applied to the piezo, we can finely position the movable mirror and maintain cavity resonance. The assembly process involves soldering electrical leads to the piezo, bonding a mirror to its surface with epoxy, connecting the actuator to a high-voltage amplifier, and monitoring cavity transmission using a photodetector and oscilloscope.

Mirror displacement is characterized using interferometry, where the piezo motion is measured by analyzing the interference signal generated by a single-wavelength laser

as a function of the applied voltage. Demonstrating reliable, controlled mirror motion is a critical step toward achieving stable cavity resonance and ultimately enhancing Raman scattering signals. The long-term goal of this project is to develop a cost-effective method for detecting and characterizing low-concentration molecules in solution-based environments that mimic the composition of living cells.

MWRM 2026 MW295

Chemical vapor deposition synthesis of hydrazone-linked covalent organic framework (COF-42) thin films

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Covalent organic frameworks (COFs) are crystalline, porous polymers that have recently emerged as a candidate materials platform for interconnect dielectrics in integrated circuits, following a report that a wafer-scale, oriented boronate-ester COF film can combine an ultralow dielectric constant with a cross-plane thermal conductivity an order of magnitude higher than conventional porous low-k dielectrics. Realizing this potential at scale, however, requires a synthesis route compatible with the solvent-free, wafer-scale processing used in back-end-of-line semiconductor fabrication - a requirement poorly met by the solution-based and interfacial growth methods used to produce COF thin films to date. Chemical vapor deposition (CVD) offers a solvent- and catalyst-free alternative directly compatible with this processing standard and was first demonstrated in 2023 for COF thin films with hydrazone, imine, and β-ketoenamine linkages grown by direct co-evaporation of two organic monomers onto a heated substrate. This vapor-phase approach is still in its infancy, and two aspects remain particularly underdeveloped: a general methodology for selecting precursor evaporation conditions for monomers without established vapor-pressure data, and detailed, multi-scale characterization of the resulting film surfaces. Building on the co-evaporation approach and monomer pair previously reported for hydrazone-linked COF-42, we address both gaps: precursor evaporation temperatures are determined directly from thermogravimetric analysis of each monomer, rather than adopted from literature values obtained under different reactor conditions, and film surfaces are characterized across several length scales to more completely capture morphology and roughness than is typically reported for CVD-grown COF films. We will report on the chemical bonding, crystallinity, elemental composition, and surface morphology of the resulting films, characterized using a combination of vibrational spectroscopy, X-ray diffraction, X-ray photoelectron and energy-dispersive spectroscopy, electron and atomic force microscopy, and spectroscopic ellipsometry, establishing successful hydrazone-linked framework formation and thickness-uniform films across the deposition zone.

MWRM 2026 MW278

Chemistry under nanoconfinement: From MAX phase etching to functional MXenes

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MXenes are an emerging family of two-dimensional transition-metal carbides, nitrides, and carbonitrides that are promising for applications ranging from energy storage and electronics to gas sensing and electromagnetic interference shielding. Most MXenes are synthesized by selectively removing the A-element layers from layered MAX-phase precursors, a chemical transformation that occurs within atomically confined spaces between strongly bonded transition-metal carbide or nitride slabs. The accessibility and reactivity of these nanoconfined A layers, together with the diffusion of etchants and reaction products through the evolving interlayer galleries, govern the efficiency of etching, the structural integrity of the resulting MXene sheets, and their surface terminations. Thus, chemistry under nanoconfinement provides the foundation for converting three-dimensional MAX phases into functional two-dimensional MXenes. Different synthetic approaches to MXenes, including traditional fluoride-based etching and molten-salt methods, as well as complementary chemical vapor deposition routes, will be discussed.

Advancement of MXene applications requires an understanding of their intrinsic physical properties, which can be determined through experiments performed on individual MXene flakes. The results of such experiments on monolayer flakes of $Ti_3C_2T_x$, Ti_2CT_x, $Nb_4C_3T_x$, $Ta_4C_3T_x$, TiVC, and $Cr_2TiC_2T_x$ MXenes will be discussed in this presentation. Electrical measurements of individual monolayers reveal that MXenes can be either n-type ($Ti_3C_2T_x$, $Nb_4C_3T_x$) or p-type ($Cr_2TiC_2T_x$) with very high electrical conductivities of up to 11,000 S cm^{-1} ($Ti_3C_2T_x$). Furthermore, MXenes show very high breakdown current densities of >10^8 A cm^{-2}, which exceed those for conventional metals. Mechanical measurements of individual MXene monolayers reveal their high Young's moduli of >300 GPa, establishing their potential for mechanically reinforced composites, protective coatings, and nanoresonators. These examples demonstrate the importance of single-flake measurements, which expand our understanding of the physical properties MXenes and broaden the already impressive range of their future applications.

MWRM 2026 MW243

Chiral bifunctional urea-based MOF catalyst with simultaneous basicity and dual-hydrogen-bond-donor activation for the Henry reaction

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The Henry reaction is an important carbon–carbon bond-forming transformation between aldehydes and nitroalkanes, and recently urea-functionalized metal–organic frameworks (MOFs) have gained popularity as potential catalysts. However, most reported MOF-based urea catalysts require the use of an external base for the reaction to proceed, which can promote uncatalyzed background reactions and diminish the benefits of catalytic confinement within the MOF pores, as well as reducing the selectivity of the catalyst. In this work, we investigate a bifunctional MOF catalyst that integrates both the hydrogen-bond-donating urea moiety and a chiral basic catalytic site within a single porous framework to suppress background reactivity, thereby increasing selectivity. KSU-1, a Zn-based pillared MOF containing both amine (-NH2) and hydroxyl (-OH) functionalities. The urea catalytic functionality is introduced through a post-synthetic modification (PSM) of the amine groups using 2,5-dioxopyrrolidin-1-yl methylcarbamate, generating a catalyst that combines dual hydrogen-bond activation for the reactants. A second PSM of the hydroxyl groups with the chiral base (1R,2R)-N1,N1-dimethylcyclohexane-1,2-diamine further incorporates the steric and chiral environment surrounding the active site. Our work investigates the effects of confinement on the selectivity and activity of a MOF-based urea catalyst while suppressing background reactions and achieving easy catalyst separation and recyclability.

MWRM 2026 MW26

Cholesterol inhibition may alter the production and the molecular profile of microvesicles

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Microvesicles are extracellular vesicles that are formed by the outward blebbing of the cell’s plasma membrane. They are then released into the extracellular space, where they can travel between cells, transporting materials such as lipids, proteins, DNA, and RNA/miRNA. The formation of these microvesicles is determined by the flexibility of the plasma membrane, which is influenced by sterol content. By comparing the structure of microvesicles in normal cells versus those with inhibition of specific enzymes involved in the cholesterol formation pathway, we aim to determine the effect of cholesterol

inhibition on microvesicle formation. In our study, we isolated and characterized microvesicles from three different cell lines: human embryonic kidney cells (HEK293T), human keratinocytes (HaCaT), and human microglial cells (HMC3). Different cell types can exhibit varied biochemical responses to the inhibition of cholesterol synthesis, and differences in the basal amount of cholesterol present within human cells suggest differences in cholesterol synthesis, turnover, or usage.
We were able to confirm microvesicle isolation by using the alpha-CD9 antibody. We were also able to measure the diameter of the microvesicles through dynamic light scattering. This showed that their size does not significantly change with cholesterol inhibition, with an average diameter of 192 nm.

MWRM 2026 MW129

Cholesterol metabolism and recycling in response to demyelination

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Myelin damage is a major feature of multiple sclerosis and is also observed in other neurological diseases including Alzheimer's disease, however, there are no FDA-approved therapies that directly target myelin repair. Myelin is a lipid-rich membrane containing up to 70% lipids with a high percentage of cholesterol. When myelin damage occurs in the central nervous system (CNS) during disease, the myelin lipids and cholesterol are metabolized and potentially recycled into newly forming myelin. This process, which is critical for successful myelin repair, is not well understood. A major goal of our research is to define the mechanisms of cholesterol metabolism and recycling during demyelination. Recently, we discovered that cholesterol levels were dramatically reduced in isolated remyelinated myelin as compared to healthy myelin – dropping from 45% of the total lipids to 25%. Biophysical studies revealed that reduced cholesterol in the remyelinated myelin reduced the stability of the lipid membrane. In the same mouse model, we also discovered that cholesterol ester levels in the brain and spinal cord were elevated up to 100-fold during peak periods of myelin damage. Normalization of cholesterol esters correlated with remyelination in the brain, whereas the spinal cord had continued elevation of cholesterol esters and limited remyelination. Thyroid hormone agonists promote both faster myelin repair and reduced accumulation of cholesterol esters. Efforts are underway to characterize cholesterol and cholesterol ester metabolism during demyelination and remyelination. We are using pharmacological inhibition and mouse knock-out lines to identify which enzymes and cells are involved in cholesterol ester metabolism during demyelination and remyelination. We are also developing analytical methods to track and isolate CNS cholesterol during demyelination and remyelination. Finally, we are exploring the mechanistic basis for how thyroid hormone modulates cholesterol metabolism and if this contributes to successful myelin repair. Overall, our goal is to define how CNS lipids and cholesterol are metabolized, stored, and recycled during disease, which has the potential to reveal new therapeutic strategies for neurological diseases affected by myelin.

MWRM 2026 MW327

Comparative assessment of the environmental degradation of polylactic acid (PLA) and starch-based bioplastics under simulated environmental conditions using mass loss and ATR-FTIR analysis

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Conventional petroleum-based plastics are widely used because of their durability and low cost; however, their slow degradation contributes to long-term environmental pollution. Bioplastics, including polylactic acid (PLA) and starch-based plastics, have been developed as more sustainable alternatives, but their degradation behavior under different environmental conditions is not fully understood. The objective of this study was to compare the degradation of PLA and starch-based bioplastics under simulated acidic, basic, and aqueous environments. Samples were cut into 2 × 2 cm squares, weighed before treatment, and placed in hydrochloric acid (HCl), sodium hydroxide (NaOH), or deionized water in aerated containers maintained at room temperature for five weeks. Fresh solutions were added weekly, and samples were monitored for physical changes throughout the experiment. Percentage mass loss was determined by comparing the initial and final masses of each sample. Chemical changes were evaluated using attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy to monitor changes in functional groups associated with polymer degradation. The starch-based bioplastic showed greater physical deterioration, higher mass loss, and more noticeable spectral changes than the PLA samples under the tested conditions. These results indicate that starch-based bioplastics degrade more readily than PLA under the environmental conditions examined and may provide a more environmentally sustainable alternative for applications where biodegradability is desirable.

MWRM 2026 MW445

Comparative photochemical oxidation behavior for different aldehydes over mixed oxide nanoparticles

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TiO_2-SiO_2 binary metal oxides were prepared by the sol-gel process. TiO_2-SiO_2 exhibits different photochemical properties from TiO_2. The adsorption of acetaldehyde and 2-butenal on TiO_2-SiO_2 has been studied by FT-IR. The oxidation reaction of acetaldehyde and 2-butenal under both dark and UV light conditions have been investigated and compared. The oxidation product of aldehyde may result in the formation of corresponding acid and carboxylate species. Detailed analysis of infrared

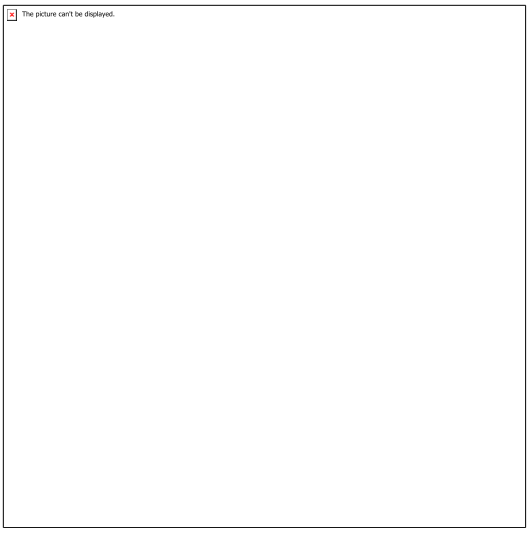
data has been used to investigate the byproducts and the kinetics of photochemical oxidation reaction for both aldehydes.

MWRM 2026 MW337

Comparing machine-learned interatomic potentials for diamond stability in liquid metals

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Machine-learned interatomic potentials (MLIAPs) enable reactive molecular dynamics at time and length scales inaccessible to ab initio molecular dynamics, but their transferability to metastable carbon chemistry remains uncertain. We compare MACE-MPA-0, Matlantis PFP v8.0, GRACE-2L/3L-OAM-L, and PET-OAM-XL for liquid Ga-Ni-Fe-Si environments relevant to diamond synthesis. Partial radial distribution functions for metal-only and carbon-containing liquids at 1448 K were first benchmarked against ab initio trajectories.
All models captured the principal metal-metal coordination shells, whereas carbon-containing distributions showed larger model- and density-sensitive discrepancies, particularly for C-C and Si-C structure. We then followed 87-carbon nanodiamonds in liquid Ga with 25-50% surface hydrogen coverage using up to ten independent replicates per condition.
At 50% coverage, median post-equilibration disassembly times were 17.8 ps for MACE-MPA-0, 41.8 ps for GRACE-2L-OAM-L, and 672 ps for Matlantis PFP.V.8.0.0. Matlantis and GRACE-2L-OAM-L also predicted stronger stabilization with increasing hydrogen coverage.
Finally, unbiased carbon-rich nucleation screens at 1300-1448 K produced model-dependent aggregation, with clusters containing up to approximately 20-23 carbon atoms, but no persistent connected all-carbon tetrahedral nucleus. MACE-MPA-0 occasionally produced isolated diamond-like carbon centers, whereas Matlantis PFP.V.8.0.0 and GRACE-2L-OAM-L predominantly generated non-diamond carbon aggregates or mixed Si-C tetrahedral motifs. Agreement in liquid structure therefore did not ensure agreement in rare-event kinetics or metastable-phase stability. Cross-potential comparisons, replicated trajectories, and targeted first-principles validation of transition-state and interfacial configurations are essential before universal MLIAPs are used to infer diamond-growth mechanisms.



MWRM 2026 MW43

Comparing the electronic properties of uranyl complexes featuring imine and amine ligands

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One of the striking features of uranium chemistry is the tendency for individual oxidation states to display unique coloration. The elusive uranium(V) oxidation state, for example, often appears colorless in coordination complexes. However, a number of U(V) species supported by imine-containing ligands have recently been reported that display vibrant colors, suggesting that imine moieties could drive ligand non-innocence when bonded to U(V). In this presentation, the synthesis of uranyl (UO_2^{n+}) complexes supported by two types of ligands will be presented, with a focus on studying how ligand conjugation influences the coloration and potential purity of the U(V) oxidation state in the complexes. Two new U(VI) compounds have been synthesized, characterized and used as starting material to obtain formal U(V) species for study; one features two imine moieties and the other contains amine donors in place of the imines. Studies with nuclear magnetic resonance, UV-visible and near-IR absorption spectroscopy, vibrational spectroscopy, cyclic voltammetry, bulk electrolysis and X-ray crystallography have been carried out to examine the role of imine vs amine ligation in the complexes. Our findings will be discussed, highlighting differences in the coloration of the complexes, and thus differences in their electronic structures. Additionally, the possibility of photochemically promoted reactivity in the U(V) complexes will be presented.

MWRM 2026 MW233

Comparing the thermodynamic properties and reactivity of FeIII- and MnIII-hydroxo complexes

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In biology and synthetic chemistry, transition metal oxidation processes often involve coupled transfer of a proton and an electron. In many of these cases, metal-oxygen species (M=O or M-OH) initiate C-H or O-H bond oxidation by concerted proton-electron transfer (CPET) reactions that involve electron transfer to the metal and proton transfer to the oxygen ligand. Enzymes such as lipoxygenase (LOXs) use MIII-hydroxo centers to oxidize fatty acids. Traditionally associated with iron, LOXs were later found to utilize manganese in the pathogenic fungi that target wheat and rice. The examination of FeIII-hydroxo and MnIII-hydroxo model complexes is significant in understanding the initial substrate oxidation step in LOXs. The scarcity of MnIII-hydroxo and FeIII-hydroxo complexes with the same coordination sphere poses a challenge in understanding the steric and electronic factors that govern the thermodynamic and kinetic properties of these complexes. This work discusses the generation and examination of the properties of a FeIII-hydroxo complex, [FeIII(OH)(dpaq)]+, and compare it to its MnIII-hydroxo analogue. Electrochemical methods are used to calculate the bond dissociation free energy (BDFE) of the FeII-aqua complex. When combined with the kinetic studies of CPET reactions by both MnIII-hydroxo and FeIII-hydroxo complexes with 1,2-diphenylhydrazine, this approach yields a comparison of the thermodynamic properties and reactivity of MIII-hydroxo complexes at parity of coordination sphere.

MWRM 2026 MW233

Comparing the thermodynamic properties and reactivity of FeIII- and MnIII-hydroxo complexes

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In biology and synthetic chemistry, transition metal oxidation processes often involve coupled transfer of a proton and an electron. In many of these cases, metal-oxygen species (M=O or M-OH) initiate C-H or O-H bond oxidation by concerted proton-electron transfer (CPET) reactions that involve electron transfer to the metal and proton transfer to the oxygen ligand. Enzymes such as lipoxygenase (LOXs) use MIII-hydroxo centers to oxidize fatty acids. Traditionally associated with iron, LOXs were later found to utilize manganese in the pathogenic fungi that target wheat and rice. The examination of FeIII-hydroxo and MnIII-hydroxo model complexes is significant in understanding the initial substrate oxidation step in LOXs. The scarcity of MnIII-hydroxo and FeIII-hydroxo complexes with the same coordination sphere poses a challenge in understanding the steric and electronic factors that govern the thermodynamic and kinetic properties of

these complexes. This work discusses the generation and examination of the properties of a FeIII-hydroxo complex, [FeIII(OH)(dpaq)]+, and compare it to its MnIII-hydroxo analogue. Electrochemical methods are used to calculate the bond dissociation free energy (BDFE) of the FeII-aqua complex. When combined with the kinetic studies of CPET reactions by both MnIII-hydroxo and FeIII-hydroxo complexes with 1,2-diphenylhydrazine, this approach yields a comparison of the thermodynamic properties and reactivity of MIII-hydroxo complexes at parity of coordination sphere.

MWRM 2026 MW33

Computational and photophysical investigation of fluorogenic Pepper RNA aptamers

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Fluorogenic RNA aptamers have gained significant attention for being used in cellular RNA imaging. Specifically, the Pepper aptamer variant has attracted considerable interest because of its strong photophysical performance while maintaining foundational RNA functions. Certain fluorogenic dyes, such as the HBC525, HBC530, and their derivatives demonstrate exceptionally high quantum yields and fluorescent intensities within their family when bound to the aptamer, creating the fluorogenic RNA aptamer complex. Currently, less is known on how fluorescence is activated in these complexes and the reasons why the fluorogenic dyes display little to no fluorescence on their own remain unclear. To better understand these experimental observations, density functional theory was used to model the interactions of the fluorogenic RNA complex, reproduce experimental data, illustrate the electronic behavior, and provide insight in probable HBC derivative structures. Along with the computational modeling, RNA X-ray crystallography was conducted to identify the structural effects of Pepper aptamer mutations and HBC derivative modifications in complex formation. Fluorometry evaluation of different RNA aptamer mutants and fluorophore derivatives demonstrated that change the position of an electron withdrawing fluorine substituent resulted in measurable changes in both absorption and emission maxima, in addition to the overall fluorescent intensities. Computational analysis indicated that incorporation of the HBC fluorogenic dye might induce structural changes to the fluorophore, favoring electronic activation for fluorescence. Collectively, computational calculations and RNA crystallography provided a comprehensive approach to understand the performance, structural behaviors, and electronics of fluorogenic Pepper aptamers.

MWRM 2026 MW167

Computational investigation of demercuration mechanisms in alkylmercuric hydroxides

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The reduction of alkylmercuric hydroxides by sodium borohydride is a key step in oxymercuration-demercuration of alkenes and alkynes. However, the exact mechanism of the demercuration remains uncertain. Likely mechanisms were proposed in the 1960's and studied by available means at that time. This work examines those proposed mechanisms using molecular modeling techniques within Wavefunction's Spartan 24 program. Two proposed mechanisms were found to be plausible with one being much more likely energetically. Computational methods and results will be presented.

MWRM 2026 MW85

Computational modeling of aryl diazonium degradation products relevant to neuropeptide receptor protein labeling

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Peptides bearing substituted aryl diazonium groups are useful labels for neuropeptide receptor proteins, but their application is limited by degradation of the reactive diazonium group. Experiments show that degradation rates depend on the aryl diazonium substituent. Here, computational methods were used to investigate possible mechanisms for hydride and hydroxyl degradation products in three substituted aryl diazonium compounds (Ar-Z-CH3, where Ar is the aryl diazonium group and Z = CH2, O, or S). Charge distribution and bond length analyses show that the diazo group is largely unaffected by the substituent. However, electron donation to the aryl ring increases in the order Z = O < CH2 < S and correlates with longer Z-C bonds adjacent to the substituent. These trends are consistent across the parent aryl diazonium compounds and their hydride and hydroxyl degradation products. Relaxed potential energy scans of the methyl dihedral angle relative to the aryl ring show that the Z = CH2 compound is stable in two conformations, whereas the Z = O and S compounds adopt more rigid geometries with only one stable conformer. Highest occupied molecular orbital distributions suggest that this rigidity results from enhanced π orbital overlap between the substituent and aryl ring when the methyl group lies in the ring plane. The greater conformational flexibility of the Z = CH2 compound is consistent with its faster experimental degradation relative to the Z = O and S analogs. For hydride product formation, citrate in the experimental buffer was identified as the most likely hydrogen atom donor because it is energetically favored relative to other buffer components, including trifluoroacetic acid, sulfamic acid, and dibasic phosphate. Isotopic exchange experiments support this assignment, although not all possible hydrogen atom donors in the reaction mixture have been tested. Potential energy surfaces for heterolytic and homolytic pathways leading to hydride and hydroxyl degradation products provide further insight into substituent-dependent degradation trends. Overall, this work offers structural and mechanistic details that may help reduce diazonium degradation during the synthesis of neuropeptide receptor protein labels, thereby optimizing these synthetic

routes and improving the efficiency of labeling neuropeptide receptor proteins for subsequent analysis.

MWRM 2026 MW416

Computational study of CO_2 solubility in the ionic liquid [bmim][PF_6] using Monte Carlo simulations

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Ionic liquids (ILs) are promising alternatives to conventional organic solvents because of their negligible vapor pressure and potential applications in carbon capture. In this work, Grand Canonical (GC) and Gibbs Ensemble (GE) Monte Carlo (MC) simulations were performed using the GOMC software package to investigate the solubility of CO_2 in 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF_6]) at 298, 313, and 353 K and pressures up to 70 bar. The ionic liquid was modeled using the refined all-atom force field of Bhargava and Balasubramanian, and CO_2 using the EPM2 model of Harris and Yung. Gas-phase non-ideality was accounted for using fugacity coefficients calculated from the Peng-Robinson equation of state. Henry's constants on the molality scale were obtained by fitting ln(f/m) versus molality and extrapolating to infinite dilution following the method of Kamps et al., which was validated by reproducing reported Henry's constants within 2%. The simulations reproduce the expected decrease in CO_2 solubility with increasing temperature and agree well with previous Monte Carlo simulations using the UA1 force field (Urukova et al., 2005). However, both force fields systematically underpredict experimental solubility measurements. This discrepancy is attributed to the reduced ionic charges in the Bhargava force field, which weaken electrostatic interactions between the CO_2 quadrupole moment and the PF_6 anion, a key contributor to CO_2 absorption. These results assess the performance of the Bhargava force field for predicting gas solubility and provide a foundation for future simulations of alkane absorption in CO_2-expanded ionic liquids.

MWRM 2026 MW342

Computational study of how molecular structure governs energy absorption, storage, and release in organic chromophores for quantum battery applications

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Quantum batteries store energy in the excited electronic states of light-absorbing molecules rather than chemical reactions, offering theoretically degradation-free energy cycling for use. Device performance depends critically on how much energy a chromophore dissipates as heat during the absorption-emission cycle, which is quantified by the Stokes shift and the accompanying ground-to-excited-state geometry

change. Initially, a benchmarking phase compared six density functionals and dispersion treatments, and three basis sets to identify the combination offering the best balance of accuracy, computational efficiency, and reliability for the class of molecules tested, establishing time-dependent density functional theory (TD-DFT) with B3LYP, PBE0, CAM-B3LYP, LC-ωHPBE, and ωB97X-D at the 6-311+G(d,p) and aug-cc-pVDZ levels as the validated method set for the remainder of the study. Applying this method set across twelve organic chromophores spanning benzene-derived and diazine/triazine scaffolds, results reveal that the character of the first excited singlet state, rather than substituent electron-donating or -withdrawing strength, is the dominant predictor of reorganization energy. Molecules whose excited state is a delocalized π→π* transition show minimal geometric distortion, with the phenoxide anion showing the smallest Stokes shift measured (0.11 eV). In contrast, molecules whose excited state is a localized n→π* transition undergo substantially larger reorganization, culminating in a Stokes shift of 2.04 eV for 1,2,3-triazine, the largest in the series. Within this n→π* group, the severity of reorganization is governed by nitrogen-nitrogen bond adjacency in the ring. Guided by this trend, a current batch of calculations tests whether protonating or oxidizing the ring nitrogen lone pair, as in pyridinium and pyridine N-oxide, can suppress the unfavorable n→π* state and restore favorable π→π* character, alongside a parallel series probing anionic donor substituents near their electron-detachment limit. These findings establish a predictive design principle for chromophore selection and advance toward the rational design of next-generation quantum battery materials.

MWRM 2026 MW274

Confinement-driven catalysis in metal–organic frameworks

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Metal–organic frameworks (MOFs) offer a unique platform for controlling chemical reactivity through confinement, combining high surface area, well-defined pore architectures, and tunable metal nodes and linkers. In this work, we develop a reactive machine-learned simulation framework to understand how the local environment of Zr-based MOF nodes governs alcohol dehydration mechanisms. The central goal is to connect pore-scale confinement, acidity, and interfacial structure with molecular reaction pathways that are difficult to resolve using conventional molecular dynamics or direct ab initio simulations.
We focus on alcohol dehydration at Zr-based MOF interfaces, where competing pathways can produce either ethers through substitution-type chemistry or alkenes through elimination-type chemistry. High-quality density functional theory reference data, generated with the ωB97X-V functional, are used to train a MACE-based machine-learned interatomic potential capable of describing adsorbed alcohols, surface alkoxy species, proton transfer, C–O bond formation and cleavage, and C–H/C–C rearrangements. Active learning is used to improve coverage of reactive configurations, while model validation is performed using chemically meaningful observables such as Zr-node bond distances, intermediate-state energetics, force consistency, and reaction-

coordinate behavior.
The trained potential is combined with OPES enhanced-sampling molecular dynamics to construct free-energy surfaces for alcohol dehydration reactions under confinement. Our simulations for ethanol dehydration have produced barriers consistent with prior calculations, validating the machine-learned potential and enhanced-sampling protocol. The current workflow enables long-timescale simulations that preserve near quantum-mechanical accuracy while accessing reaction events beyond the reach of standard DFT-based dynamics.
This study provides a transferable strategy for investigating confinement-driven catalysis in MOFs. By resolving the competition between substitution and elimination pathways across different alcohol substrates, the work aims to quantify reaction barriers, intermediate stabilities, and pathway selectivity, ultimately revealing how MOF pore environments control chemical reactivity at the molecular level. These insights can guide future catalyst design by linking structural confinement to measurable mechanistic and kinetic outcomes.

MWRM 2026 MW212

Conformational sampling of biomolecules via generative modeling

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Molecular dynamics and Monte Carlo simulations are traditional approaches for generating conformational ensembles subject to high computational cost and limited time scales. Generative modeling via artificial intelligence has become an alternative technique that has the potential for the rapid generation of structural ensembles without consideration of kinetic barriers that hinder efficient sampling via traditional approaches such as molecular dynamics simulations or Monte Carlo sampling. The focus is on generating conformational ensembles for proteins, ranging from intrinsically disordered proteins, ensembles of folded proteins, and unfolded state ensembles at higher temperatures at different levels or resolution up to atomistic detail including side chains. Examples from the idpGAN, idpSAM, and aSAM(t) models will be presented along with recent progress in developing strategies for biasing the conformational ensemble generation at inference time with applications to the incorporation of experimental restraints.

MWRM 2026 MW302

Contact lens modification & microparticles production for ocular drug delivery

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Currently, eye drops and intravitreal injections are the standard methods for delivery of ocular medications. Eye drops deliver only 1-5% of the medication and can lack patient compliance. Injections can lead to serious complications including blindness or eye loss. Slow elution from modified contact lenses would be less stressful for the patients and increase drug absorption and ergo drug efficacy. This study investigates contact lenses that have been subjected to surface addition of amino groups and electrostatic LbL (Layer by Layer) treatment of two biopolymers, hyaluronic acid (HA) and chitosan (CS). These compounds are biodegradable and biocompatible and provide many beneficial properties including: antimicrobial, wound healing, increased water retention, decreased protein absorption and increased viscoelasticity. Carboxymethyl calcium carbonate (CMCS) microparticles will be loaded via direct permeation or a LbL treatment with norfloxacin (common ocular antibiotic). These lenses will be evaluated for medication elution time. Zingerone, a naturally occurring phenolic compound found in dried ginger, is a known natural antimicrobial agent. Drug release of zingerone incorporated lenses (HA layer) will also be evaluated. Microparticles were characterized by Optical Microscopy, TGA, SEM, ATR-IR, and PXRD. Lenses will be characterized by wettability, equilibrium water content (EWC), transparency, protein deposition, and bacterial studies.

MWRM 2026 MW138

Continuous monitoring of tumor necrosis factor alpha using online affinity micro free-flow electrophoresis

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Real-time monitoring of biochemical messengers such as Tumor Necrosis Factor Alpha (TNF-α) is essential for understanding dynamic biological processes. However, current methods are limited in their ability to provide continuous data. To address this limitation, we are developing a noncompetitive platform that integrates micro free-flow electrophoresis (μFFE) with aptamer-based affinity interactions to enable selective separation and analysis. μFFE is a separation technique that enables continuous separation of analytes as a sample flows through a planar channel under an electric field applied perpendicular to the direction of flow. In affinity μFFE, binding between an affinity reagent and the target causes electrophoretic mobility shifts, enabling separation of bound and unbound species. Aptamers are used as the affinity reagent due to their small size and high stability, which produce enhanced electrophoretic mobility shifts upon target binding. Significant outcomes included clear separation of bound and unbound aptamer peaks, establishment of a linear calibration curve for TNF-α that confirms the feasibility of the assay, and reproducible signals achieved through optimization of buffer composition and aptamer handling. Ongoing work is focused on enhancing temporal response and improving the assay's limit of detection. Overall, this work demonstrates a compact, non-competitive platform capable of continuous, real-time monitoring of TNF-α. This approach provides a foundation for improving temporal

resolution in biomolecular detection and has strong potential for future diagnostic and analytical applications.



MWRM 2026 MW297

Controlled aqueous RAFT polymerization of amino-functional polymers for antimicrobial applications

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Antimicrobial resistance is a growing global health challenge that has increased interest in synthetic cationic polymers as potential alternatives to conventional antibiotics. Controlled polymerization methods provide an opportunity to tailor polymer molecular weight and structure, which can strongly influence antimicrobial performance. This project investigates thermal and light-mediated reversible addition–fragmentation chain-transfer (RAFT) polymerization as controlled aqueous methods for synthesizing amino-functional polymers for antimicrobial applications. Thermal RAFT polymerization produced well-defined polymers across a range of targeted molecular weights with narrow molecular weight distributions (1.05–1.14). Preliminary photoiniferter and oxygen-tolerant PET-RAFT polymerizations also successfully generated these polymers under mild aqueous conditions, demonstrating the feasibility of light-mediated synthesis without prior deoxygenation. Preliminary broth microdilution assays against *Pseudomonas* aeruginosa showed that lower-molecular-weight polymers exhibited greater antibacterial activity than higher-molecular-weight analogues, suggesting that polymer chain length is an important design parameter for antimicrobial performance.

These results demonstrate that aqueous RAFT polymerization provides a versatile platform for preparing well-defined antimicrobial polymers and establish molecular weight as an important variable for the future design and optimization of polymer-based antimicrobial materials.

MWRM 2026 MW227

Controlled release of oxygen from hydrogen peroxide using recycled HotHand packet solid

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The solid in a spent HotHands packet was combined with an equal amount, by weight, of both a suppressing agent, disodium hydrogen phosphate, and an approximate 30% hydrogen peroxide solution. The resultant reaction, kept cool in a room temperature water bath, allowed for a steady release of oxygen gas. Combining ten grams of each component, this simple procedure was used to support two undergraduate general chemistry lab activities. The first lab activity was quantitative in nature. Students determined the weight of oxygen lost from the peroxide solution and then, through stoichiometry, determined the exact concentration of hydrogen peroxide in the original hydrogen peroxide solution. The second lab activity was more qualitative, wherein students used the oxygen gas generated to burn steel wool vigorously. Although there are other well known catalysts for the decomposition of hydrogen peroxide, this particular approach allows students to be active participants in the recycling and use of a well known single-use commercial product to support an undergraduate chemistry lab.

MWRM 2026 MW258

Controlling ambident reactivity in organic synthesis via catalysis

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We have discovered and developed a highly chemoselective O-benzylation of ambident 2-quinolinone nucleophiles via Pd-catalysis. Detailed reaction analysis using direct-injection high resolution mass spectrometry (DI-HRMS) combined with *in situ* ^{31}P NMR implicate a phosphine mono-oxide Pd(II) benzyl complex as a key intermediate on the catalytic cycle. Extrapolation of this method to selectively O-alkylate a series of substituted 2-quinolinones using several benzylic electrophiles providing 2-benzyloxy quinolines in good yields and impressive O:N selectivities (up to 100:1) utilizing as little as 1 mol % Pd-catalyst to achieve high selectivities and yields will be discussed.



MWRM 2026 MW95

Co-occurrence of nitrate, nitrite, and arsenic in Lower Elkhorn Natural Resources District groundwater wells

***Elizabeth Chhoeung**, echhoeung2@unl.edu, Martha G. Rhoades. School of Natural Resources, University of Nebraska-Lincoln, Lincoln, Nebraska, United States*

Nearly 85% of Nebraska residents rely on groundwater for drinking. Over the past 70 years, agricultural production has contributed to widespread groundwater contamination. This study examined the relationships and co-occurrence of arsenic, nitrate (as nitrate-N), and nitrite (as nitrite-N) concentrations in 49 Lower Elkhorn Natural Resources District (LENRD) groundwater wells. Descriptive statistics, correlation, and regression were used to assess associations between well characteristics and contaminant concentrations. Spearman's rank-order correlation test determined a significant ($p<0.05$) negative correlation between arsenic concentration and nitrate concentration. No statistically significant correlations were observed between total well depth and nitrate or nitrite concentrations or between nitrate/nitrite and arsenic concentrations. Multiple pesticides detected in the wells showed significant ($p<0.05$) correlations against each other. Consistent with the initial Spearman's nitrate and arsenic correlations, logistic regression analysis further confirmed a statistically significant negative trend between arsenic and nitrate ($p<0.05$). Out of 49 wells, 24 wells were determined to have all three contaminants present. These quantified associations provided critical groundwork for epidemiologists and public health professionals to identify joint toxicological risks and associated adverse health outcomes, such as birth defects and cancer risks. These findings contribute to public health research, water quality awareness, and guide decisions regarding groundwater usage by identifying key groundwater contaminants and exposure routes.

MWRM 2026 MW276

Correlating solvent structure and single-molecule transport in nanoconfined ethanol–water–salt mixtures using confocal Raman and fluorescence correlation spectroscopy

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Understanding molecular transport under nanoconfinement is essential for advancing membrane separations and in the development of nanofluidic devices. In this work, confocal Raman spectroscopy (CRS) and confocal fluorescence correlation spectroscopy (CFCS) were employed to investigate the influence of Cs_2SO_4 (0-3 wt%) concentration on 60:40 (wt%) ethanol–water mixtures confined within anodic aluminum oxide (AAO) nanopores having diameters of 10, 20, and 30 nm. Raman measurements revealed systematic salt- and pore-size-dependent variations in the O-H stretching region, consistent with changes in solute interactions and local solvent organization relative to bulk solution. Complementary CFCS measurements of Rhodamine B (RhB) demonstrated distinct fluorescence fluctuation patterns in confined nanopores compared with bulk solution, consistent with pore size-dependent molecular transport. The combined structural and dynamical measurements reveal important correlations between solvent organization and single-molecule diffusion under nanoconfinement. These findings provide new insights into ion-induced solvent heterogeneity in nanoporous environments and contribute to fundamental understanding of mass transport processes under nanoconfinement.

MWRM 2026 MW423

Correlation of high molecular weight-glutenin subunit allele *Glu-B1-al* with seed, milling, dough, and baking characteristics in hard winter wheat

***Bruna Mattioni**[2], mattioni@ksu.edu, Michael Tilley[1], Rhett C. Kaufman[1], Donghai Wang[2]. (1) USDA Agricultural Research Service, Washington, District of Columbia, United States(2) Biological and Agricultural Engeneering Department, Kansas State University, Manhattan, Kansas, United States*

High Molecular Weight glutenin subunits (HMW-GS) strongly regulate the technological properties of bread wheat, making them fundamental genetic markers for wheat breeding. Overexpression of HMW-GS 7 (7^{oe}) has been shown to significantly increase gluten strength and dough mixing tolerance. The *Glu-B1-al* allele, which expresses this subunit, is frequently selected by breeders. However, establishing a precise mathematical correlation between this qualitative genetic marker and quantitative dough characteristics remains a significant challenge. This study aimed to establish the mathematical relationship between the *Glu-B1-al* allele and diverse wheat quality

characteristics to provide breeders with an effective tool for a precise, early-generation prediction and selection. Data were compiled from the Wheat Quality Council 2026 report, which evaluated 26 Hard Winter Wheat (HWW) samples grown across the US Midwest in 2025. The dataset encompassed 104 parameters correlating seed characterization, milling quality, dough rheology, baking performance, and protein composition. The presence or absence of the *Glu-B1-al* allele was encoded as a binary variable (1 = presence, 0 = absence). Principal Component Analysis (PCA) and Pearson correlation analyses were performed, with a of correlation threshold of r > 0.40 denoting a moderate to strong linear relationship. Strong positive correlations were observed between the *Glu-B1-al* allele and key technological parameters, specifically farinograph, extensograph, and alveograph metrics. Additionally, the allele correlated significantly with the falling number, pasting temperature, and the polymeric/monomeric protein ratio, all of which serve as direct indicators of gluten strength. PCA successfully differentiated the wheat varieties into distinct clusters based on these quality profiles. These findings corroborate existing qualitative literature by providing a concrete, quantitative link between the *Glu-B1-al* allele and flour technological properties. Furthermore, the PCA-based clustering offers millers a clearer tool for variety classification. Future research will expand the sample size to validate these mathematical correlations across a broader range of growing environments.

MWRM 2026 MW423

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MWRM 2026 MW192

Covalent modification of Kevlar fabric with oxime for improved detoxification of organophosphates and its use in protective fabrics

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Nerve agents, categorized as organophosphorus compounds, present considerable threats due to their high toxicity. Detoxification methods frequently utilize small-molecule organophosphate scavengers, especially in non-aqueous environments. Recent developments indicate that functionalized cotton materials may be transformed into protective textiles that can effectively neutralize nerve agents upon contact. Nevertheless, the modified Kevlar fabric, a key element of military textiles, has yet to be investigated for its effectiveness in detoxifying organophosphates. Therefore, this advancement is crucial for improving the safety of military uniforms, potentially providing soldiers with enhanced protection against chemical warfare agents.
In this study, novel oxime compounds are developed as organophosphate scavengers featuring an imidazole group. These compounds are effective in decontaminating organophosphate substances in non-aqueous environments at room temperature and ambient pH. Additionally, these compounds can be attached to materials like cotton and Kevlar, potentially functioning as protective textiles that neutralize nerve agents upon contact, which may have applications in protective military uniforms (Figure 1).

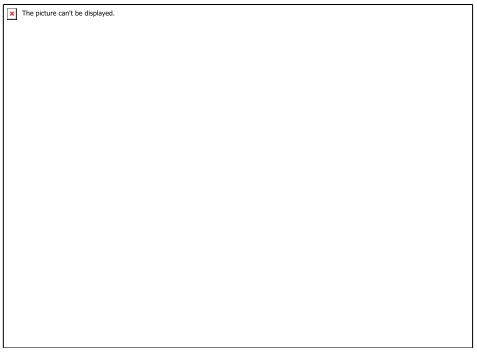


Figure 1. Modified Kevlar designed for the detoxification of organophosphate pesticides.

MWRM 2026 MW15

CRISPR knock-in to identify tethering factor association of recombinant adeno-associated virus (rAAV) to the human genome

***Josie Diffendaffer**, jdiffendaffer@drury.edu. Drury University, Springfield, Missouri, United States*

Recombinant Adeno Associated Virus (rAAV) is engineered from Adeno Associated Virus (AAV) that functions as a viral vector to deliver transgenes that are used in gene therapy. rAAV has been identified to associate extra-chromosomally with distinct sites on the human genome. How rAAV persistently associates with these loci remains unknown. Using a cluster regularly interspaced short palindromic repeats (CRISPR) knock-in of green fluorescent protein (GFP) that is activated by rAAV-delivered enhancer elements, we propose to perform a time course imaging experiment to assess the tethering of rAAV to the human genome chromosome 1.109. Leveraging this system, a CRISPR screening with Neomycin (Neo) clones will be used to identify the host protein tethering rAAV persistently at the association site. Single cell knock-in clones will be used for the future time course imaging assay and CRISPR screening to identify host tethering proteins. Identification of the host factor could help modify and direct rAAV-CRISPR systems to perform directed genome engineering strategies.

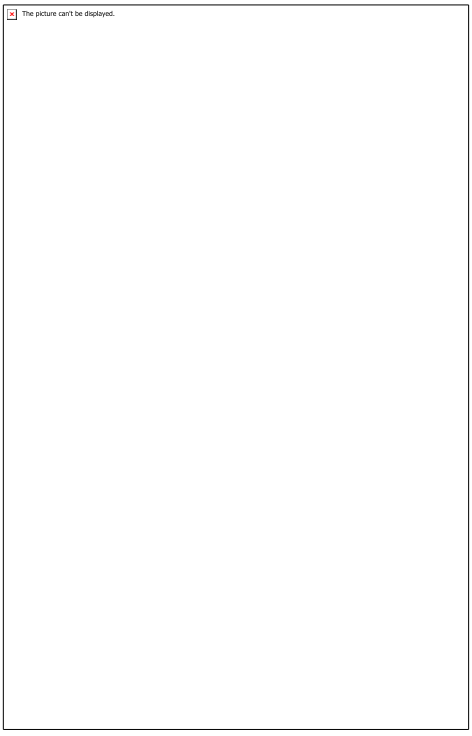


Figure 1: Sanger Sequence plasmid samples 4D (part A) and 16I (part B) viewed in SnapGene

showing the donor DNA: 5' overhang_MUL1 promoter_GFP/NEO_3' overhang in a TOPO vector.

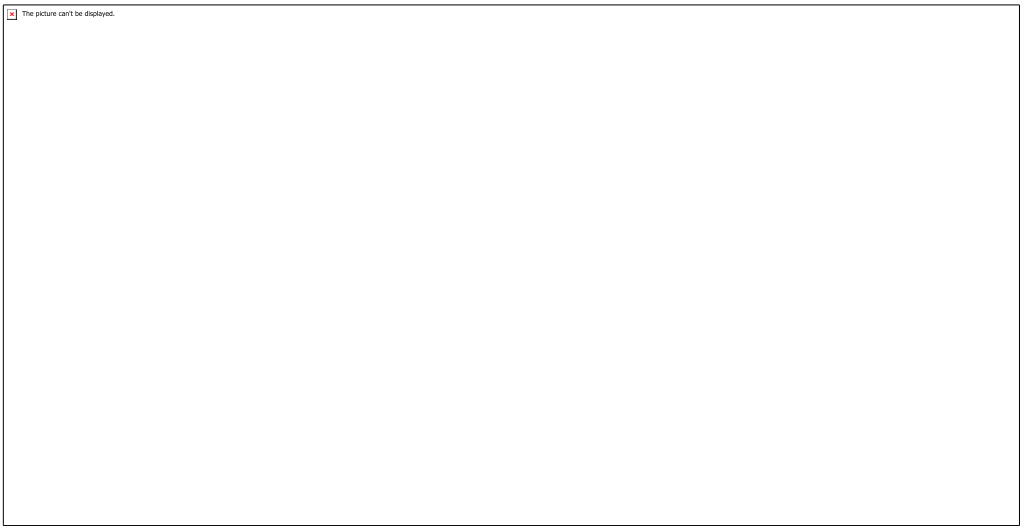


Figure 1: Donor DNA in a 1.5% gel with PCR samples that underwent a temperature gradient (50-70°C) turning plasmic DNA into linear DNA with verified extracted fragments. Part A was sample 4D: 5'_MUL1p_GFP_3' and part B was sample 16I: 5'_MUL1p_NEO_3' both showed a band around 3kb.

MWRM 2026 MW96

Critical developments towards using coaxial electrospun nanofibers for AgCl-based water disinfection in long-duration spaceflights

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Current water disinfection technology aboard the International Space Station relies on a two-part iodine dosage system, necessitating the removal of iodine before human consumption. In an effort to reduce complexity and required mass of the water treatment system, alternative methods of disinfection are being investigated. To this end, silver ion has been proven as an effective broad-spectrum biocide compatible with the National Aeronautics and Space Administration's long-duration mission requirements. In our on-going project, coaxial electrospinning is used to produce nanofiber membranes with silver chloride nanoparticles (AgCl NPs) embedded inside the nanofibers to achieve controlled release of silver ions as a disinfectant in a flow-through setup. Polyacrylonitrile (PAN) is used as an outer layer, and polymethyl methacrylate (PMMA) is mixed with the AgCl NPs as an inner component to prepare core-shell fibers. The nanofiber membrane is subjected to post-processing treatment with acetone to remove PMMA and expose AgCl NPs in the hollow channels. This presentation reports two critical developments towards this goal. First, in order to facilitate characterization of Ag+ release rate testing over a continuous period of more than 20 hours, an autosampler was designed to automate sample collection. 3-D printed

and laser-cut components formed the base of the design, while a custom circuit supported an ESP32 microcontroller programmed to collect samples at specified intervals. Further integration using Bluetooth communication allowed for ease of operation and variation in collection parameters. After collection, flow-through samples were analyzed for silver ion concentration using a silver sulfide ion-sensitive electrode. The autosampler has successfully enabled sample collection over greater time intervals without human presence. Second, different polymer formulations are being explored to optimize electrospinning of core-shell nanofibers. The viscosity of different PAN and PMMA solutions is measured and correlated with the Taylor cone stability during electrospinning. Transmission Electron Microscopy is used to characterize the fiber morphology and correlated with the Ag+ release testing.

MWRM 2026 MW157

Crystal engineering for water: Molecular design meets artificial intelligence

***Zhiling Zheng**, z.z@wustl.edu. Washington University in St Louis, St. Louis, Missouri, United States*

Addressing global challenges in water and resource sustainability requires both innovative materials and new discovery paradigms. In this seminar, I will describe the molecular engineering of porous crystalline materials, particularly metal-organic frameworks (MOFs), for atmospheric water harvesting. By establishing design principles governing water adsorption, pore architecture, energy efficiency, and scalable synthesis, our work has enabled portable water-harvesting devices that were successfully field-tested in the extreme conditions of Death Valley National Park.

Building upon these design principles, I will highlight recent collaborative efforts to engineer water-stable MOFs for the selective capture of rare earth elements from aqueous environments, extending crystal engineering from water harvesting to resource recovery. Throughout the seminar, I will compare traditional intuition-driven design with AI-enabled materials discovery, mentioning our efforts since 2022 to integrate large language models and robotics into porous materials research.

MWRM 2026 MW411

Crystallization kinetics and structural signatures of phase transition in supercooled water

***Christopher Zhou**, zhouchri@grinnell.edu, Rajendra Maharjan. Chemistry, Grinnell College, Grinnell, Iowa, United States*

Water exhibits anomalous thermodynamic behavior that becomes increasingly pronounced in the metastable supercooled regime, where rapid ice crystallization limits direct experimental investigation of supercooled water and the proposed liquid–liquid phase transition. In this study, direct coexistence molecular dynamics simulations were

performed to investigate crystal growth along the basal, primary prismatic, and secondary prismatic ice crystal faces at different temperatures. The secondary prismatic face grew faster relative to the other two faces of the crystal surface. Structural ordering was characterized using thermodynamic properties, radial distribution functions, structural order parameters, and hydrogen-bond ring statistics. Analysis of pure water at different temperatures revealed increasingly ice-like structural features with decreasing temperature, providing a basis for examining structural changes associated during crystallization and potential phase transitions. Ongoing work aims to determine the critical ice nucleus required to initiate crystallization in supercooled water below the melting temperature. Future studies will extend these analyses to investigate high density and low density liquid phase transitions, as well as amorphous phase transitions among the high density, low density, and very high-density amorphous phases under elevated pressures.

MWRM 2026 MW283

Crystallographic insights into ionic-liquid phase behavior: σ-hole interactions, melting, and supercooling

Patrick Hillesheim[1]*, pchille@ilstu.edu, Arsalan Mirjafari*[2]*, Matthias Zeller*[3]*. (1) Chemistry, Illinois State University, Normal, Illinois, United States(2) Chemistry, State University of New York at Oswego, Oswego, New York, United States(3) Chemistry, Purdue University, West Lafayette, Indiana, United States*

Ionic liquids (ILs) are salts that melt at unusually low temperatures and can be tuned by changing their cations, anions, or attached functional groups. This versatility also makes phase behavior difficult to predict: small structural changes can produce large differences in melting points and induce supercooling behavior. Single-crystal X-ray diffraction provides atom-resolved models of ion arrangement, noncovalent interactions, and coexisting molecular configurations. Combined with thermal and computational measurements, crystallography can therefore connect molecular organization to bulk properties.

We illustrate this approach through two case studies. First, we examine a series of thiazolium ILs containing sulfur-centered σ holes—directional regions of positive electrostatic potential that can guide anion approach. Crystal structures and melting-point data are compared to evaluate how the accessibility, geometry, and competition of these contacts influence lattice organization. These comparisons distinguish the strength of an individual interaction from its ability to generate a recurring, cooperative packing motif.

Second, we examine benzyl-functionalized ILs that crystallize directly or only after long-lived supercooling. Some remained liquid for weeks, and one for nearly two years, before crystallizing. Their structures show that conformational heterogeneity, competing π-mediated interactions, steric blocking, and changes in effective molecular volume can frustrate long-range order. Crystallographic disorder is therefore not merely a refinement complication; it preserves evidence of competing arrangements that delayed crystallization.

Together, these studies demonstrate how crystal structure analysis can test mechanistic hypotheses about intermolecular forces and guide the design of ILs with targeted melting and metastability.

MWRM 2026 MW309

Ctrl-X, Ctrl-V, Ctrl-PET: Rapid, selective, and mild depolymerization of poly(ethylene terephthalate)

Benjamin Heiderscheit[1]*, benheid@iastate.edu, Dhananjay Dileep*[1]*, Jared Kaczor*[1]*, Deep Patel*[1]*, Aadhi Subbiah*[1]*, Samuel Chambers*[1]*, William Teggatz*[1]*, Lucas Showman*[2]*, Michael J. Forrester*[1]*, George A. Kraus*[3]*, Luke Roling*[1]*, Eric W. Cochran*[1]*. (1) Department of Chemical and Biological Engineering, Iowa State University of Science and Technology, Ames, Iowa, United States(2) W.M. Keck Metabolomics Research Laboratory, Iowa State University of Science and Technology, Ames, Iowa, United States(3) Department of Chemistry, Iowa State University of Science and Technology, Ames, Iowa, United States*

As plastics continue to plague our landfills, it is becoming increasingly important to find a better way of recycling plastics. Current methods for recycling plastics, specifically poly(ethylene terephthalate) (PET), have many drawbacks: mechanical recycling deteriorates material quality with each reuse cycle, and chemical recycling produces virgin-grade plastic at the expense of high cost and energy; thus, leading to only 9% of total plastics being recycled globally. This research proposes a novel rapid method of selectively depolymerizing PET at low temperatures and near ambient pressures. This method selectively attacks PET, alleviating the presorting burden required for mechanical recycling. Compared to other conventional chemical recycling processes, like methanolysis, which uses temperatures of 200 °C, pressures of 20 bar, uses extremely corrosive catalysts, and can take up to 10 hours, the proposed method of recycling uses temperatures at 60 °C, near ambient pressures, uses mild solvents (0.5 to 1 M KOH on a MeOH basis), and can depolymerize PET in under one hour. Feedstock form factor and crystallinity proved decisive in determining rates of depolymerization. Cryomilled powders with a surface area to volume (S/V) ratio of about 17 mm^{-1}, relative crystallinity ~ 30%, depolymerized in about an hour, while injection molded bars (S/V ~ 2 mm^{-1} and relative crystallinity ~ 16% for amorphous and ~ 30% for crystalline bars) required over 10× the time depending on crystallinity and temperature using methanolic KOH. We also observed that water-rich conditions severely suppressed reaction kinetics as sluggish hydrolysis competed over the more rapid methanolysis cascade. Experimentally changing solvent composition to 30% water and 70% 0.5 M methanolic KOH dropped reaction yield from 89% to 29% at the 30 min timestamp. Thus, we were able to objectively discern governing factors for rapid depolymerization of polyesters, which would allow for process optimization and scale-up, eventually evoking commercial appeal to a closed-loop recycling process.



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MWRM 2026 MW355

Cu(II) adsorption behavior of an organic nanotube having inner amine groups

***Mikynzie Tatro**, mikynzie@ksu.edu, Anuththara D. Karunarathn, Takashi Ito.*
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This research project aims to understand the properties of organic nanotubes (ONTs) as adsorbents for heavy metal ions. Our ONTs are formed from bolaamphiphiles via self-assembly, and have nanoscale, tubular structures (10 nm in diameter) with distinct functional groups on the inner and outer surface. Previously, we quantitatively assessed the Cu(II) adsorption behavior of an ONT with inner carboxyl groups (COOH-ONT) using an electrochemical method with the Langmuir model. We showed that the

adsorption was pH-dependent, and the adsorption affinity of the COOH-ONT was significantly higher than other adsorbents based on carboxyl groups, which we attributed to the enhancement of Cu(II) binding onto the inner surface with nanoscale concave curvature. In this study, we measured the Cu(II) adsorption behavior of an ONT with inner amine groups (NH2-ONT) using the same methods for comparison. As with the COOH-ONT, the NH2-ONT exhibited more efficient Cu(II) adsorption at higher pH. More importantly, the Cu(II) binding affinity of the NH2-ONT was one order higher than that of the COOH-ONT. We also employed SEM to verify the stability of the tubular structure of the NH2-ONT upon Cu(II) binding. These results will assist in developing nanomaterials that will specialize in capturing and separating heavy metal ions from aqueous systems.

MWRM 2026 MW355

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MWRM 2026 MW371

Data-driven predictive synthesis of metal–organic frameworks

***Zhiling Zheng**, z.z@wustl.edu. Washington University in St Louis, St. Louis, Missouri, United States*

The art of reticular chemistry lies in connecting well-defined building blocks through strong bonds to create materials with targeted functions. Metal–organic frameworks (MOFs) embody this principle, offering vast structural and chemical diversity. Yet, their synthesis remains labor-intensive, governed by empirical intuition and repeated trials to achieve single-crystal quality. Here we present data-driven methods that simplifies MOF synthesis for chemists of all backgrounds. By data mining over 15000 experimental MOF publications, a large language model extracts synthesis conditions including metal source, linker, stoichiometry, solvent, temperature, reaction time, and resulting properties such as surface area and thermal stability. From these data, an algorithm infers likely unsuccessful attempts, which captures the unreported side of experimentation. Integrating both successful and failed outcomes enables machine learning models to predict MOF crystallization success with 83% accuracy. Complementing this, an automated high-throughput platform collects new synthesis data and refines conditions through Bayesian optimization. This closed-loop system learns iteratively, much like a human chemist developing intuition. Together, these approaches outline a path toward predictive synthesis, where artificial chemical insight guides discovery and accelerates the realization of novel, functional frameworks.

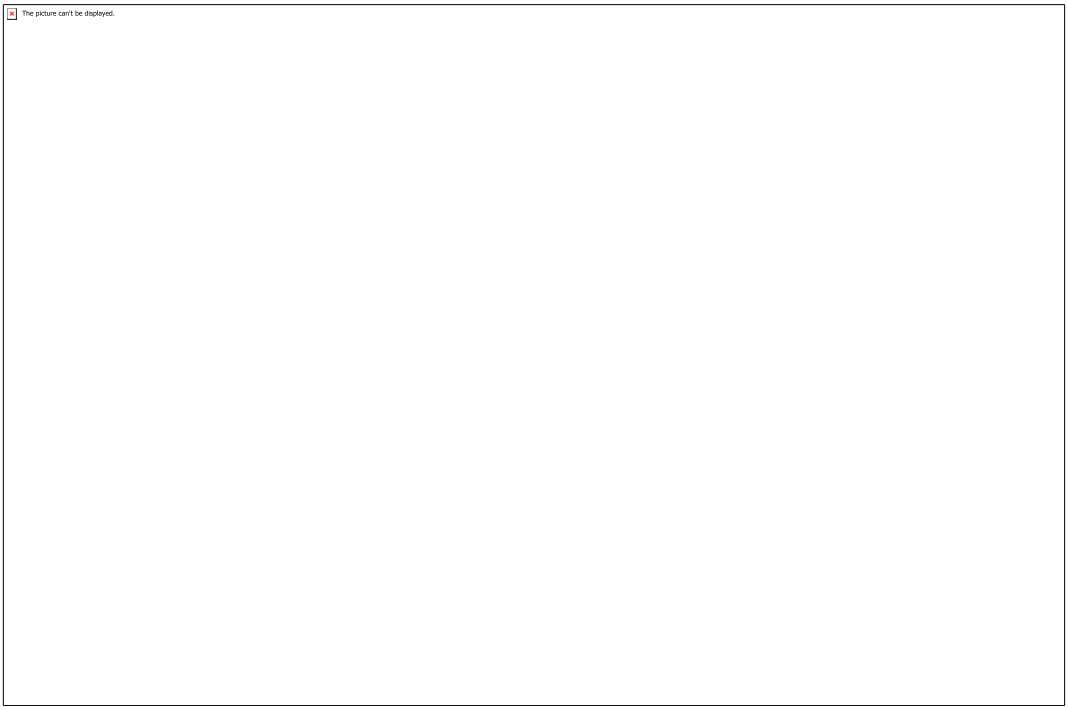
MWRM 2026 MW336

Data-efficient energy correction for quantum-informed molecular dynamics using Gaussian process delta learning

***Vibhav Chinta**, vchinta30@gmail.com. 12th Grade, Marquette High School, Chesterfield, Missouri, United States*

The accurate prediction of molecular binding energies is important for designing covalent kinase inhibitors, which are a promising class of cancer drugs. Quantum chemistry methods such as CCSD(T) can provide the accuracy needed to distinguish between reversible and irreversible binding. However, computational costs limit the amount of calculations to be performed. This data scarcity issue is prominent in the context of quantum hardware where limited qubit counts restrict available data. Current approaches address sequential transfer learning, which retain neural network force fields at each new level. In this project we present a Gaussian delta learning framework that learns the energy correction between density functional theory and CCSD(T). This occurs without retraining the underlying model. We combined predictions from a pretrained MACE neural network force field with SOAP geometric descriptors as input features to a Gaussian process regression model trained on 330 CCSD(T)/aug-cc-pVTZ single-point energies across both the direct water attack and relay proton transfer

mechanisms of metaphosphate hydrolysis. The combination of MACE and SOAP achieves a validation mean absolute error of 42.3 meV, reaching chemical accuracy and representing a 7.4-fold improvement over geometric descriptors alone. The Gaussian process provides uncertainty estimates that can directly extend active learning loops to guide calculations. The results show that lightweight correction models can extract chemical accuracy from sparse high-fidelity datasets. This suggests applications where expensive quantum calculations are limited. Future work can examine the L11 covalent inhibitor system and explore deeper neural network embeddings as input features.



MWRM 2026 MW155

Defluorination of perfluorooctanesulfonate (PFOS) by vanadium carbide (V_2C) mxenes catalyzed by hydrogen peroxide

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Per- and polyfluoroalkyl acids (PFAS) are persistent, acutely toxic synthetic organic chemicals that are widespread in environmental waters. The high thermal stability of their characteristic C–F bonds lends itself to applications in industrial processes and consumer products such as flame retardants, non-stick coatings and other industrial and consumer products. Exposure to PFOS and other PFAS have been linked to

negative toxicological and epidemiological health effects in humans and mammals resulting in upcoming Environmental Protection Agency regulations in drinking water. Common chemical disinfectants (e.g., hydrogen peroxide, H_2O_2) used in advanced oxidation processes to degrade organic contaminants during drinking water treatment are incapable of degrading PFAS due to inefficient energy transfer of the C–F PFAS bonds. To enhance degradation of PFAS in water, we employ vanadium carbide (V_2C) MXene nanosheets: a new family of 2-dimensional, conductive nanomaterials that have been used in energy storage applications (e.g., Li-ion batteries, electrochemical conversion). Data will be presented which characterizes V_2C MXene nanosheet properties, reactive species generation and PFOS transformation during this novel treatment process. Furthermore, results will be presented for enhanced V_2C MXene stability towards future electrochemical PFAS treatment.

MWRM 2026 MW51

DEL-GPT: Generative pretrained transformer to design targeted DNA-encoded libraries

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DNA-encoded libraries (DELs) have become an important technology for identifying ligands against challenging biological targets. Traditional DEL workflows, however, rely on untargeted libraries containing billions of compounds to maximize chemical space coverage. This scale comes with important drawbacks, including high production and screening costs, variable synthesis success, incomplete sampling, and potential errors during downstream hit triage.

Our previous work questions the assumption that successful DEL-based hit discovery requires ultra-large libraries. We have demonstrated that smaller libraries, tailored to individual targets or target families, can also deliver potent hits. Such focused libraries are less expensive, produce cleaner data, and are readily accessible to academic groups and smaller biotechnology companies.

A central challenge in designing focused libraries is selecting a compact yet relevant set of synthons that maximizes hit rates while minimizing library size. With thousands of commercially available synthons, identifying the optimal subset is a combinatorial problem, making random or manual selection strategies impractical.

The key difficulty in building focused DELs is selecting a compact yet relevant set of synthons that maximizes hit rates while minimizing library size. Because thousands of commercially available synthons can be considered, selecting the best subset is a difficult combinatorial problem, making purely manual design or random selection unlikely to provide an efficient solution.

To address this challenge, we developed DEL-GPT, a generative pretrained transformer for targeted DEL design. DEL-GPT is designed to identify useful synthons more effectively than random selection or expert-curated strategies, while remaining computationally inexpensive to train and apply. The model is self-trained on ordered synthon sets, in which the position of each synthon reflects its estimated contribution to overall library performance. During generation, DEL-GPT proposes the next most valuable synthon to add to an iterative library design, drawing candidates from the full available synthon pool. Synthon utility is assessed through its contribution to DEL efficiency, based on docking scores, molecular diversity, lead-likeness, and selectivity for the target. Architecturally, DEL-GPT follows the framework of a large language model.

We present encouraging results obtained on available DEL datasets.

MWRM 2026 MW40

Demonstration of a thermodynamic cycle for interpreting cation-driven tuning of redox chemistry

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Although it has been established that the properties of molecules and materials can be tuned via incorporation of secondary cations, a rigorous thermodynamic framework for interpreting the origins of such effects has remained elusive. In this presentation, a thermodynamic cycle for cation-driven tuning will be discussed that describes the fundamental relationship between shifts in the association constants of cations and shifts in reduction potentials. This cycle treats incorporated cations as guests and their redox-active acceptors as hosts and addresses the thermodynamic properties that underly the chemical behavior of the resulting host/guest complexes. Experimental validation of the thermodynamic cycle was carried out here with a macrocyclic uranium complex and $Mg(TFSI)_2$ (where TFSI is bis(trifluoromethyl)sulfonylimide), enabling calculation of high-correlation linear free energy relationships (LFERs) that demonstrate that the Lewis acidity of cations is correlated with swings in host/guest association constants which are, in turn, important drivers of previously studied but poorly parametrized relationships involving the redox properties of multimetallic species. Spectroscopic and electrochemical confirmation of the equilibria displayed by both the oxidized and reduced species involved in this study will be presented, as well as findings on the reactivity of reduced species prepared both electrochemically and chemically.

MWRM 2026 MW145

Design, synthesis, and characterization of mixed-linker Ln-MOFs with ligand and metal luminescence for cellular imaging applications

***Ashlyn Erdmann**, aeerdmann24@ole.augie.edu, Blen Lemma, Bjorn Eide, Ryan Schulte, Zachary M. Schulte. Augustana University, Sioux Falls, South Dakota, United States*

Cellular bioimaging using fluorescence microscopy is an essential tool for observing and identifying cellular species or features in vitro. However, the maximum quantity of subjects for simultaneous detection is limited by the broad emission profiles of common fluorophores. Lanthanide-based metal-organic frameworks (Ln-MOFs) offer a promising alternative through their highly tailorable structures, narrow emission peaks, and resistance to photobleaching and quenching. In MOF-76 (Ln3+(BTC)(H2O)1.5, BTC = trimesic acid), Yb3+, Tb3+ and Eu3+ ions have been effectively sensitized by the organic ligand, BTC, resulting in NIR, green, and red emission wavelengths, respectively. We hypothesize that using 2,4,6-pyridinetricarboxylic acid (PTC) as an organic ligand, we can use the ligand fluorescence to obtain a blue emitter, thus expanding the number of detectable signals in the visible spectrum. Herein, we have synthesized and characterized the luminescent properties of the PTC ligand using experimental and computational methods. Using a mixed-linker approach, we aim to incorporate PTC into MOF-76 and investigate subsequent changes to the crystal structure and photophysical properties. Finally, we will functionalize the surface of the PTC-MOFs to adhere to the exteriors of cells and determine their efficacy in fluorescent multiplexing cellular imaging applications.

MWRM 2026 MW132

Design, synthesis, and computational evaluation of novel alkyl sulfur-linked pomalidomide CRBN recruiters

***Tosin A. Oladosu**, olado012@d.umn.edu. Chemistry, University of Minnesota Duluth, Duluth, Minnesota, United States*

Proteolysis-targeting chimeras (PROTACs) represent a powerful strategy for targeted protein degradation, enabling selective elimination of disease-associated proteins. The design of effective PROTACs relies heavily on the properties of the linker connecting the protein-of-interest (POI) ligand to the E3 ligase recruiter, as linker geometry, flexibility, and physicochemical properties can influence ternary complex formation. In this study, we designed and synthesized a focused library of sulfur-linked pomalidomide-based cereblon (CRBN) ligands containing thioether and sulfone linkers with varying linker lengths and exit vector orientations (C4 vs C5). These ligands were developed as modular building blocks for future estrogen receptor alpha (ERα)-targeting PROTACs using toremifene as the POI ligand. The synthesized compounds were evaluated for intrinsic cytotoxicity across multiple cancer cell lines, including 4T1, 67NR,

MDA-MB-231, and MIA-PaCa-2, using MTT assays.
All compounds exhibited minimal cytotoxicity (IC50 greater than 100 micromolar), confirming that the sulfur-linked CRBN ligands function as non-toxic scaffolds suitable for PROTAC construction rather than standalone cytotoxic agents. To further characterize linker behavior, computational analyses were performed using RDKit-based workflows. For each ligand, multiple low-energy conformers were generated and energy-minimized to assess conformational flexibility, spatial reach from the pomalidomide core, and key physicochemical descriptors, including LogP, TPSA, molecular weight, and rotatable bonds. The analyses revealed that linker length primarily governs molecular size and flexibility, while oxidation state influences polarity, and exit vector orientation has minimal impact on overall property space. Several ligands demonstrated a balanced combination of conformational flexibility and spatial reach, suggesting favorable geometries for productive ternary complex formation. Overall, these results provide structure-property insights into sulfur-linked CRBN ligands and establish a rational framework for linker selection in PROTAC design. The identified scaffolds will serve as promising components for the future development of ERα-targeting PROTACs through conjugation with toremifene for targeted degradation studies in ER-positive breast cancer models.

MWRM 2026 MW119

Design and *in silico* computational assessment of hydrocaffeic acid functionalized PAMAM derivatives for antimicrobial application: An integrated DFT, molecular docking, dynamics simulation and pharmacokinetic study

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Poly amidoamine (PAMAM) dendrimers are highly branched, multivalent and easily modifiable scaffolds that have emerged as promising antimicrobial agents, while hydrocaffeic acid (HA) is a natural catechol derivative, consist of strong antimicrobial and antioxidant properties. Thus, the potent conjugation of these two bio-functional molecules is anticipated to yield a multifunctional antimicrobial candidate with unprecedented biological activity. The current study focused on the successful synthesis of first generation PAMAM-HA derivatives, covalently anchored with different numbers of HA catechol groups. The structures of the newly synthesized PAMAM-HA analogues were comprehensively characterized by ^{1}H NMR, ^{13}C NMR and FTIR spectroscopy. The molecular geometries were optimized by DFT/3-21G method to investigate the thermodynamic behavior of PAMAM-HA along with the parent molecules, resulting insight into the improved reactivity and electronic properties of conjugates. The PASS web tool was utilized to predict the antimicrobial potential which revealed enhanced antibacterial and antifungal efficacy in comparison to antiviral activity. To rationalize these observations, molecular docking was performed against a panel of bacterial (*S. aureus, E. coli, P. aeruginosa, B. subtilis,* and *S. mutans*), fungal (*A. flavus, A. niger,* and *C. albicans*) and viral (SARS-CoV-2, HSV and HIV) target proteins, exhibited that PAMAM-HA derivative persistently showed greater binding

energies and more preferable interactions with the active site of the proteins. Furthermore, molecular dynamics simulation was implemented to the protein-ligand complexes to confirm stability and behavior over time under in silico physiological environment. Moreover, an extensive pharmacokinetic, toxicity and QSAR study illustrated that PAMAM-HA conjugate comprises promising physicochemical properties along with permissible toxicity and better drug-likeness profile. Overall, theoretical and computational analysis evidenced the greater effectiveness of PAMAM-HA over the parent compounds, especially with encouraging antibacterial and antifungal activity. These outcomes recognize PAMAM-HA as an emerging lead molecule for antimicrobial drug design study and offer a significant scientific rationale for future experimental biological assessment to substantiate the therapeutic efficiency.

MWRM 2026 MW02

Design and development of a reactive intermediates concept inventory

Sachin Nedungadi*, snedungadi@unomaha.edu, Teresa Gibbons, Mary Simon. Chemistry, University of Nebraska Omaha, Omaha, Nebraska, United States*

Reactive intermediates such as carbocations, radicals, and carbanions, are featured in fundamental elementary steps of organic chemistry reactions. Concepts related to reactive intermediates are commonly misunderstood by students, leading to the development of alternate conceptions that inhibit a thorough understanding of reactions and their mechanisms. The large-scale assessment of student alternate conceptions could be beneficial to organic chemistry instructors so that instructional interventions and modifications can be made. A concept inventory is an assessment that can be used for such large-scale identification of student alternate conceptions. The development of a reactive intermediates concept inventory started with obtaining information from organic chemistry faculty regarding the importance and level of emphasis placed on different reactive intermediates through a national survey. The results were used to develop open-ended items related to carbocations, radicals, and carbanions. Student alternate conceptions were obtained through an open-ended administration of these items to second-semester undergraduate organic chemistry students. Student responses were used to generate answer options for multiple-choice items. Evidence for validity based on test content, response process, and internal structure were obtained through feedback from organic chemistry faculty, open-ended student interviews, and Rasch analysis respectively. The results together with implications for practice will be presented.

MWRM 2026 MW144

Design and development of Ln-MOF fluorophores for cellular multiplexing imaging applications

***Brayden Schut**, braydenschut7@gmail.com, Bjorn Eide, Ryan Schulte, Zachary M. Schulte. Augustana University, Sioux Falls, South Dakota, United States*

Cellular imaging is an essential tool for visualizing, identifying, and characterizing cells in a constrained system under similar conditions to their native environments. However, common fluorescent labels are plagued by photobleaching, small Stokes shifts, and broad emission profiles, complicating the use of many emitters at once. Lanthanide ions (Ln3+), when assembled into metal-organic frameworks (MOFs), are an enticing alternative due to their narrow emission peaks, high densities of fluorescent emitters, resistance to quenching, and tailorable structural and fluorescent properties. In this project, we developed fluorescent biomarkers based on MOF-76 (Ln3+(BTC)(H2O)1.5, BTC = trimesic acid). We produced nanoscale variants of MOF-76 with Tb3+ and Eu3+ and studied their fluorescent properties after incorporating an additional amine (NH2) group onto the BTC linker. The exterior of the Ln-MOFs were then functionalized with boronic acid or quaternary ammonium moieties to interact with the outer layers of eukaryotic HEK cells and gram positive and gram negative bacterial cells. With this design, we studied the efficacy of the cellular binding using flow cytometry and visualized the cells directly using fluorescence microscopy. Finally, we imaged several varieties of cells simultaneously for potential multiplexing studies.

MWRM 2026 MW144

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MWRM 2026 MW315

Design and synthesis of multifunctional bio-inspired polymers for metal chelation

***Destinee Shaffer**, dshaffer22@ksu.edu, Ayesha Imiya Mudiyanselage, Patricia R. Calvo. Kansas State University, Manhattan, Kansas, United States*

Selective metal ion recognition is essential for applications ranging from environmental remediation to chemical separations and biomedical technologies. Inspired by the diverse metal-binding motifs found in metalloproteins, this project seeks to develop multifunctional polymers capable of selectively chelating metal ions through the incorporation of multiple ligand types within a single macromolecule. Reversible addition–fragmentation chain-transfer (RAFT) polymerization is employed to synthesize well-defined linear polymers containing tetrafluorophenyl acrylate (TFPA), an activated ester that enables versatile post-polymerization functionalization. The TFPA repeat units are subsequently modified with biologically inspired metal-chelating ligands, including histamine, dopamine, glycine, and aspartic acid, either individually or in controlled combinations to create polymers with tunable ligand composition. This modular synthetic strategy provides precise control over ligand identity and ratio while maintaining consistent polymer molecular weight and architecture, enabling systematic investigation of structure–property relationships in metal chelation. The polymers are characterized using 1H NMR, 19F NMR and IR spectroscopy to confirm successful functionalization. Ongoing work focuses on evaluating the metal-binding properties of these multifunctional polymers and determining how ligand composition influences metal-ion affinity and selectivity. This work establishes a versatile platform for the rational design of multifunctional metal-chelating polymers and provides fundamental insight into how polymer composition governs metal recognition.

MWRM 2026 MW331

Designing antimicrobial polymers to combat antibiotic-resistant bacteria

***Marie Kerschen**, mrosekerschen@gmail.com, Dean Afsar, Patricia R. Calvo. Chemistry, Kansas State University, Manhattan, Kansas, United States*

Antibiotic-resistant bacteria represent an increasing global health challenge, creating an urgent need for new antimicrobial materials. Cationic polymers have emerged as promising alternatives to conventional antibiotics because their antibacterial activity can be tuned through molecular design. This project investigates how polymer structure and compositioninfluence antimicrobial performance by systematically varying the chemical structure and architecture of amino-functional polymers. Homopolymers containing aminoethyl methacrylamide (AEMA) or aminopropyl methacrylamide (APMA) were

synthesized and compared to copolymers prepared with N-isopropylacrylamide (NIPAM) or N-isopropyl methacrylamide to produce pseudo-gradient and statistical copolymers, respectively. By varying spacer length, hydrophobic comonomer incorporation, and monomer distribution along the polymer chain, this work aims to establish structure–property relationships that govern polymer–bacteria interactions. Preliminary minimum inhibitory concentration (MIC) studies demonstrate antibacterial activity against model bacterial strains and suggest that polymer architecture and molecular weight influence antimicrobial efficacy. These results provide valuable design principles for the development of next-generation polymeric antimicrobial materials.

MWRM 2026 MW331

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MWRM 2026 MW03

Designing a student-driven environmental chemistry CURE: Integrating water quality research, community partnerships, and science communication

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Environmental chemistry provides a natural framework for connecting laboratory research with environmental regulation, public health, and municipal water treatment, making it well suited for course-based undergraduate research experiences (CUREs). To leverage these connections, an upper-level Environmental Chemistry course at a

primarily undergraduate institution was developed in which student teams designed independent research projects investigating atrazine in water samples using a common analytical technique. The course was intentionally structured to place laboratory research within the broader context of how environmental data are generated, interpreted, and communicated. Students first examined the Love Canal disaster as a case study in community advocacy and the evolution of environmental regulation before exploring atrazine, its environmental significance, and methods used to monitor water quality. The teams then developed independent research questions, conducted literature reviews, formulated hypotheses, designed sampling strategies, collected their own samples, and quantified atrazine using ELISA immunoassays. Projects included regional surface water, groundwater, municipal tap water, bottled water, and sparkling water, allowing each team to investigate a distinct scientific. Students communicated their findings to audiences beyond the scientific community through scientific poster presentations and evidence-based letters written to policy stakeholders. A visit to KC Water further reinforced these connections by allowing students to observe municipal water treatment and atrazine monitoring using the same analytical approach employed in their own projects. This presentation highlights the course design, implementation, and practical considerations for faculty interested in developing an accessible environmental chemistry CURE.

MWRM 2026 MW242

Designing metal-organic supercontainers for direct air capture

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Increase in global atmospheric CO_2 concentration is a direct cause of global warming, and CO_2 removal is necessary. However, reducing carbon dioxide emissions alone would not be sufficient. Post-combustion carbon capture mitigates new carbon emissions from the point source, but does not address legacy CO_2 emissions. In contrast, direct air capture (DAC) removes CO_2 directly from ambient air and represents a negative-emissions technology. Current methods for DAC include solid and liquid sorbents. However, both systems use strong organic or inorganic bases and remove CO_2 through covalent acid-base reactions, presenting obstacles such as high energy costs. Metal-Organic Supercontainers (MOSCs) offer a noncovalent alternative for DAC. MOSCs are composed of both endo and exo nanocavities, which offer binding sites for small molecules, including CO_2, through non-covalent interactions such as hydrogen bonds. MOSCs are highly tunable and can be diversely constructed through a variety of different building blocks including metal ions and organic linkers . The purpose of this research was to design MOSCs with varying metal ions capable of optimal CO_2 capture from ambient air, to successfully perform DAC. To date, we have successfully designed several new MOSCs structures through metal modification. Further testing of their DAC performance is currently on-going.

MWRM 2026 MW231

Design of $NiMoO_4$/Ni-Mo-S MOF composite electrodes for supercapacitor applications

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Supercapacitors (SCs) have attracted considerable attention as advanced energy-storage devices because of their rapid charge–discharge capability, high power density, long cycle life, and excellent operational stability. The rapid development of portable electronics and emerging energy technologies has further increased the demand for efficient and environmentally sustainable electrode materials. Among transition-metal-based electrode materials, $NiMoO_4$ has attracted significant attention due to its multiple oxidation states, rich redox chemistry, and promising electrochemical activity. However, the limited charge-transfer kinetics of $NiMoO_4$ can restrict its overall energy-storage performance. In this work, $NiMoO_4$ nanorods were synthesized and investigated as electrode materials for SC applications. The pristine $NiMoO_4$ nanorod electrode exhibited a specific capacitance of 739 F/g at a current density of 2.5 A/g, demonstrating its promising charge-storage capability. To further improve the electrochemical properties of $NiMoO_4$, a Ni-Mo-S MOF is introduced to construct a $NiMoO_4$/Ni-Mo-S MOF composite electrode. The MOF component provides an abundant number of electrochemically active sites. Incorporating Ni, Mo, and S is expected to enhance redox activity and facilitate ion and electron transport. The integration of $NiMoO_4$ with the Ni-Mo-S MOF is therefore anticipated to yield synergistic effects that enhance charge-storage kinetics and overall electrochemical performance. This work provides a strategy for combining transition-metal molybdates with MOF-based materials to design composite electrodes for high-performance SC applications.

MWRM 2026 MW437 - Withdrawn

MWRM 2026 MW127

Determining substituent effects on photodeprotection rates of antiseptic 1,2,3-triazolium salts

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Quaternary ammonium compounds (QACs) prevalent in various disinfectant products such as sanitizers, herbicides, soaps, cosmetics, and more. Because degradation of the commonly used QAC benzalkonium chloride is relatively slow due to its chemical stability, its accumulation in the environment can increase the opportunity for antiseptic resistance to emerge. Development of new QACs that are similarly effective as commercial QACs while also possessing molecular features allowing their controlled

decomposition when exposed to light may be a way to address such harmful environmental accumulation. The goal of this project was to prepare triazolium salts possessing established photolabile protecting groups and examine how substituents on the triazole subunits impact both their rates of photodecomposition and overall antiseptic properties. A series of 1,5-diaryl-1,2,3-triazoles was prepared using base-catalyzed cycloaddition between azide and alkyne reactants. Variables included comparison of 1-naphthyl and 2-naphthyl subunits on the C5 position of the triazole, para-substituents (chloro, methyl and methoxy) of the arene on the N1 position of the triazole, and photolabile protecting group identity. Antiseptic properties were evaluated using minimum inhibitory concentration assays against Gram-positive bacteria, Gram-negative bacteria and yeast. Relative rates of UV-light promoted removal of PPG groups to regenerate 1,5-diaryl-1,2,3-triazoles was determined by HNMR monitoring in d_6-DMSO. Details regarding the preparation and characterization of such compounds, as well as substituent impacts on antiseptic properties and photodeprotection rates, will be presented.

MWRM 2026 MW87

Determining the effect of coformer alkyl chain length on cocrystal melting points

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Cocrystal formation is a powerful strategy in supramolecular chemistry for modifying the physical properties of a compound—such as solubility or thermal stability—without changing its chemical identity. This approach is particularly valuable in pharmaceutical research, where promising drug molecules may possess desirable biological activity but unsuitable physical characteristics for manufacturing or delivery.
Building on previous studies of cocrystals formed between 2-amido-3,5-dibromopyridines and substituted benzoic acids, this project investigates how increasing the alkyl chain length of the coformer influences cocrystal formation and melting behavior. Five new coformers were synthesized by acylation of 4-aminobenzoic acid and combined with the target molecule using liquid-assisted grinding. The resulting products were characterized by infrared spectroscopy (IR) and differential scanning calorimetry (DSC), and successful cocrystal candidates were subsequently crystallized by slow evaporation for structural analysis. The results presented here provide insight into how systematic changes in coformer structure influence cocrystal formation and thermal properties, helping to establish design principles for the rational development of new cocrystals.

MWRM 2026 MW103

Determining the role of acetylation on α-melanocyte stimulating hormone (α-MSH) neuropeptides

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Cell-to-cell signaling peptides (neuropeptides, peptide hormones) undergo functionalization after translation like acetylation, phosphorylation, epimerization, etc. to mature into their bioactive forms. These post-translational modifications change the chemical properties of the peptide by altering binding, stability and physiological function. Alpha-melanocyte stimulating hormone (α-MSH) is a signaling peptide that recognizes the melanocortin receptor (MCR) family as its primary target which is responsible for production of steroids and melanin, energy homeostasis and several other physiological functions. There are two known isoforms of α-MSH, the unmodified and N-terminal acetylated sequences, which demonstrate different binding affinities to MCR 1, 3, 4, and 5 as well as resistance to degradation. We previously used mass spectrometry to identify additional forms of α-MSH, including several di-acetylated and tri-acetylated forms. We hypothesize that these additional forms of α-MSH have distinct signaling activities or demonstrate varying resistance to degradation. To test this, we synthesized all isoforms of α-MSH, tested their ability to activate MCRs using cell-based assays and determined their half-lives in serum. From this, we can determine what role acetylation has on α-MSH peptides. These results can aid in the synthesis of high-affinity drugs used to target the melanocortin receptor family and other receptors who use peptides as their primary signaling molecule.

MWRM 2026 MW220

Developing an interdisciplinary first-year seminar connecting chemistry, neuroscience, and student well-being

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First-year college students face increasing academic, social, and emotional challenges that can negatively influence learning, persistence, and overall well-being. At the same time, introductory chemistry is often perceived as disconnected from students' daily experiences. To address both challenges, we developed a three-credit interdisciplinary first-year seminar that uses chemistry as the central concept for exploring the molecular basis of stress, attention, sleep, emotion, and resilience.
The seminar integrates concepts from general chemistry, biochemistry, neuroscience, and physiology to examine neurotransmitter signaling, hormonal regulation, chemical equilibrium, thermodynamics, oxidative stress, inflammation, and epigenetic regulation.

Students investigate these topics through the lens of current research on meditation and mindfulness, treating these practices as evidence-based scientific phenomena rather than philosophical or religious traditions. The course emphasizes scientific literacy through analysis of peer-reviewed literature, interpretation of experimental data, collaborative case studies, reflective writing, and inquiry-based learning activities. A semester-long project provides opportunities for students to communicate scientific concepts to diverse audiences.
The course is intentionally designed to help students connect molecular-level chemistry with everyday experiences while developing critical thinking, information literacy, scientific communication, and evidence-based reasoning. This poster will present the course rationale, learning outcomes, course map, assessment strategy, sample assignments, and instructional resources developed for implementation at a liberal arts institution.

MWRM 2026 MW344

Development and validation of an UHPLC/MS/MS method for quantitative measurements of per- and polyfluoroalkyl substances using a linear ion trap

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Increased attention and regulation of per- and polyfluoroalkyl substances (PFAS) have created a global need for accurate quantification of PFAS, for which triple quadrupole (QQQ) and quadrupole-time-of-flight (Q-ToF) mass spectrometers are widely used. However, the availability of QQQ and similar advanced instruments can be limited due to start-up costs, maintenance, and training. Our group seeks to utilize alternative mass spectrometry instrumentation to increase the utility of PFAS analysis and quantitation. Thus, a solid-phase extraction (SPE), ultrahigh-performance liquid chromatography/tandem mass spectrometry (UHPLC/MS/MS) method was developed using a linear ion trap (LIT). A Thermo LTQ XL LIT was used to quantify 16 compounds using multiple reaction monitoring (MRM). The liquid chromatography was performed using a Thermo UltiMate 3000 equipped with a Millipore Sigma Ascentis Express 90 Å C18 PFAS column. The method was validated in accordance with the guidelines of EPA Method 537.1. This method shows that a wider variety of mass spectrometry instrumentation can be used for the quantification of PFAS in drinking water samples.

MWRM 2026 MW323

Development and validation of a physiologically based pharmacokinetic (PBPK) model for dihydrocaffeic acid, a pharmacologically active antioxidant metabolite

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Background/Objectives: Antioxidants are found in many natural substances and are beneficial for reducing the effects of harmful reactive oxygen species. Caffeic acid is a common antioxidant found in many natural substances, such as coffee and Polypodium leucotomos extract, which is sold as Heliocare for protection against damage to skin due to UV radiation. This study aimed to develop a physiologically based pharmacokinetic (PBPK) model for dihydrocaffeic acid, an active metabolite of caffeic acid. Model differences based on ethnic groups were also investigated.
Methods: PK-Sim (Open Systems Pharmacology) was used for model development, using interspecies extrapolation and in vitro secondary data obtained from the literature. The PBPK model validation was completed using graphical and mathematical statistical comparisons of the predicted PK profiles and parameters with those obtained from in vivo PK studies in the literature. The models' accuracy was also compared for European and Black American ethnic groups.
Results: Two similar "middle-out" models were developed. The models used non-mechanistic dissolution functions (Weibull and Lint80) to simulate GI tract transit time to the colon, where bacterial metabolism occurs. The models passed all validation tests. There were no significant differences in the results for the two ethnic groups.
Conclusions: The parsimonious approach resulted in models that should be versatile enough to apply to other ethnic groups and to minor changes in colon microbiota and in the source of the polyphenol. The procedures followed and models developed provide a guide for future model development for other polyphenols.

MWRM 2026 MW48

Development of accurate and efficient machine-learned quantum dynamics methods for vibrational spectra

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Accurate vibrational spectral simulations using molecular dynamics (MD) methods present a two-fold challenge. First, an accurate potential energy surface (PES) needs to be constructed for neutral, charged, or interfacial environments. Second, nuclear quantum effects (NQEs) must be efficiently accounted for, especially in condensed-phase and interfacial simulations involving light nuclei. We have developed custom-trained 4th-generation high-dimensional neural network potentials (4G-HDNNPs) that include long-range electrostatics and polarization effects, a missing feature in most existing NNP architectures. In this work, we combine our 4G-HDCNNPs with machine-learning centroid MD (ML-CMD) methods to build new fast and reliable real-time path-integral methods, which we coin 4G-ML-CMD, for capturing NQEs and simulating accurate dynamical properties, including vibrational spectra. To showcase the efficiency and accuracy of our combined framework, we have calculated dynamical and vibrational surface-enhanced infrared absorption spectra (SEIRAS) of interfacial water on various low- and high-index gold facets as test cases compared to experiments.

MWRM 2026 MW121

Development of activated iodinated alkynyl esters for halogen-bond-driven crystal engineering

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Halogen bonding has emerged as a highly reliable and directional noncovalent interaction in supramolecular chemistry, arising from an electron-deficient region of electrostatic potential, commonly referred to as the σ-hole, associated with a covalently bound halogen atom. The magnitude and accessibility of the σ-hole govern the strength and directionality of halogen-bonding interactions and can be systematically tuned through rational molecular design. In this work, we explore a new family of highly activated iodinated alkynyl esters designed to maximize σ-hole potential through electronic activation by conjugated electron-withdrawing ester functionalities and aromatic substitution. Building on previously reported triply activated iodopropiolate systems, we investigate mono- and bis(propiolate) architectures based on ortho-, meta-, and para-substituted phenylene scaffolds to determine how molecular geometry and substitution patterns influence electrostatic potential distributions, halogen-bond donor strength, and supramolecular assembly.
A combination of synthetic organic chemistry, computational electrostatic potential mapping, and single-crystal X-ray diffraction will be used to establish relationships between molecular structure, electronic activation, and supramolecular behavior. The multifunctional nature of these compounds also provides an opportunity to examine the interplay among halogen bonding, hydrogen bonding, and π–π interactions in directing molecular organization and crystal packing. Elucidating the cooperative and competitive effects of these complementary noncovalent interactions will provide insight into the factors governing solid-state assembly and enable the more rational design of predictable supramolecular architectures. Ultimately, this work will expand the toolbox of highly activated halogen-bond donors available for applications in crystal engineering, pharmaceutical cocrystal design, molecular recognition, porous materials, and other functional organic solids.

MWRM 2026 MW335

Development of a free, open-source Python kinetic simulation package for modeling, fitting, and mechanism discovery

***Taylor Paez**, tmpaez25@ole.augie.edu, Lin-Lin Elliott, Charles Weiss. Chemistry & Biochemistry, Augustana University, Sioux Falls, South Dakota, United States*

Computer modeling of chemical kinetics is an important step in the proposal and validation of reaction mechanisms. To support these efforts, we are developing a free, open-source Python package for the simulation of chemical kinetics. This package contains three key functionalities: 1) the simulation of chemical kinetic data based on a

reaction mechanism, 2) the fitting of a mechanism to time series data to extract elementary step rate constants, and 3) the automated proposal of reaction mechanisms that fit experimental kinetic data. The package has been tested for features 1 and 2 on both simulated and experimental data and has demonstrated a good ability to quickly simulate and fit a variety of reaction mechanisms. It is also designed to be intuitive to use and to make building reaction mechanisms quick because the package generates the differential equations for the user. The package also contains useful features such as the ability to calculate the empirical rate law based on a reaction mechanism and species concentrations, set known equilibrium values, and set reactant concentrations to fixed values. Feature 3 uses numerical methods to fit data to possible reaction mechanisms that are consistent with the experimental data. Efforts are underway to further test the package and add more algorithms for the discovery of viable reaction mechanisms.

MWRM 2026 MW335

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MWRM 2026 MW343

Development of a reactive Py-GC/MS methodology for the mass quantification of microplastics in water samples

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The pervasive contamination of microplastics (MPs) (particles <5 mm) has raised significant environmental and public health concerns, necessitating accurate quantification. While spectroscopic techniques such as micro-FTIR provide particle counts, they are often limited by a 10 µm size threshold and by interference from organic matter. To address these challenges, this study presents the development of a reactive Pyrolysis Gas Chromatography-Mass Spectrometry (Py-GC/MS) method for the identification and quantification of seven common polymers: Polymethyl Methacrylate(PMMA), Nylon, Polypropylene(PP), Polystyrene(PS), Polyethylene (PE), Polyvinyl Chloride (PVC), and Polyethylene Terephthalate (PET). The methodology employs in situ thermochemolysis at 600 °C using 5 µL of tetramethylammonium hydroxide (TMAH) as an alkylating reagent to enhance the volatility and chromatographic elution of polar pyrolyzates. A critical focus of the method development was the PET detection mechanism, in which TMAH induces a saponification-transesterification reaction, cleaving the ester bonds in the polymer chain to produce dimethyl terephthalate (DMT) as a stable, quantifiable marker. This approach bypasses the poor volatility of standard PET thermal degradation products. Calibration was performed using a microplastic standard in a $CaCO_3$ matrix, yielding excellent reproducibility and sensitivity. Limits of Detection (LOD) were achieved as low as 0.35 µg for PMMA and 0.54 µg for PET, with the highest precision demonstrated by a 0.48% RSD for PS. Ongoing work applies this optimised workflow to evaluate microplastic occurrence in bottled water. This research provides a robust, mass-based analytical tool essential for understanding the fate and transport of MPs.

MWRM 2026 MW98

Development of a reporter-based assay to identify VraSR inhibitors and enhance vancomycin activity in *Staphylococcus aureus*

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Staphylococcus aureus is a major cause of serious bacterial infections, and increasing antibiotic resistance continues to limit effective treatment options. Vancomycin is widely used as a last-line therapy for methicillin-resistant *S. aureus* (MRSA), but strains with reduced susceptibility, including vancomycin-intermediate *S. aureus* (VISA), have emerged. One important mechanism contributing to this reduced susceptibility is

activation of the VraSR two-component regulatory system. In response to cell wall stress caused by vancomycin, VraSR auto-upregulates by reduced repression of the vra operon; then, it promotes expression of genes involved in cell wall synthesis and repair, leading to cell wall thickening and decreased antibiotic effectiveness. Despite its promise as a therapeutic target, few scalable tools for monitoring VraSR activation or systematically identifying pathway inhibitors have been reported.
We aim to develop a fluorescence-based assay that can be used to detect inhibition of the VraSR signalling pathway in *S. aureus*. The assay is based on a fluorescent reporter system designed to enable real-time monitoring of VraSR pathway activation and provide a platform for inhibitor discovery in *S. aureus*. We have chosen a fluorescence-based method for increased sensitivity, in the hope that we will be able to detect initial low-potency hits and also use the same assay for detailed structure-function optimization. Accordingly, we are generating an assay using green and red fluorescent proteins (GFP and DsRed) in the hope that we can segregate <10-fold changes in vraSR auto-upregulation activity. In this presentation, we will report details of assay development, its validation, and its use in identifying candidate VraSR inhibitors. Additionally, we will report how VraS inhibition restores susceptibility to β-lactam and glycopeptide antibiotics in resistant strains.

MWRM 2026 MW191

Development of a self-sufficient biomass hydrothermal liquefaction process for the future biorefinery

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Hydrothermal liquefaction (HTL) is a promising method for biomass liquefaction. Mixtures of low-boiling point C1-3 alcohols and water are commonly used as HTL solvents. High-pressure reaction vessels, difficult water-alcohol separation and loss of the alcohols to waste gas stream are potential engineering challenges associated with these alcohols. To address these challenges, a novel solvent system of 1:2.7:5 vol water: X : Y is designed for biomass HTL. At 280 °C the vapor pressure is reduced from 1468 psi for 1:3 water:EtOH to 460 psi. The water is easily separated from Y by phase separation and from X by distillation. Their high Tbs also minimize their loss to the waste gas stream. Corn stover HTL reactions were run at 280 °C from 2h to 15h. Greater than 99% of Y and 97–98% of X survived the 15h HTL. Oxygen content in heavy biocrudes decreased from 21.71% to 18.69%, accompanied by a decrease in glass transition temperature. The high efficiency in liquefaction, characterized by low hydrochar yields (4.75 to 1.57%) and high biocrude yields (39.6 to 44.1%), is attributed to the hydrophobic nature of Y, which keeps water out of the organic phase, thus facilitating the dissolution of liquefaction products, reducing their condensation, and driving the conversion of carboxylic acids to esters. The light biocrude, with a boiling point slightly higher than that of Y and a moderate polarity, is a potential substitute for Y and may further enhance the sustainability of the new HTL process

MWRM 2026 MW79

Development of a thermoresponsive simvastatin prodrug for the treatment of periodontal bone defects

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Periodontitis is a chronic inflammatory disease that leads to destruction of gingival tissue and alveolar bone, resulting in tooth loss and systemic complications. Conventional therapies reduce symptoms but do not restore lost tissue. Simvastatin (SIM) has anti-inflammatory and osteogenic properties, but systemic delivery limits local efficacy and may cause off-target effects. This study evaluates ProGel-SIM, a thermoresponsive polymeric prodrug of Simvastatin (SIM) designed for localized and sustained delivery within the periodontal pocket. Through a highly efficient one-pot reaction, a SIM-containing monomer was synthesized and then copolymerize with N-(2-hydroxypropyl) methacrylamide (HPMA) to produce ProGel-SIM. The prodrugs were characterized for their SIM content, molecular weight, dispersity, and thermoresponsive behavior. Sol–gel transition and gel stability were evaluated across concentrations. The therapeutic efficacy was assessed using a ligature-induced periodontitis model in SD rats (n = 40; five groups: ProGel-SIM, free SIM, vehicle, saline, and healthy control). Following disease induction and ligature removal, a single local injection was administered into the periodontal pocket. Rats were monitored for 4 weeks. Outcomes were evaluated using micro-CT to measure alveolar bone loss and cementoenamel junction to alveolar bone crest (CEJ–ABC) distance, followed by histological analyses. ProGel-SIM treatment significantly reduced inflammatory infiltration and preserved alveolar bone compared to controls. Micro-CT analysis showed decreased CEJ–ABC distance and reduced bone resorption in ProGel-SIM treated rats. Histological evaluation demonstrated improved tissue organization and reduced inflammation when compared to saline and vehicle groups. These results support ProGel-SIM as a clinically translatable strategy for better clinical management of bone loss associated with periodontitis.

MWRM 2026 MW427 - Withdrawn

MWRM 2026 MW141

Development of multiplex electrochemical biosensors for quantifying overexpressed proteases in cancer

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Proteases are important biomarkers for cancer due to their overexpression during metastasis. Detecting these enzymes quickly and accurately can improve early diagnosis and disease monitoring. In this study, we developed an electrochemical biosensor based on a 3 × 3 gold (Au) microelectrode array (MEA) to measure the activity of three cancer-related proteases: cathepsin B (CB), MMP-9, and ADAM-17. When a protease cleaves its peptide substrate labeled with aminoethyl ferrocene (Fc), the electrochemical signal decreases over time following an exponential pattern, and the inverse of the decay time constant (1/τ) is directly related to the enzyme's catalytic activity according to heterogeneous Michaelis-Menten kinetics. We found that the commonly used activation reagents, dithiothreitol (DTT) for CB and 4-aminophenylmercuric acetate (APMA) for MMP-9, caused unwanted signal loss by likely disrupting the bond between gold and sulfur on the sensor surface. To overcome these, DTT was removed after CB activation, while EDTA was added to preserve enzyme activity. Similarly, APMA was removed after MMP-9 activation without affecting its activity, minimizing non-specific signal changes. We then studied how different peptide sequences show different proteolysis rates to different proteases and at different pH values. The results showed that proteolysis rates strongly depended on both the peptide sequence and the target protease, demonstrating the importance of substrate design for achieving selective detection in a common buffer at physiological conditions (with pH ≈ 7.4), possibly leading to implementing a multivariate data analysis approach. We further confirmed that the sensor platform remained stable in 3% human serum (H.S) without significant interference, and different peptide substrates exhibited distinct cleavage rates. In addition, varying the concentration of H.S produced a linear electrochemical response, demonstrating the sensor's ability to quantify protease activity in complex biological environments. These findings contribute to the development of multiplex electrochemical biosensors for cancer diagnosis using liquid biopsy.

MWRM 2026 MW20

Development of novel fluorogenic dyes to explore the role of fluorine in fluorescence activation

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Fluorogenic RNA aptamer-ligand complexes are a powerful tool for imaging, as target RNAs can be visualized in live cells through fluorescence activation. A well-established model system using the RNA aptamer Pepper and fluorogenic dye HBC525 provides sufficient binding affinity and specificity for visualization purposes, but there is limited understanding of how dye functionalization and substituent location impacts photophysical properties and RNA binding. Here, electronegative fluorine substituents were added at varying positions on HBC525 to investigate their impacts on fluorescence activation. Because fluorine acts as an electron acceptor and was added to the electron acceptor region of the chromophore, a stronger push-pull system was created. This generally lowers the energy band gap, resulting in a red shift. Because the choice of fluorine is predicted to produce drastic photophysical changes, it is an ideal substituent

to evaluate differences in locant placement. Three derivative dyes, HBC525-5F, HBC525-6F, and HBC525-7F, were synthesized and characterized using multiple spectroscopic measurements in the presence and absence of RNA. The emission of HBC525-5F in complex with the Pepper RNA aptamer shows a Stokes shift of about 60 nm, while HBC525-6F and HBC525-7F show anti-Stokes shifts of about 2-3 nm. Fluorescence-based binding assays of HBC525-5F in complex with the Pepper RNA aptamer shows about 4-fold less fluorescence intensity than the HBC525 parent molecule. Fluorescence-based binding assays of HBC525-6F and HBC525-7F were performed to compare fluorescence intensity for the three derivative dyes. The collection of these experiments reveals the vital role of chemical composition and substituent location in fluorogenic dye activation.

MWRM 2026 MW168

Development of second-generation RARα antagonists for nonhormonal male contraception and strategies to enable large-scale synthetic routes for YCT-529

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Even with the current contraceptive methods, nearly half of all pregnancies worldwide are unintended. In the United States, the taxpayer burden from unplanned pregnancies is between $5.5 billion and $21 billion per year. An active metabolite of dietary vitamin A, all-trans retinoic acid (ATRA), binds to retinoic acid receptors (RAR) in germ cells and activates genes responsible for several phases of sperm differentiation. Our lab has characterized the first orally bioavailable, reversible RARα-selective antagonist, YCT-529, which selectively targets RARα by forming hydrogen bonds to a unique serine 232 present only in RARα. YCT-529 exerts antagonism through a bulky substituent that prevents conformational activation of RARα. With its advancement to Phase 1a/2b clinical trials, its kilogram-scale synthesis suffers from the expensive and challenging removal of iridium and palladium catalysts. A new synthesis route that relies on a modified Kulinkovich 1,4-diketone synthesis using the $ZnCl_2$.*t*-BuOH.Et_2NR complex improved efficiency and production cost (33% in 4 steps). Density functional theory of a model Kulinkovich reaction provided insights into the optimal halo-ketone to use in the synthesis. The Matzuk group performed a DNA-Encoded Library (DEL) screen with 6 billion compounds targeting RARα to diversify our current ligand space. After resynthesis of the binders, only one compound showed potent and selective RARα inhibition (6.7 nM) in our cellular-based functional assay. With this novel structural motif, structure-activity relationship studies are underway to improve potency, selectivity, and drug-like properties, with the aim of advancing to ADMET and mating studies.



RAR antagonists prevent binding of the natural agonist (ATRA) hence halts the maturation of germ cells to spermatids.

MWRM 2026 MW293

Diblock copolymers with LCST behavior for conformance control in carbonate reservoirs

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As global oilfields mature, recovering oil through conventional methods is becoming more and more challenging. In a typical oil well, only about one third of oil is recoverable by conventional means and the rest will remain unproduced unless Improved Oil Recovery (IOR) methods are employed. In reservoirs with high permeability zones, cracks, and voids, conformance control methods have been used to divert water flow into previously unswept portions of the reservoir. Preformed particle gels (PPGs) have been used to seal large cracks, and micro- and nanogels have been used to plug smaller cracks and high permeability rock. Gels rely on the mechanical force of swelling in order to resist flow, but can be difficult to inject when swollen. A conformance agent made of linear, soluble polymer that could adsorb onto the rock surface would be easier to inject and would allow tight pores to be targeted. Stimulus-responsive polymers that swell or shrink in response to temperature will provide the potential to fine-tune the IOR treatment. We have synthesized novel diblock copolymers of sodium styrene sulfonate (NaSS) with alkyl acrylamides N,N-dimethylacrylamide (DMA) and N,N-diethylacrylamide (DEA) using RAFT polymerization. The block copolymers were designed such that the NaSS block is capable of adsorbing to the carbonate rock surface, while the alkyl acrylamide block remains extended in aqueous solution, providing stimulus responsive behavior at relevant temperatures and resistance to water

flow. We will present the synthesis and characterization of the block copolymers using NMR, DSC, and GPC, and demonstrate adsorption behavior on calcium carbonate. The NaSS-DEA copolymer has an LCST below 100°C, and this copolymer will be used to demonstrate stimulus responsive swelling and de-swelling of polymer while adsorbed on calcium carbonate. We will present results of ^{1}H NMR relaxation experiments that characterize the adsorbed polymer layer at temperatures above and below the LCST for the NaSS-DEA block copolymer and at temperatures below the LCST for the NaSS-DMA copolymer.

MWRM 2026 MW62

Direct photochemical glycosylation via a fluorenol-based photoactive leaving group

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The formation of glycosidic bonds is a fundamental transformation in carbohydrate synthesis, yet conventional glycosylation methods frequently require strong acids, stoichiometric activators, or catalyst systems that can limit functional group compatibility and reaction control. Photochemical approaches offer attractive alternatives; however, most reported methods rely on photosensitizers or additional reagents to generate reactive intermediates for donor activation. Herein, we report a photoactive leaving group, derived from a 9-arylfluoren-9-ol scaffold, that enables direct light-mediated glycosylation without any external activating agents, catalysts, or photosensitizers. Upon irradiation at 300 nm, direct activation of the leaving group generates a reactive glycosylating species that couples efficiently with alcohol acceptors under neutral room temperature conditions. The method has been applied to a range of primary, secondary, and tertiary alcohol acceptors, affording the corresponding glycosides in excellent yields (>90%). These findings establish directly photoactivated fluorenol-based leaving groups as a promising platform for glycosyl donor activation and provide a streamlined approach to light-controlled glycosylation. Ongoing studies are focused on further expanding substrate scope, determining anomeric selectivity, and investigating the mechanism of photochemical activation.

MWRM 2026 MW99

Discovery and development of novel quinoxaline analogs to treat hearing loss

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Sensorineural hearing loss (SNHL) is a prevalent and irreversible condition caused by the loss of auditory hair cells, with no currently available pharmacological treatments to restore function. Current management options, such as hearing aids and cochlear implants, are limited and often invasive, requiring external devices or surgical

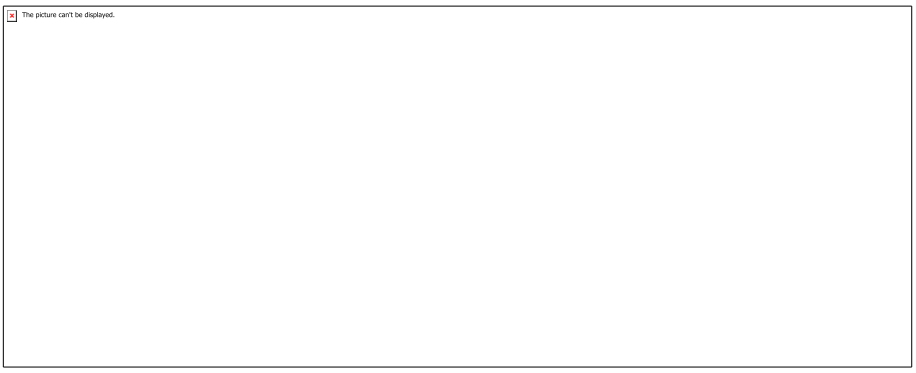
implantation that do not address the underlying cellular damage. The most accepted hypothesis for hearing loss restoration or prevention is the ability to regrow auditory hair cells, and currently, there are no FDA-approved drugs to restore or prevent hearing loss. We have identified a novel small molecule (Quinoxaline) that has shown proliferative effects for auditory hair cells, with in vivo efficacy in mice. Recently, we identified novel substituted 2-aminoquinoxaline analogs with improved cellular proliferative effects in the ear, that has also been achieved in vivo efficacy. However, these lead compounds suffer from poor aqueous solubility and currently must be injected into the ear for therapeutic effects. We hypothesize that expanding the structure-activity relationships (SAR) at the 2-position of quinoxaline will not only expand the SAR of this novel chemotype, but will also improve physical, chemical, and pharmacokinetic properties, leading to lead drug compounds, poised for further drug development. Substitutions at the two positions include aromatic, heteroaromatic, aliphatic, and ionizable functional groups. Compounds will undergo an iterative drug discovery cycle to include cellular proliferative effects, cytotoxicity, aqueous solubility, permeability, metabolic stability, and human plasma protein binding. Current lead compounds have achieved cellular proliferative effects against the HEI-OC1 cell line, have an aqueous solubility 365±28 - 551±24 mg/mL, Parallel Artificial Membrane Permeability Assay (PAMPA) permeability of 0.77±0.91 - 3.5±3.0 x10-6 cm/s-1, metabolic stability against the S9 fraction of 9.1±8.4 - 57.2±4.7 t1/2 = hr, 32.3±4.3 - 88.5±4.0 percent plasma protein bound. Future studies include robust pre-clinical physical-chemical and formulation studies to identify not only a lead preclinical drug candidate, but also a preclinical drug product.

MWRM 2026 MW09

Discovery and optimization of thienopyrazine RNA-splicing modulators for the treatment of Huntington’s disease

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Huntington’s disease (HD) is a progressive neurodegenerative disorder caused by a CAG-repeat expansion in the Huntington gene (HTT). We discovered a series of HTT pre-mRNA-splicing modulators that promote the inclusion of a cryptic stop codon that could in turn lower levels of mutant Huntington protein (mHTT). Optimization of the starting thienopyridine amide core resulted in the discovery of the potent, CNS-penetrant, selective, and orally bioavailable HTT-splicing modulator BIO-6553. This compound demonstrated a favorable pharmacokinetic profile and significant reduction of canonical HTT transcript levels in both human cells and mouse YAC128 models. Additionally, RASL-seq assessment revealed that most tested compounds in this series, including BIO-6553, exhibited a favorable genetic off-target profile compared to existing HTT splice modulators. RNA-seq analysis further confirmed BIO-6553 has attractive off-target efffects on alternative splicing and gene expression across the whole transcriptome.



MWRM 2026 MW134

Discovery of protein-binding peptides: From computational screening to biological applications

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Protein-binding peptides are emerging as versatile molecular probes and therapeutic candidates because of their high target specificity, predictable metabolism, and reduced off-target effects compared with many small molecules. However, the discovery of target-specific peptides has been hindered by the lack of efficient methods for large-scale *in silico* screening. The intrinsic flexibility and enormous sequence diversity of peptides make conventional virtual screening computationally challenging.

In this talk, I will present MDockPeP2_VS, a computational platform for the rapid discovery of novel protein-binding peptides. The method integrates molecular docking with a newly identified principle of structural conservation between protein folding and protein–peptide binding: when interfacial residues are conserved, a sequence fragment from a monomeric protein often binds its target in a conformation resembling its native folded structure. By leveraging this principle, MDockPeP2_VS dramatically reduces the peptide conformational search space while maintaining high prediction accuracy, enabling efficient large-scale virtual screening.

I will demonstrate how MDockPeP2_VS can accelerate the discovery of peptide-based molecular probes and therapeutics through the identification of peptide inhibitors targeting TEM-1 β-lactamase from *Escherichia coli*, a key enzyme responsible for antibiotic resistance. This work illustrates how physicochemistry-driven computational methods can transform peptide discovery, providing a general strategy for developing next-generation molecular probes and peptide therapeutics.

MWRM 2026 MW360

DNA origami–chitosan hybrid nanocarrier enables sustained intracellular antioxidant delivery for protection against oxidative stress in early cataract

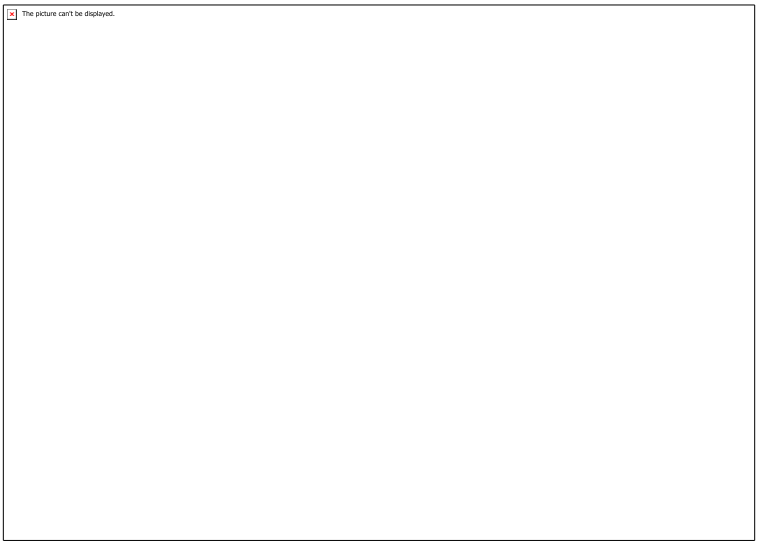
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Oxidative stress is a major contributor to early cataract formation through excessive reactive oxygen species (ROS) production and damage to lens epithelial cells. Although tiopronin (MPG), a thiol-containing antioxidant, effectively scavenges ROS, its therapeutic application is limited by rapid ocular clearance and poor intracellular retention. We developed a DNA origami–chitosan hybrid nanocarrier for sustained intracellular delivery of tiopronin.

DNA origami nanostructures were coated with EPTMAC-modified chitosan to improve stability and drug loading. Hybrid nanocarrier formation were confirmed by atomic force microscopy, dynamic light scattering, zeta potential analysis, and agarose gel electrophoresis, while dextran sulfate displacement confirmed reversible encapsulation. The nanocarrier exhibited high drug-loading efficiency and sustained tiopronin release for more than 72 hours.

Biological performance was evaluated in HLE-B3 human lens epithelial cells exposed to tBHP-induced oxidative stress. Compared with free tiopronin and carrier controls, the tiopronin-loaded DNA origami–chitosan nanocarrier reduced intracellular ROS, improved cell viability, and reduced apoptosis. Ocular compatibility was assessed using the Hen's Egg Test on the Chorioallantoic Membrane (HET-CAM), where the formulation showed no hemorrhage, vascular lysis, or coagulation (irritation score = 0.00; non-irritant).

These findings demonstrate that integrating DNA origami with modified chitosan creates a stable, biocompatible nanoplatform for sustained antioxidant delivery. This strategy provides a promising platform for non-invasive antioxidant therapy targeting oxidative stress associated with early cataract development.



MWRM 2026 MW69

Driving uranium redox at positive potentials with crown ether chelation

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Interconversion of actinide oxidation states underpins most steps in the nuclear fuel cycle and, thus, fundamental studies of strategies for controlling actinide redox chemistry could inform improved processes for handling of nuclear materials. In this presentation, the encapsulation of uranium in crown ether ligands will be discussed as a strategy for controlling metal-ligand bonding and shifting the reduction potentials associated with uranium redox to more positive values. The synthesis, characterization, and redox properties of uranyl-crown complexes supported by both conventional organic crowns as well as more specialized transition-metal-templated crown-like species will be discussed. Data will also be presented from spectroscopic and computational studies designed to illuminate bonding patterns in select complexes as well as electrochemical studies targeted at quantifying stability and reactivity under various conditions.

MWRM 2026 MW377

Dual lithiophilic promotors for dendrite-less lithium metal batteries

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Lithium metal as an anode provides a high theoretical capacity of about 3.8 A/g, which is about ten times higher than the existing graphite anode for lithium (Li)-ion batteries. Despite, there are critical bottlenecks in cycling Li metal anode such as dendrite formation, low Coulombic efficiency, and poor cycle life, along with safety issues. Here, nitrogen (N) and fluorine (F)-based heterostructure is developed as a lithiophilic regulator for Li metal. The as-developed NF-based heterostructure employed Li metal cell demonstrated good cycling behavior for over 500 and 800 cycles at low and high current densities of 1 and 2 mA/cm^2, respectively. In addition, the Coulombic efficiency of the cell was about 94% at the end of 100 cycles in a $LiPF_6$ based carbonate electrolyte. Through density functional theory studies, it was found that the presence of N and F certainly involves the hybridization of orbitals in heterostructure, which meticulously allows the Li deposition in a smooth and controlled manner.

MWRM 2026 MW214

Dynamic modulation and allosteric mechanisms underlying ACKR3-mediated arrestin2/3 activation

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G protein-coupled receptor (GPCR)-mediated signal transduction is the primary means by which cells respond to external stimuli and maintain proper function. Extracellular ligand binding induces conformational changes in the receptor that propagate to intracellular binding interfaces, where the receptor engages three classes of transducer proteins: G proteins, GPCR kinases, and arrestins. Arrestin binding can terminate GPCR signaling by blocking G protein pathways, promote receptor-mediated endocytosis or internalization, and activate arrestin-dependent signaling pathways. Despite the essential role of arrestins in GPCR signaling, the detailed mechanisms of arrestin activation remain elusive. In humans, more than 800 GPCRs couple diverse extracellular ligands to specific intracellular pathways, yet only four arrestin isoforms mediate this information transfer. How such a large diversity of ligand-GPCR complexes selectively regulates distinct signaling pathways through a small number of hub molecules remains a fundamental unresolved question. Our hypothesis is that ligand binding to GPCRs modulates arrestin dynamics in a ligand-, receptor-, and arrestin isoform-dependent manner, leading to distinct functional outcomes. Here, we test one aspect of this hypothesis: how different arrestin isoforms engage the same ligand-receptor complex to exhibit distinc conformational dynamics and function. We investigated arrestin2 and arrestin3 activation by atypical chemokine receptor 3 (ACKR3) complexed with the chemokine ligand CXCL12 using all-atom molecular dynamics simulations. These two arrestin isoforms are ubiquitously expressed and, despite their high sequence and structural similarity, produce distinct functional outcomes upon interaction with ACKR3. Initial complex structures were modeled based on the recent cryo-EM structure of CXCL12-ACKR3-arrestin2 (PDB: 9E82). Conformational dynamics were characterized using both hypothesis- and data-driven approaches. Mechanisms underlying allosteric coupling among distant arrestin, receptor, and membrane binding interfaces were elucidated using a graph-centric approach.

MWRM 2026 MW81

Dynamic polymers for energy, sustainability, and human health

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Dynamic polymers are an emerging class of materials whose properties arise from the addition of reversible covalent or non-covalent interactions along an amorphous or

semicrystalline polymer backbone. These polymers can exhibit ordered morphologies due to the formation of supramolecular nanostructures, self-heal autonomously, and have improved recyclability. These properties enable their use in a wide range of applications including for actuators for soft robotics, wearable electronics for improved human health, solid-state electrolytes in batteries, recyclable underwater adhesives, and the design of more sustainable plastics. In this talk, I will discuss how dynamic polymers can achieve unprecedented material properties for multilayer self-healing electronics (through selective self-healing and interfacial toughening), soft actuators (through supramolecular assembly into nanostructures), and recyclable underwater adhesives (through nanophase separation). These examples will show how next-generation dynamic polymer molecular design can be translated to applications in energy, sustainability, and human health.

MWRM 2026 MW390

Dynamics of microplastics occurrence in residential environments following Southern California wildfires: A multi-matrix assessment

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Wildfires are increasing in scale and frequency, raising concerns regarding the occurrence, transformation, and redistribution of microplastics (MPs) within wildland–urban interface (WUI) environments. This study provides one of the first field-based multi-matrix assessments of MPs occurrence in residential environments following the January 2025 Southern California wildfire. Soil, ash, and indoor-outdoor PM_{10} samples were collected from 50 households located within burn-area, adjacent, and further-distance houses, and household surveys were conducted to identify potential residential sources for MPs and to evaluate their distribution across indoor and outdoor environments. Target polymers, including styrene-butadiene rubber (SBR), polymethyl methacrylate (PMMA), nylon-66 (N66), polypropylene (PP), polystyrene (PS), and polyethylene (PE), were quantified using pyrolysis gas chromatography–mass spectrometry (Py-GC/MS). MPs were consistently detected across all the matrices investigated. Ash samples exhibited the greatest MPs abundance and polymer diversity, with total MP loadings higher in burn-area households (1.61×10^5 µg/kg) than adjacent households (1.21×10^5 µg/kg). Soil MPs were highest in further-distance households (7450 µg/kg), followed by burn-area (6850 µg/kg) and adjacent households (6050 µg/kg). Airborne PM_{10}-associated MPs ranged from 0.17 to 0.22 µg/m^3 across indoor and outdoor environments. PE dominated most matrices, while indoor SBR and PP loadings varied significantly ($p < 0.05$) among residential distance categories. The widespread occurrence of synthetic household materials identified through the survey, together with the observed polymer distributions, suggests that the measured MPs

represent a combination of pre-existing residential contamination and particles influenced by wildfire-related thermal alteration and environmental redistribution. The findings demonstrate that wildfire can act as an important contributor to the occurrence and redistribution of MPs in residential environments, with potential implications for prolonged human exposure through inhalation of airborne PM_{10}-associated MPs and contact with contaminated ash and residential soils.

MWRM 2026 MW277

Dynamics of water in mesoporous silica. confinement and interfacial effects

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The dynamics of nanoconfined water differ dramatically from those of the bulk liquid, yet the origins of these behaviors remain poorly understood. Here, we address this gap through an investigation of the changes in water dynamics, ***e.g.,*** diffusion, hydrogen-bond exchange, and vibrational spectra, upon confinement in nanoscale silica pores. A key question we consider is whether the modifications of water dynamics in mesoporous silica is attributable to confinement or interfacial effects. We make use of force fields developed for silica and silica-water interfaces to reproduce density functional theory data. The results demonstrate that the issue of confinement versus interfacial effects requires some nuance and the answer can depend strongly on the property of interest.

MWRM 2026 MW111

Effect of *N*-amide substitution on the sensitivity of lysosome-targeted H_2S sensors using 1,8-naphthalimide scaffold

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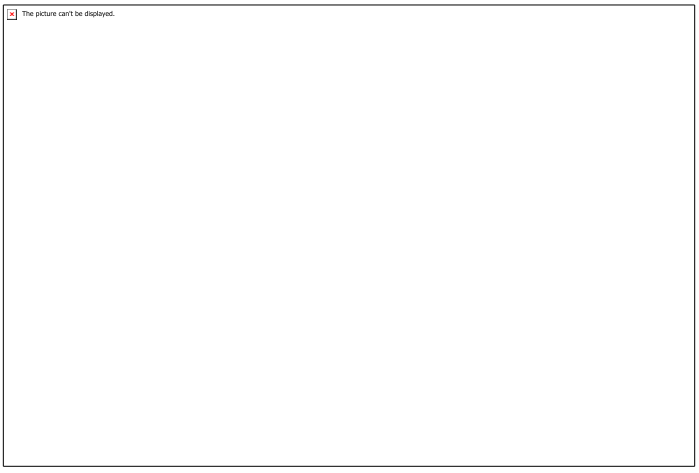
1,8-Naphthalimides are widely used fluorophores for building fluorescent sensors, especially for detecting hydrogen sulfide (H_2S). In our work, we used 3-hydroxy-1,8-naphthalimide as the fluorescent core and 2,4-dinitrobenzenesulfonate (DNBS) as the H_2S-responsive group to develop a series of H_2S sensors with high selectivity and sensitivity. *N*-amide substitution on the 1,8-naphthalimide is commonly used to improve solubility and tune fluorescence properties, but its effect on sensing performance has not been well studied. We found that the variation in the *N*-amide structure strongly influences sensor sensitivity, particularly in aqueous solutions. To understand this effect, we synthesized and tested a series of DNBS-based sensors with different *N*-amide substituents. Our results show a relationship between *N*-amide structure and H_2S sensitivity, which provides useful guidance for designing sensitive 1,8-naphthalimide-based fluorescent probes for H_2S detection.

MWRM 2026 MW100

Effects of agricultural biomass-derived hydrochar on soil fungal growth

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Hydrochar derived from agricultural biomass is a promising carbon-rich soil amendment with the potential to improve soil quality and influence soil microbial communities. However, the interactions between hydrochar and soil microorganisms remain poorly understood. In this study, hydrochar was produced from corn stover through hydrothermal liquefaction (HTL) under controlled temperature and retention time conditions. Saprobic fungus *Marasmius rotalis* was cultivated in potato dextrose broth (PDB) supplemented with 0%, 0.5%, 1.0%, and 1.5% hydrochar. Cultures were incubated for six days, with hydrochar-free cultures serving as the control. Fungal biomass accumulation following freeze-drying was measured. Preliminary experiments using unwashed hydrochar showed no significant improvement in fungal biomass. We hypothesized that residual low-molecular-weight compounds present in the raw hydrochar inhibited fungal growth. To test this hypothesis, the hydrochar was washed with acetone and oven-dried overnight before repeating the experiment under identical conditions. The washed hydrochar resulted in higher fungal biomass with 0.5%, 1.0%, and 1.5% hydrochar amendment ($P<0.05$). Scanning electron microscopy (SEM) revealed enhanced fungal hyphal development with increasing hydrochar concentration, supporting the observed biomass measurements. These findings suggest that removing inhibitory compounds from hydrochar improves its microbial compatibility. Further evaluations with a variety of microbes are recommended to determine hydrochar effects on soil biota.



SEM image of *Marasmius rotalis* growth on hydrochar

MWRM 2026 MW10

Effects of propylene glycol on the stability of nanostructured lipid carriers

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Nanostructured lipid carriers (NLCs) have emerged as promising dermal drug delivery systems because they enhance drug encapsulation, improve skin permeation, and provide greater stability than conventional lipid-based carriers. Propylene glycol (PG) is commonly incorporated into topical formulations as a penetration enhancer and lipid-modifying agent, yet its effects on NLC stability remain formulation dependent. This study investigated the influence of PG concentration on the encapsulation efficiency and stability of NLC formulations prepared by the solvent injection method.
Five NLC formulations containing 0, 1, 5, 10, and 20% (v/v) PG were prepared using oleic acid, stearic acid, and Tween 80, with Sudan III serving as a model lipophilic compound. Encapsulation efficiency was evaluated over a four-week storage period using heated hexane extraction followed by UV–Vis spectrophotometric analysis. Formulation stability was further assessed through qualitative observations of lipid expulsion, phase behavior during extraction, and resistance to ultrafiltration.
This work demonstrates that the effects of propylene glycol on NLC performance are highly formulation dependent and highlights the importance of optimizing excipient concentration to balance particle flexibility with long-term stability. Future studies will investigate the incorporation of polymeric stabilizers to mitigate PG-induced destabilization while preserving its beneficial effects on drug delivery.

MWRM 2026 MW57

Electrochemical and ^{13}C NMR determination of Hammett substituent constants using a 2,6-azulenic π-linker

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Hammett parameters (substituent σ constants) provide a quantitative measure of electron-donating and electron-withdrawing effects and remain indispensable for correlating molecular structure with reactivity and physicochemical properties across virtually all areas of chemistry. In our recent work, we demonstrated that linearly functionalized 1,1′,3,3′-tetraethoxycarbonyl-6,6′-biazulenes provide an electrochemical platform for quantitative determination of Hammett substituent constants from reversible reduction potentials of the biazulenic core. Owing to the intrinsic polarization and exceptional electronic polarizability of the azulene framework relative to benzenoid aromatics, this scaffold efficiently transmits substituent effects over long distances. However, the four ethoxycarbonyl groups required in our original design impose steric constraints that limit accurate evaluation of bulky substituents capable of strong π-

resonance donation, including dialkylamino groups. In this presentation, we will introduce a complementary molecular design based on two families of linearly functionalized 1,3-diethoxycarbonylazulenes. In the first, the substituent of interest is installed at the 6-position, eliminating the issue of steric interference. In the second, the molecules additionally incorporate a terminal [–NCCr$(CO)_5$] fragment at the 2-position of the azulenic nucleus, thereby offering a highly sensitive ^{13}C NMR reporter. We will discuss extraction of effective Hammett constants (σ_{eff}) from electrochemical reduction potentials of the azulenic core and demonstrate how ^{13}C NMR signatures of the [–NCCr$(CO)_5$] reporter anchor the electrochemically derived σ_{eff} values to the conventional Hammett scale. Synthetic details, spectroscopic characterization, and analyses of the molecular and electronic structures will also be presented as time permits.

MWRM 2026 MW378

Electrochemical and computational analysis of organic cathodic corrosion inhibitors: The effect of polarizability on corrosion inhibition

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Corrosion, the natural degradation of metallic materials through electrochemical oxidation, results in chronic financial drain and severe safety issues. Economically, the global cost of corrosion is estimated to be $2.5 trillion as of 2013, equating to approximately 3.4% of the global GDP. Furthermore, corrosion has directly led to catastrophic material failures in airplanes, bridges, sewer systems, and other critical infrastructure that resulted in the loss of human life. While corrosion is naturally spontaneous, the rate of corrosion can be accelerated by the environment and is especially escalated in saline environments. Corrosion inhibitors prevent corrosion by aiding formation of a barrier layer between the metal substrate and the corrosive environment. Heteroatomic organic molecules with polar functional groups and conjugated π-electrons, through their metal surface adsorption, can be used as corrosion inhibitors. Effectiveness of the corrosion inhibitor is typically inversely proportional to charge polarity of the functional groups, but we hypothesize that the polarizability of a functional group directly affects the corrosion inhibition ability of an organic molecule. To test this, we designed corrosion inhibiting organic heteroatom molecules containing nitrogen, oxygen, and/or sulfur heteroatoms for corrosion prevention of AISI 1008 cold-rolled carbon steel in saline media. Using electrochemical methods, including electrochemical impedance spectroscopy and cyclic polarization, in conjunction with computation analysis, the corrosion inhibition efficiency of these polarizable molecules will be explored. The synthesis, characterization, and corrosion inhibition of these molecules will be presented with implications for future research.

MWRM 2026 MW245

Electrochemical studies of lanthanide complexes supported by a di-aza crown ether ligand

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Lanthanide redox chemistry has applications in separations and a variety of technologies, but electrochemical studies of lanthanide coordination complexes have not received the attention that they deserve. In this presentation, the synthesis and study of a series of di-aza crown lanthanide (Ln) complexes where Ln = La, Sm, Eu, Tm, or Yb will be described, with a particular focus on the redox properties of the complexes. A variety of characterization methods have been used to study the isolated Ln(III) complexes, including cyclic voltammetry, X-ray diffraction analysis, and various spectroscopies. The corresponding Ln(II) complexes have been generated and studied by chemical and electrochemical reduction methods as well. The results show that the di-aza crown ligand used in this work enables appealing chemically reversible Ln(III)/Ln(II) redox with select lanthanide ions.

MWRM 2026 MW372

Electrochemistry-induced deposition for formation of mixed metal ZIF thin films

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Metal organic frameworks (MOFs) are the subject of growing interest in recent decades owing to their high porosity, surface area and tuneability. MOFs characterized by two or more metal centers are especially interesting for catalysis and sensing applications, but limitations of current synthesis methods restrict the study of these material for use in devices. Additionally, the design of these materials for use in devices often requires the formation of thin films with controlled thickness and shape, and current methods require tedious or expensive procedures and/or equipment. To address these issues, we demonstrate the applicability of electrochemical methods for the formation of patterned bimetallic cobalt/zinc zeolitic imidazolate framework (ZIF) thin films. In particular we aim to extend a method previously demonstrated by our group with Zinc(II)-based ZIF, electrochemistry induced (EC-Induced) deposition, to the synthesis of mixed metal Co/Zn(II)-ZIF. In contrast to the commonly utilized cathodic deposition, EC-induced deposition permits the formation of a film mimicking the cathodic electrode size and shape onto a substrate placed directly below, regardless of substrate conductivity. Monometallic and bimetallic ZIF films were synthesized under varying conditions via both EC-induced deposition and direct cathodic deposition, allowing for a thorough analysis and comparison of the two electrochemical methods. Characterization methods including XRD and ICP-MS were used to confirm the structure and metal uptake of the synthesized films. AFM, SEM-EDX and spectroscopic ellipsometry revealed differences

in film morphology and metal composition between the two electrochemical methods, with EC-Induced deposition consistently producing higher cobalt-content in films. The results of these investigations will provide fundamental insights necessary to establish a facile and highly tunable electrochemical method for the fabrication of mixed metal MOF thin films for catalysis and sensing applications.

MWRM 2026 MW153

Electronic properties of heterobimetallic complexes incorporating vanadyl and uranyl ions

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Heterobimetallic complexes offer the opportunity to understand how metals influence each other's properties when placed in close proximity. However, the properties of complexes containing both uranium and one or more redox-active transition metal have received less attention than they deserve. In this presentation, the synthesis and study of heterobimetallic complexes featuring both vanadyl, [VO]n+, and uranyl, [UO2m+] moieties will be reported. Particular to this study, the use of the redox-active vanadyl cation in the complexes provides unique spectroscopic handles and enables exploration of the influence that changing the oxidation state of uranium can have on nearby species. Findings from cyclic voltammetry as well as optical and vibrational spectroscopies suggest that significant interactions are possible between the [VO]n+ and [UO2m+] moieties, and evidence regarding the nature of these interactions will be discussed.

MWRM 2026 MW449

Electronic transitions of copper oxide in the 15,000 – 16,000 cm-1 Region

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Copper Oxide has a rich electronic structure, and numerous electronic transitions are found from the near infrared through the ultraviolet spectral regions. This project focuses on four electronic transitions in the 15,200 – 15,600 cm-1 spectral region, with particular emphasis on the previously assigned β 2Δ5/2 - X 2Π3/2 and β 2Δ3/2 - X 2Π1/2 transitions with bandheads at 15,317 cm-1 and 15,396 cm-1, respectively, and the A′ 2Σ– - X 2Π3/2 and A′ 2Σ– - X 2Π1/2 transitions with R-branch bandheads at 15,548 cm-1 and 15,271 cm-1. In our work, new high-resolution spectra of CuO in this region were obtained using intracavity laser absorption spectroscopy. Additionally, new ab initio theoretical calculations on the electronic states of CuO are reported, including

spectroscopic constants for the predicted electronic states. Based on the ab initio calculations, the previous β 2Δ5/2 and β 2Δ3/2 states are reassigned as 4Π5/2 and 4Π+1/2 spin-orbit components of the [1]4Π state, and the A′ 2Σ– state is assigned as the 4Π-1/2 state. Rotational analyses of these transitions were successful, and molecular constants for the excited state components were obtained Hund's case(a) Hamiltonian for the [1]4Π state. Large Λ-doubling was observed in the 4Π+1/2 and 4Π-1/2 spin-orbit components, due to interaction with the A 2Σ– at 16,492 cm-1. An energy level diagram of the previously assigned states in this region are correlated to the new experimental and ab initio-based assignments.

MWRM 2026 MW77

Engineered living hydrogels: Fundamental studies of microbe-material interactions in PEG-based matrices

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Engineered living hydrogels (ELHs) integrate functional microorganisms with natural or synthetic hydrogels to create composite materials that dynamically interact with their environments. These materials are enabling advancements in cellular therapeutics, biosensing, water treatment, and bioelectricity generation, among other applications. This research establishes fundamental insights into microbe–hydrogel interactions to advance the design and performance of these emerging technologies. Poly(ethylene glycol) (PEG)-based hydrogels were selected because of their biocompatibility, widespread use, and the broad range of available PEG-based macromers. We first investigated encapsulation chemistries that provide uniform bacterial dispersion throughout hydrogels while maintaining high cell viability. Step-growth hydrogels formed via Michael-type addition reactions between vinyl- and thiol-functionalized macromers provided high cell viability, tunable degradability, and uniform cellular encapsulation. Next, we investigated the effects of hydrogel mesh size on bacterial growth and secondary metabolite production. We found that mesh size regulates growth and can stimulate and modulate quorum-mediated bioproduction processes, primarily by imposing diffusion limitations within the hydrogel. Finally, PEG hydrogels were engineered to be photodegradable and were incorporated into microfluidic channels, where patterned light exposure produced controlled reductions in crosslink density. This enabled the systematic investigation of bacterial taxis through hydrogels at different stages of degradation. Cell speed, directionality, and release from the hydrogel were tunable by controlling degradation. These findings advance the development of ELHs, particularly for cellular biotherapeutic applications. Ongoing work focuses on incorporating catalytic enzymes and stimulus-responsive nanoparticles to further expand hydrogel functionality.

MWRM 2026 MW266

Engineering AgCl-loaded nanofiber membranes for sustained antimicrobial water treatment in long-duration space missions

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Long-duration space missions recycle water from wastewater, cabin humidity, and urine, and every batch must be disinfected before crew consumption. The International Space Station currently uses iodine for this, but iodine must be removed afterward because higher intake can affect thyroid function, adding equipment and complexity that becomes harder to justify on longer missions. Silver is being studied as a replacement, as it kills microbes effectively at low concentrations and is safe to consume. The challenge is maintaining the silver ion (Ag^+) concentration within a narrow range, about 200 - 400 ppb, high enough to control microbial growth but low enough to remain safe for consumption. This requires a material that provides sustained, controlled release of silver ions. Electrospun nanofibers, particularly coaxial nanofibers, can achieve this, since fiber diameter, porosity, and nanoparticle placement can all be controlled during fabrication, tuning ion diffusion through the fiber wall upon dissolution. Polyacrylonitrile (PAN) is used as the shell polymer, and polymethylmethacrylate (PMMA) mixed with silver chloride nanoparticles (AgCl NPs) as the core. After solvent treatment, the PMMA is removed, leaving hollow PAN nanofibers loaded with exposed AgCl NPs. However, the measured Ag^+ release rate in initial tests exceeded the target range, likely due to incomplete coaxial fiber formation, where the core and shell solutions mixed during electrospinning rather than forming a distinct core-shell structure. To address this, we are pursuing two parallel approaches. The first, an engineering approach, tailors membrane assembly. The AgCl NP-containing membrane is cut to a smaller diameter and sandwiched between two larger PAN membranes at the center of the flow path. Since this sandwiched region is thicker than the surrounding PAN layer at the periphery, water preferentially flows through the thinner, lower-resistance peripheral region, diluting the released Ag^+ toward the target concentration. Several trials did not achieve the desired reduction in release rate, so we are now focusing on a materials approach, optimizing the coaxial electrospinning process by controlling core-shell solution viscosity, AgCl nanoparticle loading, and needle configuration. Progress is being made toward consistently producing well-formed coaxial fibers with a properly confined core. Full materials and Ag^+ release characterization will be presented.

MWRM 2026 MW385

Engineering a reprocessable and self-healable boronic ester vitrimer derived from epoxidized soybean oil and eugenol

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Covalent adaptable networks (CANs), typically vitrimers are covalently cross-linked materials that offer multi-functionality of both thermosets like rigidity and thermoplastics like recyclability, reprocessability, and self-healing, due the dynamic covalent bond exchange mechanism. The manufacturing of traditional thermosets has significantly increased in recent years, which has led to the rapid depletion of fossil fuel reserves and the landfilling of plastic waste because it cannot be recycled or reprocessed after its application. The development of bio-based vitrimers with dynamic covalent bonding is a practical means of overcoming the limitations of conventional thermosets. Among various reported vitrimer networks, boronic ester vitrimers are particularly desirable because they can enable dynamic adaptability through associative reversible B–O bond exchange mechanism in their cross-linked networks. In this study, we have demonstrated the one-pot synthesis of eugenol-modified epoxidized soybean oil (ESBO_Eu) as a reactive precursor for the fabrication of boronic ester vitrimer. Moreover, the as-synthesized ESBO_Eu has been characterized by FTIR, ^{1}HNMR, iodine value and %EOC titration methods. To avoid conventional acrylated systems involving acrylic acid, eugenol becomes an excellent eco-friendly alternative extracted from bio-based clove oil, which offers reactive double bonds to initiate the "*thiol-ene*" coupling reaction under a sustainable pathway. Finally, we have designed the bio-based boronic ester vitrimer by thermally triggered "*thiol-ene*" reaction between ESBO_Eu and dynamic dithiol boronic ester cross-linker (DBEDT) under catalyst-free condition followed by initial structural confirmation form the FTIR analysis. The synthesized boronic ester vitrimer exhibits a single glass transition temperature (T_g) of 16.3 °C and is quite thermally stable up to 331.7 °C according to TGA thermogram, which evaluates the vitrimer's thermos-oxidative behavior. The vitrimer also showed a balanced mechanical strength between a thermoset and thermoplastic, with a moderate tensile strength of ~5 MPa and elongation break at ~300%. Topological interchange is made possible by dynamic boronic ester connections, which enhance mechanical reprocessing efficiency, solvent recyclability by reversible hydrolysis in ethanol, and self-healing capacity.

MWRM 2026 MW46

Engineering confined phosphonate pore environments in MOF-808 for selective rare-earth recovery

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Recovering rare earth elements (REEs) from acidic mining-impacted waters and mineral-processing effluents could transform contaminated waste streams into secondary sources of critical materials. However, REEs occur at low concentrations in chemically complex acidic solutions containing sulfate and competing metal ions, limiting their selective capture by conventional sorbents. Metal-organic frameworks (MOFs) offer promising platforms for REE adsorption because of their high surface areas, accessible pore volumes, and tunable chemical functionality. Chemically robust Zr- and Al-based frameworks are especially attractive because they combine stability in acidic media with potential for scalable synthesis, yet their application to REE recovery under these conditions remains underdeveloped. We present a mechanistic strategy for the selective recovery of REEs via phosphonate grafting within the confined pore environment of the acid-stable Zr-MOF, MOF-808 [$(Zr_6O_4(OH)_4(BTC)_2(HCOO)_5(H_2O)(OH)$; BTC = 1,3,5-benzenetricarboxylate]. The resulting functionalized MOF-808 achieved 90% selective recovery of Nd from an aqueous mixture containing competing metal ions, with negligible uptake of the competing ions. Building on this result, a library of phosphonate-functionalized frameworks will be designed to vary the binding-pocket geometry, functional-group density, and pore accessibility,and confinement effects while prioritizing materials compatible with scale-up. Batch adsorption and desorption studies will quantify REE uptake capacity, selectivity, adsorption kinetics, recovery efficiency, and regeneration performance. Molecular simulations and machine-learning models will complement these experiments by resolving REE coordination within confined pores and identifying physically meaningful descriptors of selective binding and release. This integrated experimental and computational framework aims to connect pore-scale coordination chemistry with practical separation performance and establish design principles for scalable REE recovery from acidic wastewater.

MWRM 2026 MW177

Engineering dipole-parallel alignment in donor-acceptor organic molecular crystals

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The majority of polar organic molecules crystallize in centrosymmetric arrangements in which molecular dipoles align antiparallel, resulting in nonpolar crystal structures. Consequently, polar organic crystals, which are essential for nonlinear optical (NLO) and electronic applications, remain rare. This project aims to engineer dipole-parallel alignment in donor–acceptor molecular crystals by exploiting favorable aromatic interactions to overcome dipole–dipole repulsion. A series of imine and bisimine compounds derived from the isonicotinaldehyde synthon were synthesized and evaluated as potential polar crystalline materials.
Undergraduate researchers prepared the target compounds using organic synthesis techniques and characterize them by NMR and IR spectroscopy. Single crystals suitable for X-ray diffraction will be grown and structurally characterized in collaboration with the University of Iowa. Crystal structures were deposited in the Cambridge Crystallographic Data Centre (CCDC), providing publicly accessible crystallographic data. To evaluate functional properties, selected crystals will be investigated for second-harmonic generation (SHG) activity through laser-based nonlinear optical measurements in collaboration with faculty specializing in optical materials.
This research integrates synthetic organic chemistry, crystallography, and materials characterization to investigate structure–property relationships governing polar crystal formation. The project provides undergraduate researchers with interdisciplinary training in modern materials chemistry while advancing the rational design of organic molecular crystals with potential applications in photonics and nonlinear optics.

MWRM 2026 MW379

Engineering lithium storage in PAN- and PVP-derived carbon anodes through carbonization, nanofiber architecture, and C_{60} reinforcement

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Polymer-derived carbons offer a versatile platform for lithium-ion battery anodes, yet the interplay among precursor chemistry, thermal processing, electrode architecture, and molecular carbon additives remains poorly understood. In this work, polyacrylonitrile (PAN)- and polyvinylpyrrolidone (PVP)-derived carbons were synthesized by argon pyrolysis and systematically correlated with electrochemical performance through FTIR,

XRD, Raman spectroscopy, SEM, galvanostatic cycling, and electrochemical impedance spectroscopy. Increasing the carbonization temperature from 600 to 1500°C enhanced carbon ordering and coulombic efficiency but reduced defect-associated lithium-storage sites, resulting in lower reversible capacities. To investigate architectural effects, electrospun PAN and PVP nanofiber mats, with and without C_{60} incorporation, were carbonized at 600°C. C_{60} modified the carbon microstructure and improved charge-transfer kinetics, with the C_{60} reinforced PVP nanofiber mat exhibiting the highest reversible capacity. These results highlight a fundamental trade-off between defect-mediated lithium storage and thermally induced structural ordering, while demonstrating that nanofiber architecture and C_{60} reinforcement provide effective routes for tailoring lithium-storage sites and charge-transport pathways. This study establishes a practical framework for optimizing polymer-derived carbon anodes through coordinated control of precursor chemistry, carbonization conditions, and electrode design.

MWRM 2026 MW381

Engineering plasmonic nanoparticles for quantitative surface-enhanced Raman spectroscopy

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Surface-enhanced Raman spectroscopy (SERS) has enormous potential for ultrasensitive molecular detection yet achieving reliable and quantitative measurements remains a major challenge. While most studies focus on maximizing electromagnetic enhancement, we propose that hotspot accessibility is equally important. Strong hotspots alone do not guarantee high-performance sensing if analyte molecules cannot efficiently reach and occupy these regions.
Our research investigates how nanoparticle morphology, including shape, size, surface roughness, interparticle spacing, and three-dimensional architecture, controls hotspot accessibility and ultimately determines SERS performance. Plasmonic gold nanoparticles with well-defined morphologies are synthesized and characterized by electron microscopy, optical spectroscopy, and Raman spectroscopy. Rather than evaluating individual structural parameters independently, we use machine learning to analyze large experimental datasets and uncover the complex relationships among nanoparticle morphology, hotspot accessibility, spectral quality, sensitivity, reproducibility, and quantitative sensing performance. These analyses identify the structural features that most strongly influence analyte transport and hotspot utilization, providing predictive design rules for engineering high-performance SERS substrates. This work establishes hotspot accessibility as a critical design parameter for quantitative SERS and provides a framework for the rational development of plasmonic nanomaterials for chemical sensing, biosensing, and molecular diagnostics.

MWRM 2026 MW415

Enhanced sampling approaches to Li-ion transport across the solid electrolyte interphase

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Lithium-ion transport across the electrode/electrolyte boundary in a battery is complicated by the presence of a surface film known as the solid electrolyte interphase (SEI). Our group has previously applied classical molecular dynamics to show that the SEI can impact electrolyte structure and dynamics as measured by changes in ion accumulation, association, lithium coordination environment, and solvent residence time. Understanding these molecular-level features is essential for elucidating the mechanisms governing lithium transport in lithium-ion batteries. In this work, molecular dynamics simulations combined with umbrella sampling and replica exchange are used to investigate lithium transport across SEI surfaces. A comparison between conventional umbrella sampling and replica exchange simulations demonstrates improved sampling with exchange and a more natural mechanistic interpretation of the transport pathway. The influence of umbrella potential parameters, including force constants, is further investigated to understand their effects on the resulting free energy profiles and coordination changes. It will be shown that the efficacy of replica exchange comes from allowing the system to overcome kinetic barriers between solvation structures along the path to lithium-ion insertion. Our calculated free energy barriers are in excellent agreement with experimental estimates for ion transfer and provide much-needed molecular insights into the “resolvation” process. Ongoing work will consider the use of Hamiltonian replica exchange to improve sampling of electrode-electrolyte interactions as a function of salt concentration.

MWRM 2026 MW415

Enhanced sampling approaches to Li-ion transport across the solid electrolyte interphase

Hiruni Wimalasiri*, mdwimalasiri@shockers.wichita.edu, Ryan Jorn. Chemistry & Biochemistry, Wichita State University, Wichita, Kansas, United States*

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MWRM 2026 MW264

Enhancing capacitive deionization performance through safe polymeric binders

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Capacitive deionization (CDI) is an efficient electrochemical water treatment technology used to purify the brackish water into potable water through the electrosorption of ions within the electrical double layer of the activated carbon (AC) electrodes. While AC has been extensively studied as the active electrode material because of its high surface area and hierarchical pore structure, the effect of polymeric binders on electrode performance has received comparatively less attention in CDI. Beyond providing mechanical adhesion, binders contribute towards the hydrophilicity, electrode integrity, electrical contact, ion transportation, and ultimately the desalination performance of CDI electrodes. This study involves the investigation of AC electrodes fabricated using three different safe polymeric binders’ polyacrylic acid/carboxymethyl cellulose (PAA/CMC), styrene-butadiene rubber/carboxymethyl cellulose (SBR/CMC) and crosslinked poly(vinyl alcohol)-glutaraldehyde (PVA-GA). The PAA/CMC electrodes exhibited optimal wettability but lower mechanical stability and lower desalination performance. In contrast, both SBR/CMC and PVA-GA electrodes demonstrated excellent structural stability, with the PVA-GA electrodes maintaining their integrity for more than one week without observable carbon particle peeling off from the graphite substrate. Electrochemical characterization revealed that the SBR/CMC electrodes achieved the highest mass-specific capacitance 116 F/g, followed by PAA/CMC 107 F/g and PVA-GA 104 F/g. Correspondingly, the SBR/CMC electrodes exhibited the highest salt adsorption capacity (SAC) of 17.6 mg_{NaCl}/g_{AC} (the average value over 50 cycles), followed by the PVA-GA electrodes at 14.5 mg_{NaCl}/g_{AC}, whereas the PAA/CMC electrodes showed the lowest SAC of 8.0 mg_{NaCl}/g_{AC}. These results demonstrate that binder chemistry significantly influences the mechanical robustness and desalination performance of AC electrodes. Although SBR/CMC delivered the highest electrochemical and CDI performance, crosslinked PVA-GA exhibited superior long-

term structural stability while achieving desalination performance closer to SBR/CMC, highlighting its potential as a promising binder for durable CDI electrodes.

MWRM 2026 MW135

Enzyme-activatable 5-ALA prodrugs for targeted photodynamic therapy

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5-aminolevulinic acid (5-ALA) is an FDA approved drug that is used for photodynamic therapy (PDT) and diagnostic imaging. 5-ALA is a natural precursor in the heme biosynthetic pathway that is present in all cells. But a notable hallmark of many types of cancer cells is decreased ferrochelatase activity which limits the conversion of Protoporphyrin IX (PpIX) into heme. Exogenous administration of 5-ALA to a patient leads to selective accumulation of fluorescent PpIX in the cancerous tissue which can be exploited for diagnosis and fluorescence guided surgery, and also targeted cancer PDT. As a theranostic agent, 5-ALA is useful, but it is limited by some significant pharmacokinetic performance problems including poor tumor selectivity, limited cell membrane penetration, and instability in serum. These limitations drive the development of protected derivatives of 5-ALA to improve stability and delivery. We report the design and synthesis of 5-eMAL, a doubly protected derivative, whose protecting groups are cleaved at both ends of the molecule by esterase activity followed by self-immolation. We show that cancer cells treated with 5-eMAL produce much higher levels of intracellular PpIX than cells treated with 5-ALA and low doses of 5-eMAL permit efficient cell photoinactivation. These findings highlight 5-eMAL as a promising prodrug of 5-ALA to overcome the stability and delivery limitations of 5-ALA. Building on the success of 5-eMAL, we are currently developing next-generation 5-ALA prodrugs with peptide-based and tumor-targeting motifs to further enhance selectivity and cancer-specific activation. These derivatives are designed to exploit tumor-associated enzymes and receptor-mediated uptake pathways to improve localization and therapeutic index. Preliminary synthetic efforts are underway, and ongoing studies aim to evaluate their stability, activation profiles, and PpIX generation in cancer models. This work establishes a modular platform for improving 5-ALA delivery and supports the continued development of targeted theranostic strategies for photodynamic therapy in oncology.

MWRM 2026 MW272

Establishing EPA Method 1633A as the primary analytical tool for PFAS analysis of agricultural samples in Kansas

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Per- and polyfluoroalkyl substances (PFAS) are a class of persistent synthetic fluorinated compounds widely used in industrial and consumer products because of their exceptional chemical and thermal stability. Their persistence has led to widespread environmental contamination, with agricultural systems becoming important exposure pathways through contaminated irrigation water, biosolids, and other soil amendments. PFAS can accumulate in soils, be taken up by crops, and transfer to livestock, raising concerns for food safety and human health. Accurate determination of PFAS is challenging because they occur at parts-per-trillion (ppt) levels in complex matrices such as groundwater, biosolids, soil, plant tissue, and milk. This study implemented EPA Method 1633A to determine 40 priority PFAS analytes in agricultural samples. Samples were extracted using weak anion-exchange carbon-black-hybridized solid-phase extraction cartridges and analyzed by UHPLC–MS/MS using a Waters Acquity Premier UHPLC with a BEH C18 column coupled to a TQ Absolute triple quadrupole operating in electrospray ionization multiple reaction monitoring mode. Although automated processing was used, reliable quantification required expert manual review of peak integration and analyte identification to meet EPA quality control criteria. Method validation demonstrated excellent linearity ($R^2 \geq 0.990$), limits of quantitation below EPA single-digit ppt requirements, and sub-ppt method detection limits for agricultural water. Stable isotope-labeled internal standards effectively corrected for extraction losses and matrix effects, with all performance criteria satisfied. This presentation highlights PFAS occurrence in agricultural systems, analytical challenges associated with EPA Method 1633A, and strategies for reliable PFAS analysis in Kansas agricultural samples.

MWRM 2026 MW30

Estrogenic signaling imposed by standard culture conditions

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Investigating sex as a biological variable reveals sex-specific mechanisms that shape disease risk, progression, and treatment response. In ovarian cancer, it has been shown that estrogen promotes proliferation, invasion, and immune signaling and also

alters the epithelial-mesenchymal transition and metabolism in cells. Currently, there is a major gap in the ovarian cancer addendum—estrogen contamination has not been assessed extensively in ovarian cancer, as breast cancer has been the main focus for estrogen-based cancer research. Several components of cell culture media can contribute to the results of in vitro studies. These components include fetal bovine serum (FBS) and phenol red. FBS is a natural supplement added to cell media that offers essential nutrients and growth factors for the maintenance and growth of cultured cells. FBS contains low, variable concentrations of 17-beta-estradiol, often ranging between 10 and 100 pg/mL. Additionally, serum is highly heterogeneous in cell culture and can vary by species, donor, vendor, production lot, and age; this high degree of hormonal variability introduces confounding endocrine exposures into cell culture systems. Phenol red (PR), a pH indicator used in cell culture, contains two hydroxyphenyl groups attached to a central carbon; this structure closely resembles the phenolic A-ring found in many estradiol compounds, allowing PR to weakly bind estrogen receptors and mask estrogenic activity. We aim to measure the effects of PR and FBS on estrogen-receptor expression through four different conditions on four ovarian cancer cell lines: media with charcoal-stripped (CS) and PR, media with no PR and regular FBS, media with no PR and CS FBS, and finally the previous no PR and CS FBS media with estradiol supplemented back in. Our ovarian cancer cell lines include Kuramochi, OVSAHO, OVCAR3, and OVCAR8. Cell lysis was performed on each cell line under standard conditions and in no PR/regular FBS media, and analyzed by Western blot with anti-ER alpha and anti-ER beta as primary antibodies. Identifying the estrogen-specific mechanisms underlying cancer cell proliferation will aid in the identification of pathways involved in disease resistance and longevity and support the development of more effective cancer therapies.

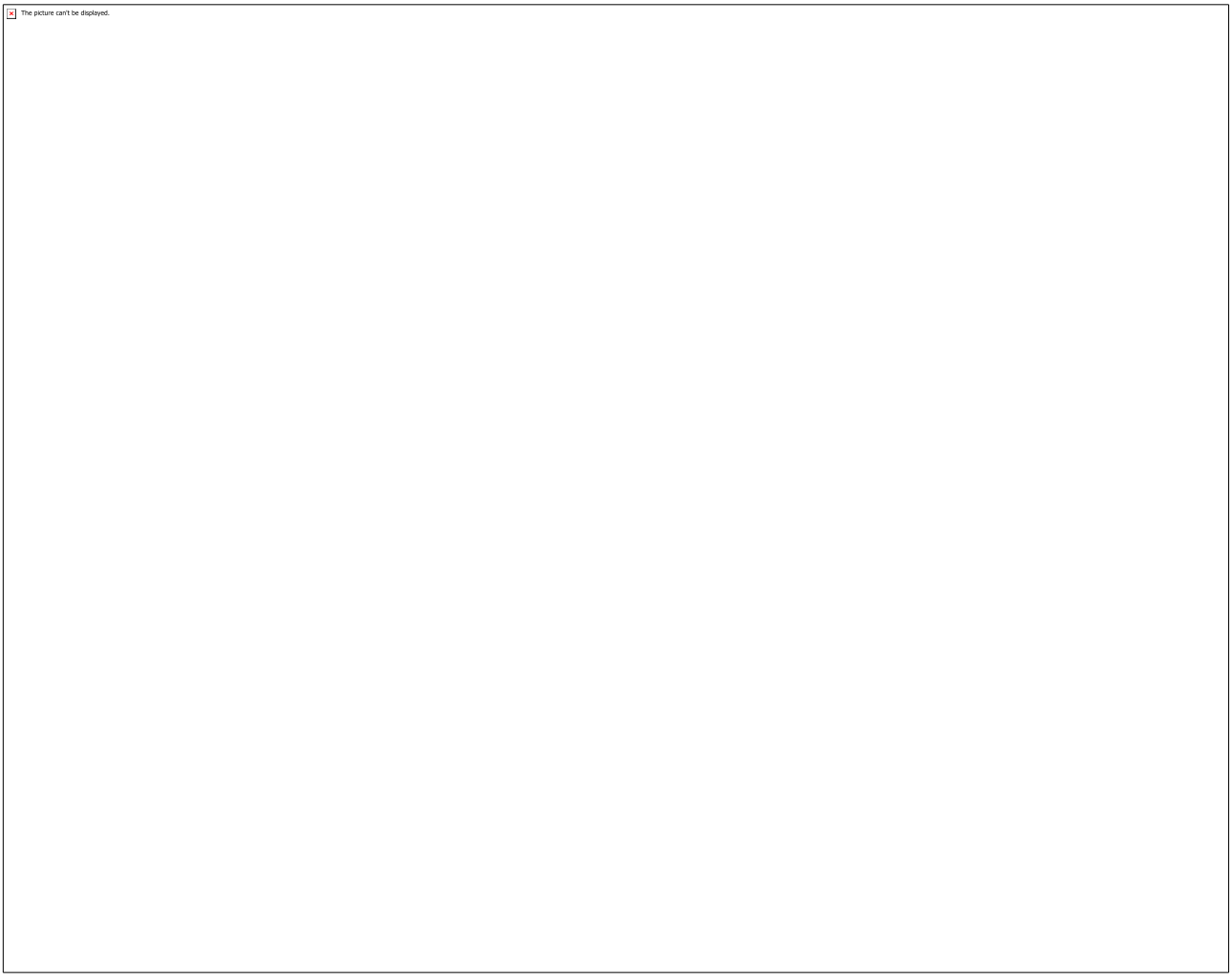
MWRM 2026 MW324

Evaluating the efficacy of aggregation propensity as a predictor of oligopeptide dimerization in redox-active conditions

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Peptide sequence determines its structure, function, ability to exhibit self-assembly behavior, and stimuli responsiveness. Different cysteine-containing amino acid sequences were synthesized and characterized to experimentally validate a computer model predicting peptide aggregation propensity. Oligopeptide aggregation occurs when the cysteine group in the peptide oxidizes to form a thiol-disulfide bond with another cysteine, forming a dimer. Those outputs yielded peptide sequences that are likely to aggregate based on the probability of the formation of thiol-disulfied bonds and dimerization. The oligopeptides' structure and redox activity will be tested using a variety of light spectroscopy and microscopy techniques that show peptide structure, aggregation, and morphology. The goal of the study is to identify if oligopeptide sequences that exhibit high aggregation propensity will experimentally demonstrate

redox-active aggregation. Experimental validation of aggregation propensity to predict oligopeptide dimerization will contribute to identifying the most precise metrics to predict oligopeptide dimerization in redox-active conditions. Oligopeptides were synthesized via solid state peptide synthesis and undertook cleavage, precipitation,and purification. MALDI mass spectrometry and UPLC determined oligopeptide purification accuracy by distinguishing mass and distribution which can be compared to the expected protein mass. Dissipative self-assembling peptides (DSAPs) require constant chemical fuel, also producing waste products which can interfere with chemical reactions. The synthesis of self-assembling oligopeptides that demonstrate self-assembly properties provide a more energy-efficient alternative compared to DSAPs. The testing of the aggregation propensity of oligopeptide dimerization in redox-active conditions will create more precise prediction methods, leading to the development of biomaterials and nanotechnologies for improved drug release precision.



This image is the final draft of the poster that will be presented.

MWRM 2026 MW358

Evaluating the functional selectivity of endogenous D-amino acid-containing neuropeptides in *Aplysia californica*

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Some neuropeptides undergo a post-translational modification where an L-amino acid residue is converted into a D-amino acid residue. The resulting D-amino acid-containing peptides (DAACPs) have been found to have different biological functions as compared to the all-L-residue peptides. Despite the biological relevance, little is known about how endogenous L-to-D-residue isomerization in peptides impacts interactions with their cell surface receptors. Based on prior studies from our lab, we hypothesized that the isomerization of an L-amino acid residue to a D-amino acid residue in a peptide may lead to preferential activation of one signaling pathway over another, a naturally occurring form of functional selectivity. To test this hypothesis, we evaluated several signaling pathways for two of the known DAACP receptors, allatotropin-related peptide receptors 1 and 2 (*ap*ATRPR1 and *ap*ATRPR2) from *Aplysia californica*. We tested the activation of G protein-dependent pathways ($G\alpha_q$ and $G\alpha_s$), G protein-independent pathway, and phosphorylation of ERK (pERK) in transiently transfected HEK-derived (HTLA) cells using cell-based receptor activation assays to determine bias factors. For *ap*ATRPR1, the DAACP seems to be biased towards activation of $G\alpha_q$ pathway as compared to pERK and $G\alpha_s$ pathway. The DAACP also seems to preferentially activate G protein-independent pathway as compared to $G\alpha_q$ pathway for *ap*ATRPR1. For *ap*ATRPR2, the DAACP seems to show preferential activation of $G\alpha_s$ pathway as compared to $G\alpha_q$ pathway and $G\alpha_q$ pathway as compared to G protein-independent pathway. These results suggest that isomerization of the endogenous peptide ligands (all-L-peptide to DAACP) for receptors *ap*ATRPR1 and *ap*ATRPR2 leads to preferential activation of one signaling pathway over another for both receptors in HTLA cells. This research demonstrates how endogenous peptide isomerization can lead to functional selectivity and how nature utilizes isomerization to regulate downstream signaling pathways. Moreover, the presence of DAACPs across phyla suggests that cellular signaling involving peptide isomerization is not restricted to *Aplysia californica*, and the knowledge of functional selectivity could be relevant to other systems across the animal kingdom. This research provides a deeper understanding of the role of isomerization of peptides in regulation of neuropeptide-receptor signaling.

MWRM 2026 MW161

Evaluating the substrate scope of an improved Blum aziridine synthesis

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N–H aziridines are valuable synthetic building blocks with medicinal relevance, serving as versatile intermediates in the synthesis of pharmaceuticals, natural products, and other biologically active molecules. The Blum aziridine synthesis is a powerful and widely used method for preparing these compounds. However, the Delaney lab has identified challenges in the cyclization step, consistent with published methods that employ a multistep workaround to bypass this difficult transformation. Our experimental and computational studies refute the canonical unimolecular mechanism and instead suggest that the reaction proceeds through a concerted chain mechanism. We hypothesize that poor reactivity in the cyclization phase is caused by a failure to initiate the chain reaction. This hypothesis led to the discovery of a catalytic initiator that can reliably access the propagation step. My work focuses on expanding the substrate scope of the optimized Blum aziridine synthesis by preparing diverse N–H aziridines to demonstrate its improved functional group tolerance and broader applicability. The substrates were subjected to the optimized reaction conditions, and the resulting aziridines were purified when necessary and characterized by NMR spectroscopy. In addition, NMR yield studies were performed to directly compare reactions conducted with and without the catalytic initiator. These results further establish the optimized Blum aziridine synthesis as a practical and efficient approach for accessing stereodefined aziridines for applications in synthetic and medicinal chemistry.

MWRM 2026 MW92

Evaluation of gold nanosphere-induced cytotoxicity in leukemia cells via MTT assay

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Leukemia is a blood cancer commonly treated with chemotherapy and targeted drug therapies, which are often limited by toxicity and drug resistance. Gold nanoparticles have emerged as promising platforms for improving therapeutic delivery due to their unique optical properties and surface tunability.
In this study, gold nanospheres were evaluated for their effects on leukemia cell viability using an MTT assay. Cells were exposed to varying nanoparticle concentrations, and

metabolic activity was measured as an indicator of viability. The results demonstrated a concentration-dependent effect, with minimal impact at lower concentrations and a significant decrease in cell viability at higher concentrations.
These findings suggest that gold nanospheres can influence leukemia cell survival and may serve as a foundation for future therapeutic applications. Ongoing work will focus on functionalizing nanoparticles with CLL-1 targeting ligand to improve specificity towards leukemia cells and enhance treatment efficacy.

MWRM 2026 MW442 - Withdrawn

MWRM 2026 MW442 - Withdrawn

MWRM 2026 MW246

Experimental studies of platinum heterobimetallic complexes to probe Lewis acid effects

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Incorporation of secondary, effectively Lewis acidic metal cations into heterometallic complexes is a useful strategy for tuning chemical properties and reactivity, but the origins of metal-driven tunability and quantitative correlation of metal-focused data have not received the attention they deserve. Prior work has shown a relationship between the properties of macrocyclic platinum(II) complexes and the charge states of the incorporated cations, but in prior work, the measured tuning could not be directly attributed to Lewis acidity as only a limited set of cations were studied. Here, the synthesis and characterization of an expanded series of diamagnetic complexes containing platinum(II) and secondary cations are reported, along with nuclear magnetic resonance (NMR) measurements of ^{195}Pt chemical shifts. Spectroscopic and electrochemical studies of the complexes demonstrate linear trends that depend on the Lewis acidity, or charge density, of the secondary cations. Such trends are maintained when comparing among mono-, di- and tri-valent cations, enabling the measured trends to be attributed to Lewis acid effects and not charge state alone.

MWRM 2026 MW84

Exploring biological sequence diversity to identify enzymes for efficient plastic degradation

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Polylactic acid (PLA) and polycaprolactone (PCL) are biodegradable bioplastics widely used in packaging, 3D printing, medical implants, and agricultural applications. Although derived from renewable resources, they degrade slowly under natural conditions, limiting their potential to reduce plastic waste. Enzymatic depolymerization offers a promising strategy to accelerate degradation and enable closed-loop recycling. Building on prior reports of a cutinase-like enzyme from *Cryptococcus* species capable of degrading PLA, we used public protein databases and BLAST to identify 14 homologous fungal enzymes with potential polyester-degrading activity. These genes were cloned into a yeast host for secretory expression and screened using a rapid solid-plate assay. Six and nine homologs exhibited high hydrolytic activities toward PLA and PCL, respectively. Computational structural analysis of enzyme-substrate interactions uncovered mechanistic features that help explain the subtle determinants of substrate specificity. Together, this work demonstrates how integrating sequence diversity mining, high-throughput functional screening, and computational structural analysis can accelerate enzyme discovery and engineering for future sustainable plastic deconstruction and circular biomanufacturing.

MWRM 2026 MW443

Exploring photophysical effects of linker modifications of MOF-76 via computational and experimental methods

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Lanthanide metal-organic frameworks (Ln-MOFs) are porous, crystalline materials whose luminescence properties make them ideal candidates for bioimaging applications. Here, Ln3+ luminescence is governed by the antenna effect, where energy from the ligand's excited triplet state is transferred to the lanthanide's excited triplet state via ligand-to-metal charge transfer (LMCT). Empirical results show that a specific range of energy differences between the two triplet states results in efficient energy transfer. In MOF-76, 1,3,5-benzenetricarboxylic acid (BTC) shows greater sensitization of Tb3+ than Eu3+. We hypothesize that shifting the linker’s energy levels by adding supplemental functional groups can enhance or limit the LMCT process and alter the material's fluorescence quantum yield. This project used computational and experimental methods to determine the triplet-state energies of functionalized variants

of BTC to optimize the fluorescence intensity of different Ln3+. Computationally, ORCA was used to calculate the triplet-state energies of several ligands using TD-DFT, Δ-SCF, and other methods at various levels of theory. The BTC variants were synthesized and their triplet energy states were experimentally determined via phosphorescence spectroscopy. The combined results guided the selection of various metals and linkers for optimized luminescence intensity and fluorescence quantum yield in MOF-76 variants.

MWRM 2026 MW150

Fabrication, characterization, and reactivity study of an Fe^{III}-OMe complex

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Current synthetic methods heavily utilize precious metals in their oxidative steps, which are very costly and environmentally toxic. An intriguing alternative to these are earth-abundant transition metals, which are much cheaper and more environmentally friendly. Lipoxygenase is an enzyme that utilizes an Fe^{III} or Mn^{III} center to conduct proton-coupled electron transfer (PCET) reactions to oxidize polyunsaturated fatty acids. Currently, literature exists that examines this reaction via the $[Fe^{III}(OH)(dpaq)]^{+}$, $[Mn^{III}(OH)(dpaq)]^{+}$, and $[Mn^{III}(OMe)(dpaq)]^{+}$ model complexes. However, the $[Fe^{III}(OMe)(dpaq)]^{+}$ complex has not been previously studied. Examining this complex could help to better understand the effects of the metal center and the methoxide ligand upon the reactivity of the complex. Metalation of the H-dpaq ligand was achieved by reacting it with $Fe(OTf)_3$ under basic conditions in methanol. This complex was then characterized with UV-Vis spectroscopy, mass spectrometry, and nuclear magnetic resonance (NMR) spectroscopy. Subsequently, the reactivity of the complex was studied by monitoring its PCET reaction with 1,2-diphenylhydrazine (DPH) by UV-Vis spectroscopy. This complex was found to react with DPH at a rate exceeding that of the $[Fe^{III}(OH)(dpaq)]^{+}$ complex.

MWRM 2026 MW441 - Withdrawn

MWRM 2026 MW441 - Withdrawn

MWRM 2026 MW356

Fabrication of spatially aligned gold nanotriangle–silver nanodot arrays using optimized nanosphere lithography masks

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Multimaterial nanostructure arrays offer advantages for both optical sensing and biomolecular organization. The plasmonic response of metallic nanostructures can enhance optical sensing signals, while chemically distinct materials on the same surface can provide separate binding sites for different biomolecules, such as the enzymes involved in an enzyme cascade. These binding sites can partially organize two enzymes at controlled distances, which may improve the transfer of reaction intermediates between them. Here, we present a nanosphere lithography method for fabricating gold nanotriangle–silver nanodot arrays with spatially aligned features on silicon. Because the quality of the resulting structures strongly depends on the particle mask, polystyrene nanosphere assembly at the air–water interface was optimized before fabrication. Marangoni-driven spreading was used to promote sphere movement and packing, while sodium dodecyl sulfate was added to the water subphase to control surface tension and packing forces. For 900 nm spheres, 0.1 mM SDS produced large, hexagonally close-packed domains with fewer defects. These improved masks support more uniform feature dimensions, spacing, and spatial alignment in the multimaterial arrays.
The close-packed sphere layer is transferred to silicon and used as a common mask. Gold is thermally evaporated through the gaps between the spheres to form nanotriangles. An octadecyltrichlorosilane self-assembled monolayer is then formed as a resist. After sphere removal, silver is electrolessly deposited at the original sphere-surface contact sites, producing silver nanodots spatially aligned with the gold nanotriangles. This approach provides a scalable route to ordered two-material surfaces for plasmonic sensing and controlled biomolecular organization.

MWRM 2026 MW238

Facile linking of lanthanide cations with soft metals via thiosulfate

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The lanthanides have been applied to profitable innovations in medicine and technology, yet a better understanding of the coordination chemistry of hard lanthanide cations with softer ligands could lead to innovative discoveries in medicine, industry and geochemistry. The thiosulfate anion ($S_2O_3^{2-}$) is a versatile, tetrahedral ligand that can exhibit bonding through both the “soft” sulfur and the “hard” oxygen atoms. Here, we are

using this softer thiosulfate ligand, which an effective metal complexing agent that has industrial and medical applications, to not only complex the lanthanide cation but also as a means to couple a lanthanide to a soft secondary metal. This is a highly desirable aim as many lanthanide mixed-metal compounds have been shown to be useful in a variety of luminescent and catalytic applications; moreover, some thiosulfate-based inorganic-organic frameworks have been shown to be effective photocatalysts. Herein, we discuss the syntheses and structures of novel lanthanide-silver thiosulfate complexes.

MWRM 2026 MW38

Fe-Co-Ru-promoted Ni/CeO_2 single-atom and nanocluster catalysts for dry reforming of methane at high space velocity

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The rational design of dry reforming of methane (DRM) catalysts requires a fundamental understanding of how catalyst synthesis governs active-site and selectivity. In this study, we systematically investigated five solution-based synthesis routes for Fe-Co-Ru-promoted Ni/CeO_2 catalysts and established direct synthesis-structure-activity-coking relationships at 700°C under high space velocity (180,000 ml/g_{cat}.h) for 20 h time on stream using spectroscopic, electron-microscopic, and temperature-programmed techniques. The synthesis methods are wet impregnation (WI), hydrothermal (HT), co-precipitation (CP), solution combustion (SC), and microwave-assisted (MW). We established that each synthesis route produces a distinct catalyst structure that directly controls CH_4 reaction rate, metal-support interactions, oxygen mobility, and resistance to coking. Among all the synthesis routes investigated, the MW method produced the most catalytically active multi-metallic alloy due to the formation of highly dispersed nanoclusters, which enhanced CH_4 activation while suppressing carbon deposition. The CP method, in particular, produced the most coke-resistant catalyst by generating single-atom sites with abundant oxygen vacancies and strong metal-support interactions that promote efficient CO_2 activation and a continuous supply of reactive oxygen radicals (O^*) for carbon oxidation. However, the HT and WI methods produce large nanoclusters, which result in a higher coking rate due to poor oxygen mobility. Although the SC method minimized carbon deposition, the excessive structural confinement significantly reduced catalytic activity. The study therefore established that the synthesis routes influence catalyst morphology, reducibility, oxygen-vacancy concentration, and coking rate. It further highlights that the optimal DRM catalyst should combine the high CH_4 activation capability of the MW method with the rich oxygen-vacancy and single-atom sites of the CP method.

MWRM 2026 MW397

Finite-resolution identifiability of molecular conformers from vibrational spectroscopy

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Computed vibrational spectra are often used to assign molecular conformers, but differences between theoretical spectra do not necessarily mean that the corresponding structures can be distinguished experimentally. In this work, we develop a finite-resolution framework for determining whether candidate conformers are distinguishable under a specified experimental resolution, noise level, and theoretical uncertainty. Each conformer is represented by the probability distribution of its measured observables rather than by an ideal spectrum alone. Exact observational equivalence defines conformer classes, while finite-noise ambiguity is represented by a graph connecting conformer pairs that cannot be resolved below a chosen decision-error threshold. Within a shared-covariance Gaussian model, pairwise Bayes errors can be evaluated directly, and the addition of an independent observable can only remove ambiguity edges.

We apply this approach to B3LYP-D3(BJ)/def2-TZVP calculations for 1,2-difluoroethane, ethylene glycol, and *n*-pentane using infrared, Raman, rotational-constant, and permanent-dipole observables. We determine which conformer pairs remain ambiguous after instrumental broadening and theoretical model error are included and examine which additional measurements are most useful for resolving those ambiguities. We find that Raman spectra can provide little additional information beyond infrared spectra, while rotational and dipole observables can distinguish chemically different polar rotamers. Mirror-related conformers remain unresolved under the achiral observables considered here, indicating that parity-sensitive measurements such as vibrational circular dichroism or microwave three-wave mixing may be required. This framework connects computational spectroscopy with experimental conformer assignment and provides a systematic approach for selecting the next measurement.

MWRM 2026 MW60

First total synthesis of Balgacyclamide C and new analog based upon computational docking

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The balgacyclamide family consists of three heterocyclic and macrocyclic peptides, balgacyclamide A-C. These natural products were isolated from *Microcystis aeruginosa*, a phototropic cyanobacteria, which is found in eutrophic water bodies worldwide. Balgacyclamide A and B have been reported to have antiparasitic activity toward *P. falciparum*; however, there has been no biological activity reported for balgacyclamide

C. Structurally, balgacyclamide A-C all contain three main components in the macrocyclic peptide: an oxazoline ring, a thiazole ring, and a dipeptide unit (linear or cyclized). There are two main differences between the structures of A/B and C that could impact the biological activity of these natural products. Balgacyclamide A and B both have valine in the oxazoline component, whereas C has phenylalanine. Another structural difference is that A and B have alanine incorporated in the dipeptide component, whereas C has glycine. Based upon our computational docking studies, the aromatic side chain from the phenylalanine is crucial to the best docking to the target of *P. falciparum*. Additionally, the extra oxazoline that balgacyclamide A contains, contributed to enhanced docking ability. In this research, the first total synthesis of balgacyclamide C has been achieved, as well as an analogue of balgacyclamide C that contains an extra oxazoline ring, as in balgacyclamide A, to confirm the biological activity and results from the computational docking studies.

MWRM 2026 MW133

Flavin-dependent enzymes as antimicrobial targets: From mechanism to inhibitor discovery

***Pablo Sobrado**, psobrado@mst.edu. Chemistry, Missouri University of Science and Technology, Rolla, Missouri, United States*

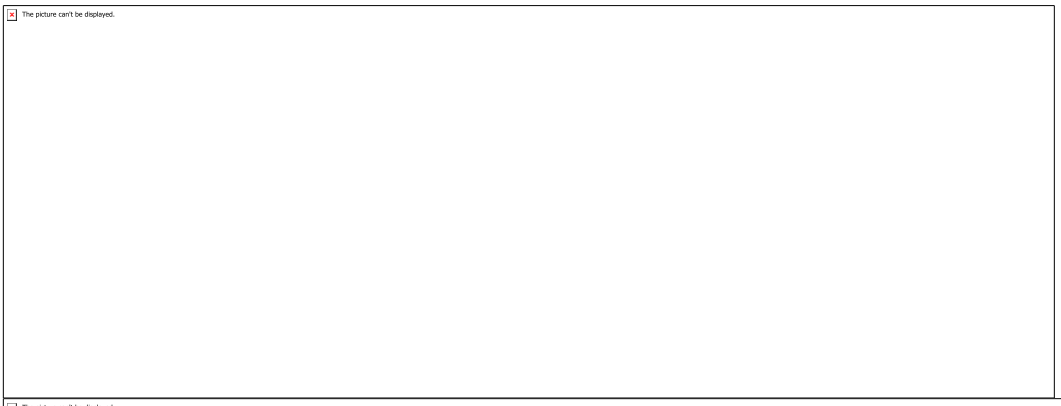
Flavin-dependent enzymes catalyze a wide range of essential redox and non-redox reactions. Their remarkable versatility arises from the ability of the protein environment to modulate the reactivity of the flavin cofactor, enabling diverse chemical transformations. Our laboratory investigates the mechanisms of flavin-dependent enzymes involved in iron acquisition through siderophore biosynthetic pathways and in cell wall biosynthesis through the production of galactofuranose in the human fungal pathogen *Aspergillus fumigatus*. These studies have uncovered novel roles for flavins in catalysis, including the formation of covalent intermediates and protein- and flavin-conformational changes that are critical for enzymatic activity. This presentation will highlight these mechanistic discoveries and discuss how they have advanced our understanding of flavin-dependent catalysis. In addition, it will describe the development of high-throughput screening approaches that have enabled the identification of inhibitors targeting these enzymes, providing promising leads for the development of new antimicrobial agents.

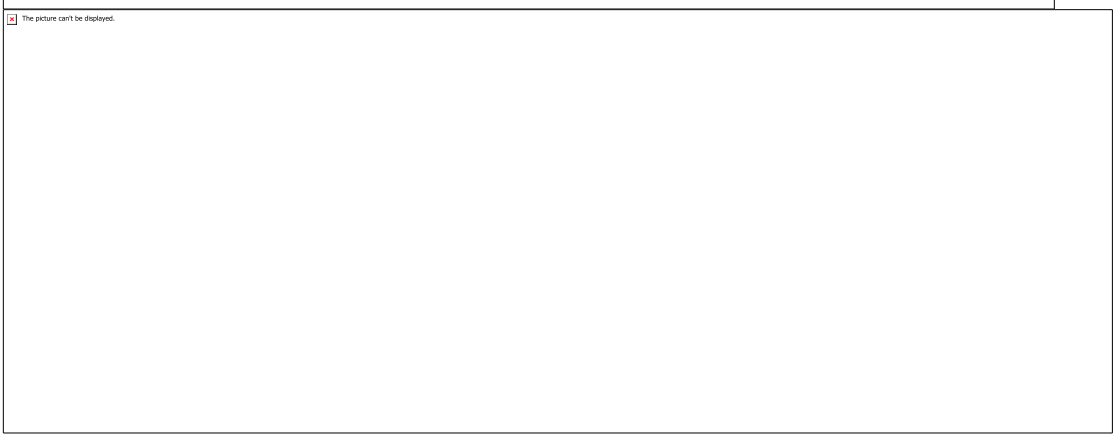
MWRM 2026 MW255

Flower-like Fe-based metallogel as a durable electrocatalyst for oxygen evolution reaction

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Metallogels (MOGs) are an emerging class of soft materials with unique structural and functional properties. Herein, a stimuli-responsive Fe-based metallogel (Fe-MOG) with a flower-like morphology was synthesized using 2-aminoterephthalic acid as the gelator in N,N-dimethylformamide. The morphology and microstructure were investigated using FESEM, TEM, and AFM, confirming the formation of a hierarchical flower-like architecture. Rheological studies demonstrated the robust mechanical behaviour of the gel. FTIR, XPS, and MALDI-TOF analyses provided detailed insights into its chemical composition, bonding interactions, and structural characteristics. The electrocatalytic performance of the dried Fe-MOG was evaluated toward the oxygen evolution reaction (OER) under alkaline conditions. The catalyst required an overpotential of only 380 mV to achieve a current density of 100 mA per cm squar and exhibited excellent durability, retaining its activity over 2000 continuous cycles. These findings demonstrate that Fe-MOG is a cost-effective, highly stable, and efficient OER electrocatalyst, offering a promising strategy for the development of advanced energy-conversion materials





MWRM 2026 MW230

Flow synthesis of cryptomelane (KMn_8O_{16}): A greener alternative to conventional batch synthesis

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Cryptomelane (KMn8O16) is a tunneled manganese oxide structure with important applications in catalysis, energy storage, and environmental remediation. In this research, cryptomelane was synthesized using a flow reactor and compared with a conventional batch synthesis under similar reaction conditions. Tetra-*n*-butylammonium permanganate (TBAMnO4) and potassium acetate were used as the precursor materials in both methods. The flow and batch synthesis produced comparable product yields, demonstrating that the flow process is an effective alternative to the conventional method. The synthesized cryptomelane samples were characterized by powder X-ray diffraction (XRD) to evaluate their crystal structure. Scanning electron microscopy (SEM) was performed to examine the morphology and microstructure of the synthesized materials. The flow process also reduced reaction time, solvent consumption, and chemical waste compared with the batch process. These improvements were consistent with the principles of green chemistry and sustainable chemical synthesis. Therefore, this study demonstrates that continuous flow synthesis is a promising, scalable, and environmentally friendly approach for the preparation of cryptomelane (KMn_8O_{16}).



MWRM 2026 MW313

Formulation and fabrication of a fluorinated polymer based material loaded with ^6Li for neutron shielding applications

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Neutron shielding is essential for the health and safety of humans and sensitive electronics that are in proximity of neutron sources in sectors such as research facilities, medical diagnostics and therapy, and space exploration. To address this concern,

materials that are hydrogen rich, such as high-density polyethylene (HDPE) are used with Boron-10 (^{10}B) fillers. ^{10}B, however, produces gamma radiation upon interacting with neutrons. This is especially problematic in research reactors that use scintillator detectors, as their crystals are highly sensitive to gamma radiation, and it creates background noise in these detectors. Our current research uses a fluorinated resin base with Lithium-6 (^{6}Li), which produces less gamma radiation upon interacting with neutrons. Two different ^{6}Li salts were used in the formulation of the material. Fabrication of the material varied parameters such as salt content, solvent type, solvent evaporation methods, solvent volume, curing time, and particle size. A flexible material with 60% ^{6}LiF loading was successfully fabricated. The material was tested at MURR and the results showed a favorable reduction in gamma radiation.

MWRM 2026 MW434

Fourier transform infrared spectrometric quantification of volatile organic compounds emitted by common commercial 3D printers

***Daphne Hedrick**, daphnemarie124@gmail.com, Kayla McCreary, Martin Spartz, Daniel A. Higgins. Chemistry, Kansas State University, Manhattan, Kansas, United States*

The 3D printing industry has grown substantially in the last decade due to increased accessibility and decreased cost. Various types of 3D printers are now used in a multitude of settings including businesses, homes, schools, hospitals, and libraries, which are environments that often lack adequate ventilation, posing elevated risks to human health. Research has confirmed that both fused deposition modeling (FDM) and vat polymerization stereolithography with digital light processing (SLA/DLP) release mixtures of ultrafine particles (UFPs) and volatile organic compounds (VOCs). FDM primarily releases ultrafine particles and thermally generated VOCs such as lactide and acetaldehyde from filament extrusion, whereas vat SLA/DLP primarily releases acrylate-based VOCs such as 2-hydroxypropyl methacrylate and 3-hydroxypropyl methacrylate that are associated with photopolymer resins and post-processing steps. These emissions have been linked to adverse health effects such as respiratory and cardiovascular issues, especially with prolonged or repeated exposure. The objective of this study was to characterize VOC emissions generated from common commercial FDM and SLA/DLP printers using various types of common filaments and resins using a unique recirculating gas experimental setup. Two types of filaments and three types of resins were tested including PLA, ABS, speed resin, flame retardant resin, and aqua clear plus resin.The results and implications of these studies will be discussed.

MWRM 2026 MW434

Fourier transform infrared spectrometric quantification of volatile organic compounds emitted by common commercial 3D printers

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MWRM 2026 MW290

From chains to cycles: Nitrilium-driven cyclization in secondary polyacrylamides

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The demand for functional macromolecular materials continues to grow in the field of polymer chemistry. Although controlled polymerization is typically the method of choice, not all desired functionalities are accessible through this approach. To bridge this gap, a new post-polymerization modification methodology, specifically through the generation of a reactive nitrilium ion intermediate, provides an alternative approach to synthesize multifunctional polymers consisting of highly distinct, functional repeat units. This presentation outlines our progress in establishing an efficient pathway to tailor the properties of a variety of secondary polyacrylamides, expanding their potential in advanced materials for targeted applications.

MWRM 2026 MW184

From chains to dimers: Structural motifs and co-crystal formation in benzothiazole amides

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Co-crystals are crystalline materials composed of two or more different molecules held together by noncovalent interactions. They are attracting considerable interest in pharmaceutical science because co-crystal formation can modify the physical properties of drug molecules without altering their chemical identity. However, predicting which molecules will successfully form co-crystals remains a significant challenge.
In this study, we investigate the co-crystallization behavior of two families of benzothiazole amides that exhibit distinct crystal packing motifs: hydrogen-bonded chains and hydrogen-bonded dimers. Each benzothiazole amide will be paired with a range of aromatic and aliphatic co-formers using liquid-assisted grinding to promote co-crystal formation. The resulting materials will be characterized by infrared spectroscopy (IR), differential scanning calorimetry (DSC), and single-crystal X-ray diffraction. By comparing the co-crystallization behavior of molecules with different structural motifs, we aim to determine how crystal packing influences co-crystal formation. These findings will improve our understanding of intermolecular recognition and may help identify molecules that are more likely to form co-crystals in future pharmaceutical and materials design.

MWRM 2026 MW117

From click chemistry to cocrystal synthesis

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Click chemistry, based on the copper-catalyzed [3+2] cycloaddition of azides and alkynes (CuAAC), is a powerful synthetic strategy for constructing triazole-linked architectures. Its high efficiency, mild reaction conditions, and exceptional regioselectivity make it an attractive approach for preparing functional materials with tunable solid-state properties. Despite its widespread use, a fundamental challenge remains in understanding how electronically distinct substituents modify the electrostatic and steric environment of the triazole core and, consequently, influence intermolecular interactions and crystal packing.
Herein, we report the design, synthesis, and supramolecular characterization of a new series of functionalized triazole derivatives prepared through CuAAC reactions between electron-deficient pyrazine-based azides and pyridine-based alkynes. The products were characterized using nuclear magnetic resonance (NMR) spectroscopy, Fourier-transform infrared (FT-IR) spectroscopy, and differential scanning calorimetry (DSC) to

confirm their structures and evaluate their thermal properties. Their ability to form cocrystals was subsequently explored through neat-grinding experiments with a series of functionalized aromatic acid coformers. To complement the experimental studies, molecular electrostatic potential (MEP) surfaces were calculated to identify preferred hydrogen-bond donor and acceptor sites, as well as potential π–π stacking interactions, providing insight into the supramolecular recognition patterns governing cocrystal formation.

MWRM 2026 MW203

From dimerization to oligomerization through solid-state photochemistry

***Kristin M. Hutchins**, kristin.hutchins@missouri.edu. Chemistry, University of Missouri, Columbia, Missouri, United States*

Crystalline phase chemical reactions are much less investigated when compared to transformations conducted in solution, often as a result of reduced motion and reactivity in the solid phase. To achieve successful reactions in the crystalline phase, reactants are frequently designed to self-assemble into specific spatial arrangements, often assisted by molecular or metal-based templates. Here, we will describe a diene-based system that self-assembles into two unique monomer structures. This difference in structure affords access to regioisomers of the products, which are obtained through [2 + 2] photocycloaddition reactions. We further show the ability to prepare a series of products in the crystalline phase, ranging from dimers to oligomers through a combination of structural control and wavelength choice. The macroscopic response of the materials to light will also be discussed.

MWRM 2026 MW417

From molecular innovation to manufacturing impact: Catalysis for sustainable chemical production

***Sachin Handa**, sachinhanda@missouri.edu. Chemistry, University of Missouri, Columbia, Missouri, United States*

Catalysis and sustainable chemistry are key drivers of modern innovation, enhancing efficient chemical processes and environmentally responsible technologies. In this talk, a journey that connects fundamental discoveries with real-world applications, demonstrating how new catalytic tools and scalable aqueous technologies can reduce the environmental impact of chemical synthesis, will be discussed. Our unified strategies promote resource-efficient transformations by applying green chemistry principles to minimize solvent use, energy demand, and waste generation while boosting reaction selectivity and scalability. By integrating novel catalysts—including heterogeneous, recyclable systems—with unconventional reaction media and technologies, we show that sustainable methods can outperform traditional methods without sacrificing chemical versatility. Through collaboration between academia and

industry, one can develop cleaner and safer chemical manufacturing pathways. These advancements not only solve longstanding synthetic challenges but also encourage next-generation technologies for a circular chemical economy.

MWRM 2026 MW257

From oxaboranes to oxaborole catalysts: Modular synthesis of and regioselective catalysis with non-benzofused boron heterocycles

Dustin Youmans, Mason Koeritz, Haley K. Banovetz, Austin T. Moore, Sean Prell, ***Levi M. Stanley****, lstanley@iastate.edu. Department of Chemistry, Iowa State University of Science and Technology, Ames, Iowa, United States*

Boron heterocycles possess distinctive structures and reactivity, but modular methods to prepare highly substituted, non-benzofused derivatives and translate their structural features into useful catalytic function remain underdeveloped. This presentation describes an integrated program that advances from the construction of oxaboranes to the synthesis and catalytic application of structurally tunable oxaboroles. Nickel-catalyzed dearylative cyclocondensation of aldehydes, alkynes, and triphenylborane provides direct access to oxaboranes through the formation of new C–C and C–B bonds. The reaction proceeds under mild conditions to furnish oxaboranes in 47–99% yield with high regioselectivity.

The resulting oxaboranes were subsequently employed in a selective Petasis borono–Mannich reaction with morpholine and salicylaldehydes. These transformations provides densely substituted, non-benzofused oxaboroles in yields up to 93% and are readily performed on gram scale. Exclusive aryl transfer over competing vinyl transfer, supported by computational studies, enables predictable assembly of these highly functionalized scaffolds.

Finally, a highly substituted oxaborole was developed as a cyclic hemi-boronic acid catalyst for the regioselective functionalization of unsymmetrical 1,2-diols. The optimized catalyst promotes benzoylation with only 2 mol% catalyst loading in 15 minutes, producing monoacylated diols in 74–99% yield with high regioselectivity. The method accommodates electronically and sterically diverse diols and multiple acylating agents while retaining greater than 20:1 regioselectivity in representative transformations. Computational analysis and ^{11}B NMR experiments support the formation of a spirocyclic boronate intermediate and provide a steric rationale for selective reaction at the more accessible oxygen.

Together, these studies establish a modular platform in which efficient heterocycle synthesis enables control over oxaborole structure, and that structural control is leveraged to achieve rapid and highly regioselective catalysis.

MWRM 2026 MW47

From reaction paths to free-energy landscapes: Exploring chemistry with machine-learned interatomic potentials

***Joseph Gomes**, joe-gomes@uiowa.edu. Chemical and Biochemical Engineering, University of Iowa, Iowa City, Iowa, United States*

Machine-learned interatomic potentials are rapidly expanding the time and length scales accessible to molecular simulation, but their utility ultimately depends on our ability to explore complex potential-energy surfaces reliably. In this talk, I will describe two complementary approaches developed and applied in our group for investigating chemical reactivity with machine-learning potentials. First, machine-learning-assisted freezing string methods provide efficient static exploration of reaction pathways and transition states, enabling rapid characterization of reaction mechanisms across diverse molecular systems. Second, constrained molecular dynamics and Blue Moon ensemble simulations extend this framework to finite-temperature free-energy landscapes by sampling thermodynamic forces along path-based reaction coordinates. Together, these methods connect stationary-point searches with dynamical ensemble sampling and allow direct comparison between machine-learned and first-principles potential-energy surfaces. Applications will illustrate both the computational opportunities offered by modern pretrained interatomic potentials and the remaining challenges associated with transferability, uncertainty, and reliability in chemically reactive regions. These developments provide a practical framework for using machine learning to accelerate mechanistic discovery while retaining close connections to physical principles and electronic-structure theory.

MWRM 2026 MW176

From total synthesis to chemical screening libraries: The story of Brocazine and new therapeutic agent discovery

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Natural products continue to be one of the dominant forces in drug discovery, with a large percentage of the currently approved therapeutics employed coming directly or from analogs of them. Since the 1980s high-throughput screening (HTS) has become allow for the rapid screening of chemical screening plates (CSL) in the efforts to identify new potential therapeutic compounds, this includes in natural products. These plates are the linchpin for any discovery via HTS, and as such new methods have been developed to populate these plates. One method our lab has developed is the utilization of synthetic intermediates within a total synthesis route as the starting point of chemical diversification for the construction of new CSL. We have disclosed the power in this method from CSL construction based upon our total synthesis route of uvaretin. In a

new avenue, we now aim to diversify synthetic intermediates in our total synthesis route and then install a portion from the original route for the targeted natural product to create new hybrids. In this, we are using our total synthesis route towards the brocazine family which are disulfide-bridged diketopiperazine (DKP) natural products. Each half of the compound is structurally similar around the DKP. To be disclosed is our route to access the required units of brocazine E/F, the skeletal rearrangement/diversification upon key synthetic intermediates and the coupling of these new fragments to one portion of the target natural product. Cytotoxicity studies will be disclosed and an overall assessment of this strategy as a new method of accessing therapeutically active compounds.

MWRM 2026 MW52

From water to biomolecules: Predictive simulations through data-driven many-body models

***Francesco Paesani**, fpaesani@ucsd.edu. Department of Chemistry, University of California San Diego, La Jolla, California, United States*

Accurately describing aqueous molecular systems remains a longstanding challenge because their properties emerge from the subtle interplay of many-body interactions and nuclear quantum effects. In this talk, I will present a unified data-driven many-body framework that enables predictive molecular simulations across environments ranging from gas-phase clusters to bulk solutions and interfaces. The resulting MB-nrg potentials, including MB-pol for water and its extensions to aqueous systems, combine physically motivated representations of molecular interactions with machine-learned terms trained on coupled-cluster reference data. This rigorous connection to high-level electronic structure theory allows the models to reproduce structural, thermodynamic, and spectroscopic properties across different phases and thermodynamic conditions, while also predicting emergent phenomena such as the liquid–liquid critical point of supercooled water. I will conclude by discussing recent developments that extend the same framework beyond water and aqueous solutions to general covalently bonded molecules, opening a path toward predictive biomolecular simulations with chemical accuracy.

MWRM 2026 MW200

Functionality for free: Interphases in composites

***Frank D. Blum**, fblum@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

The interphases in composite materials, especially those of polymers adsorbed on rigid substrates are often altered in properties compared to their bulk counterparts. This alteration can manifest itself due to chemical bonding or other interactions such as hydrogen bonding, polar interactions or dispersion forces. These often result in

interfaces graded in chemical or physical properties. In this presentation, I will examine how these interactions result in behavior that affect the mechanical properties. While the impacts of chemical bonds are obvious to chemists, the mobility of the polymer interphase between the hard surface and the bulk polymer affects the mechanics of the composites. I will also discuss how calorimetry is not always a definitive measure of the interactions in the polymer interphase.

MWRM 2026 MW205

Functionalization and crosslinking of brominated poly(lactic acid)

***Coleen Pugh**, coleen.pugh@wichita.edu, Parisa Jahangiri, Abegel Freedman. Chemistry and Biochemistry, Wichita State University, Wichita, Kansas, United States*

Poly(lactic acid) (PLA) is a popular bio-based polyester with the potential to replace traditional petroleum-based polymers in various applications, especially those that take advantage of its biocompatibility, sustainability, and degradation profile. We developed the synthesis of brominated PLA (PLB), via copolymerization of lactic acid and 2-bromo-3-hydroxy propionic acid, to provide sites for post-polymerization functionalization of PLA to expand its usefulness. This talk will discuss functionalization and crosslinking reactions via nucleophilic substitution, radical reactions, and cationic reactions via 1,3-dioxolenium ion intermediates.

MWRM 2026 MW382

Functionalized chitosan as a polymeric chelator for targeted radionuclide delivery

***Dilanka N B D Dassanayake Mudiyanselage**, dilankad@ksu.edu, Patricia R. Calvo. Chemistry Department, Kansas State University, Manhattan, Kansas, United States*

Targeted radionuclide therapy is an emerging approach for treating cancer by delivering radioactive isotopes directly to tumors while minimizing damage to healthy tissues. Polymeric chelators offer several potential advantages over traditional small-molecule chelators, including prolonged circulation, reduced off-target accumulation, and the ability to incorporate multiple metal-binding sites within a single macromolecule. Chitosan is an attractive platform for these applications because of its biocompatibility, biodegradability, and abundance of functional groups available for chemical modification. However, unmodified chitosan has limited aqueous solubility and its native amino groups exhibit relatively weak affinity and selectivity for many therapeutic radionuclides. In this study, chitosan was functionalized with phosphonate and phosphonate/carboxylate metal-chelating ligands using a modified Moedritzer–Irani reaction. A microwave-assisted synthetic strategy was developed to reduce reaction times while improving functionalization efficiency and preserving the polymer structure. The resulting materials were characterized using NMR and IR spectroscopy, elemental analysis, dynamic light scattering, and thermogravimetric analysis, confirming successful functionalization and enhanced thermal stability. Isothermal titration

calorimetry demonstrated high-affinity binding between the modified polymers and various metal ions. Importantly, incorporating both phosphonate and carboxylate ligands improved selectivity for samarium over competing calcium ions, demonstrating that ligand composition can be used to tune metal-binding selectivity. This work establishes a rapid, scalable strategy for preparing polymeric metal chelators and demonstrates the potential of multifunctional chitosan derivatives for targeted radionuclide delivery.

MWRM 2026 MW241

Functionalizing nanoporous metal-organic supercontainers for environmental remediation of illicit substances

MaKenna King[1,2]*, makennaking@hotmail.com, Robyn Cook*[1]*, Kiriti Chitrakar*[1]*, Zhenqiang Wang*[1]*. (1) Chemistry, University of South Dakota, Vermillion, South Dakota, United States(2) Wayne State College, Wayne, Nebraska, United States*

Improper disposal of illicit substances is a serious environmental problem that is often overlooked. One of the barriers is monitoring trace illicit substances in the environment. Current methods include insensitive test strips providing inaccurate results or highly technical mass spectrometry. The project objective is to design a new family of nanostructured, multifunctional molecules known as Metal-Organic Supercontainers (MOSCs) for both detection and sequestration of illicit substances. MOSCs are a subclass of synthetic container molecules with three unique components – divalent or trivalent metal ions, organic linkers with carboxylate groups, and container precursors that self-assemble to create the super-container structure. In this work, we are functionalizing MOSCs via pre-synthetic modification of linkers with extended 'floppy'-like alkyl chains to promote flexible liquid-like intrinsic properties for advantageous capture of target analytes for solid-liquid extractions. Reactions of the linker with suitable metal ions (e.g., Co2+) and container precursors (e.g., p-tert-butylsulfonylcalix[4]arene, TBSC) produced MOSCs characterized by thermogravimetric analysis (TGA), single-crystal X-ray crystallography (SC-XRD), and ultraviolet-visible (UV-Vis) spectroscopy. Preliminary results confirm the creation of a newly synthesized container molecule. Moreover, application trials uncover previously unknown water-solubility properties, enabling liquid-liquid extraction. Further study will focus on continued optimization of solid-liquid application trials with illicit analogs.

MWRM 2026 MW241

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MWRM 2026 MW209

Functionally-important protein dynamics are altered by amino acid changes at rheostat positions

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During protein evolution, amino acid changes can modulate protein function. In some proteins, such functional “tuning” requires multiple amino acid changes. However, some proteins contain individual positions where single amino acid changes are able to sample a broad functional range; at these “rheostat” positions, function can be dialed up or down, depending on which of the twenty amino acids occupies the site. This behavior is not rare: Rheostat positions occur in a wide range of protein types; within individual proteins, their prevalence can be as high as 40%; changes at rheostat positions have been observed to modulate ligand binding affinities, allosteric regulation, and substrate transport. Thus, understanding which proteins contain rheostat positions – and the

biophysical mechanisms by which amino acid changes lead to altered function – is needed to advance protein engineering and personalized medicine. This goal has numerous challenges: Many rheostat positions are far from binding sites, are not conserved in the evolutionary super-family but are conserved within subfamilies, and substitutions lead to a unexpected outcomes. Furthermore, amino acid changes at rheostat positions do not appear to cause major changes in the protein's overall fold. This suggests that functional changes arise from altered protein dynamics. Intriguingly, both molecular dynamics simulations and dynamic coupling calculations show promising correlations between measured functional changes and the locations of long-range rheostat positions. Results suggest that functional tuning is an emergent property of coupled amino acid networks and that changes in these networks produce the complex outcomes observed for amino acid changes at rheostat positions.

MWRM 2026 MW106

Gamma-secretase modulators shift the cleavage site preference and Aβ trimming process of γ-secretase: Implications for Alzheimer's disease treatment

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Alzheimer's disease (AD) afflicts 7 million Americans. AD results in dementia and the formation of amyloid plaques and tau tangles within patient's brains. Amyloid plaques are composed of amyloid beta peptides (Aβ) that are produced by the protease γ-secretase from the C-terminal domain of amyloid precursor protein (APP). Aβ peptides vary in length, but Aβ42 is the major component of plaques and is widely considered to be neurotoxic, while shorter Aβs like Aβ38 are benign. Gamma-secretase modulators (GSMs) are small molecules designed to allosterically stimulate proteolysis of Aβ42 to Aβ38 by altering γ-secretase's function. Despite ongoing clinical trials of GSMs like nivegacetor, little is known about how these compounds affect the proteolysis of other Aβ species. γ-secretase cleaves APP and then forms the various Aβ peptides by trimming that occurs via two pathways, the Aβ40 pathway (Aβ49→Aβ46→Aβ43→Aβ40) or the Aβ42 pathway (Aβ48→Aβ45→Aβ42→Aβ38). Using purified γ-secretase to conduct proteolytic assays on APP, we found that at least one GSM changes the enzyme's preference for initial cleavage site, altering which pathway the enzyme uses during trimming. We also measured the effect of GSMs on each trimming step, to understand how such compounds affect the entire proteolytic process. Our results challenge the assumption that GSMs only act on γ-secretase at the Aβ42 or Aβ40 stage and challenge the idea that substrate must be present in order for GSMs to bind the enzyme. Instead, our results suggest that some contemporary GSMs are already bound to the enzyme before substrate enters the active site. Thus, further GSM design efforts should measure cleavage site preference when testing structure-activity relationships.

MWRM 2026 MW425

Gas-phase ion-molecule reactions of protonated oxime compounds with 2-methoxypropene in a linear quadrupole ion trap mass spectrometer

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Oximes are an important class of organic compounds that are recognized for their broad utility in synthetic organic chemistry and medicinal applications. They contain the C=N-OH functional group. However, their reliable untargeted identification in complex mixtures remains a challenge due to structural similarities to many other oxygen- and nitrogen-containing compounds. For example, tandem mass spectrometry based on collision-activated dissociation (CAD) cannot be readily used to distinguish protonated oximes from similar compounds. However, gas-phase ion-molecule reactions often enable the identification of specific functional groups in protonated analytes when CAD fails. This study explores the gas-phase ion-molecule reactions of protonated aldoxime and ketoxime model compounds with 2-methoxypropene (MOP) by using a linear quadrupole ion trap mass spectrometer coupled to an atmospheric pressure chemical ionization (APCI) source. When protonated oximes were allowed to react with MOP in the ion trap for up to 3000 ms, the sequential generation of MH++MOP–methanol and MH++MOP–methanol–2-propenol product ions were observed. In contrast, structurally related protonated compounds, including *N*-oxides, C-nitroso compounds, *N*-disubstituted hydroxylamines, and amides, were either unreactive or produced only a stable adduct upon reactions with MOP, while protonated *N*-monosubstituted hydroxylamines formed only the MH++MOP–methanol product ions. Protonated *N*-nitrosamines, on the other hand, generated only the MH++MOP–2-propenol product ions. These distinct diagnostic gas-phase ion-molecule reactions enable the reliable and fast selective detection of oximes in complex mixtures. Quantum chemical calculations were performed at the M062X/6-311G++(d,p) level of theory to delineate the underlying reaction mechanisms, after which a human-made decision tree was developed to facilitate easy interpretation of the results by non-experts.
The novelty of this study lies in the development of a diagnostic gas-phase ion-molecule reaction approach to identify oximes and distinguish them from structurally related compounds.

MWRM 2026 MW28

Gene expression & structural analysis of OAZ RNA in *Neurospora crassa*

***Billy Bettis**, billybettis24@gmail.com, Juliane Soukup. Creighton University College of Arts and Sciences, Omaha, Nebraska, United States*

Riboswitches are regions of non-coding messenger RNA that regulate various cellular communication pathways following binding of specific metabolites, or small molecules. Following this binding event, the downstream gene product incurs alteration in expression. Specifically, the posited riboswitch RNA undergoes a conformational change following metabolite binding that leads to differential expression of the associated gene in a concentration dependent manner. This regulation generally precludes translation initiation but can also be a result of altered transcription and translational termination. Many riboswitches have been verified in prokaryotic organisms such as bacteria, however this mechanism of differential gene expression is being studied in higher order eukaryotic organisms such as in Neurospora crassa (N. crassa), a type of mold. The project examines the highly conserved putative mammalian RNA Ornithine Decarboxylase Antizyme (OAZ RNA) in N. crassa, which is required in the biosynthetic pathway for polyamines. Polyamines are small organic molecules ubiquitously expressed in cells and they range in function from cell differentiation to DNA stability. That is, further research on the regulation of their presence and concentration is beneficial to potential biomedical application for a number of disease pathologies such as cancer, fungal diseases, and more. The goal of my research is to examine whether the putative OAZ RNA from N. crassa exhibits the standard riboswitch characteristics of gene expression alteration and structural change upon ligand binding. Further, the extent to which the OAZ RNA exhibits those various riboswitch characteristics is being examined. In-line probing and dual luciferase assays are the main techniques to verify the putative riboswitch.

MWRM 2026 MW22

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***Billy Bettis**, billybettis24@gmail.com, Juliane Soukup. Creighton University College of Arts and Sciences, Omaha, Nebraska, United States*

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studied in higher order eukaryotic organisms such as in Neurospora crassa (N. crassa), a type of mold. The project examines the highly conserved putative mammalian RNA Ornithine Decarboxylase Antizyme (OAZ RNA) in N. crassa, which is required in the biosynthetic pathway for polyamines. Polyamines are small organic molecules ubiquitously expressed in cells and they range in function from cell differentiation to DNA stability. That is, further research on the regulation of their presence and concentration is beneficial to potential biomedical application for a number of disease pathologies such as cancer, fungal diseases, and more. The goal of my research is to examine whether the putative OAZ RNA from N. crassa exhibits the standard riboswitch characteristics of gene expression alteration and structural change upon ligand binding. Further, the extent to which the OAZ RNA exhibits those various riboswitch characteristics is being examined. In-line probing and dual luciferase assays are the main techniques to verify the putative riboswitch.

MWRM 2026 MW66

Generation of unnatural α-amino acids via photoredox-enabled radical decarboxylation

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Unnatural amino acids have garnered significant attention in organic and pharmaceutical research as their incorporation in peptides can significantly improve the biological activity and pharmacokinetic properties of peptide-based drugs. Therefore, development of new and efficient methodologies which enable their quick and direct access under mild reaction conditions are highly desirable. Current radical-based approaches involve radical addition to dehydroalanine (DHA) or its derivatives to generate a-amino esters, followed by an additional step to transform the ester into an acid, rendering the overall process less step-economical. To address this limitation, we disclose a decarboxylative cross-coupling strategy between two carboxylic acid derivatives that directly furnishes the desired amino acid in a single photocatalytic reaction. The new strategy is, operationally simple, scalable, and allows for the generation of a wide range of unnatural a-amino acids under mild reaction conditions and short reaction times.



MWRM 2026 MW338

Geometrical and electronic structure, stability, and optical absorption spectra comparisons between thiolate- and hydroxide-stabilized gold nanoclusters

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Atomically precise gold nanoclusters exhibit unique size-dependent properties that are strongly influenced by their surface ligands. While thiolate-stabilized gold nanoclusters have been extensively investigated, hydroxide-stabilized nanoclusters remain comparatively unexplored. In this work, we compare the geometrical structures, electronic properties, stability, and optical absorption spectra of a series of thiolate- and hydroxide-stabilized gold nanoclusters (Au_nL_m; L = SH, OH; n = 18 -133) using density functional theory (DFT) and linear-response time-dependent density functional theory (LR-TDDFT). The DFT and LR-TDDFT calculations were performed using Amsterdam Density Functional (ADF) using the functional BP86, a TZP basis set and ZORA scalar relativistic effects. The calculations reveal pronounced ligand-dependent trends in both the average binding energies and HOMO-LUMO gaps across the investigated nanocluster series. Hydroxide-stabilized gold nanoclusters exhibit higher average binding energies than their thiolate-stabilized counterparts, indicating enhanced ligand binding potential. A similar trend is observed for the HOMO–LUMO gaps, with $Au_{24}(OH)_{20}$ showing the largest difference between the two ligand types. Ongoing LR-TDDFT calculations will determine how these ligand-dependent structural and electronic differences influence the optical absorption spectra. These results demonstrate the significant role of surface ligands in governing the stability and electronic properties of atomically precise gold nanoclusters and provide insights into the rational design of ligand-engineered gold nanomaterials.

MWRM 2026 MW216

Get involved with the ACS Division of Chemical Education

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MWRM 2026 MW384

Going bananins: A sugary solution to stiff engineering thermoplastics

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Most high-performance engineering polymers mandate dimensional stability at high temperatures, typically met through rigid petro-derived backbones at the expense of sustainability. Here, we demonstrate the synthesis of a bioanalog of rigid adamantyl cores via ketalization of myo-inositol, a non-food-competitive sugar. Acid-catalyzed condensation of orthoformates yielded bicyclic trioxadamantane cages, also known as bananins. The rigid core offers a distinct advantage over adamantanes, retaining three pendant hydroxyl groups that can be readily modified for polymerization. Regioselective acylation of the core with aliphatic/aromatic spacers, followed by methacrylation, yielded a polymerizable monomer library spanning a broad property space. Free radical polymerization (FRP) of monofunctionalized species yields stiff polymers (Mn ≈ 16 kDa, PDI = 1.5-1.7, Tg = 120-135 °C), while controlled radical polymerization produces pseudo-living chains (Mn < 10 kDa, PDI = 1-1.3) with steric control affecting termination kinetics. Despite a flexible octanoyl spacer, the bananin core yielded a Tg > 130 °C, demonstrating that the bananin core governs stiffness, which can be tuned by appropriate pendant groups. RAFT mediated chain-extension affords a poly(bananin-monooctanoyl-methacrylate)-*b*-poly(butyl acrylate) diblock exhibiting fully resolved transitions at +132 °C and −27.4 °C, confirming microphase separation and thermoplastic elastomer behavior across that 100 °C window. The bananin triol further serves as a drop-in polyol for polyurethane networks, extending the platform across multiple polymer classes from a single scaffold. This class of rigid biobased ketal-containing thermoplastics also provides a handle for post-polymerization functionalization via mild hydrolysis of the ketals, thereby tuning surface wettability. Collectively, this establishes bananins as among the first bio-derived monomer platforms to achieve thermal performance while providing a modality for post-polymerization functionalization, a thermoplastic elastomer block architecture, and cross-platform polymer accessibility, all from a single sustainable molecular scaffold.



MWRM 2026 MW93

Gold nanoparticle mediated delivery of FDI6 for targeted glioblastoma therapy

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Glioblastoma (GBM) remains one of the most aggressive brain cancers because of the blood-brain barrier (BBB), diffuse tumor invasion, and resistance to current therapies. We report the development of FDI6-conjugated gold nanoparticles for targeted glioblastoma therapy. FDI6 is a selective inhibitor of the transcription factor FOXM1, a central regulator of tumor cell proliferation, invasion, stemness, and therapeutic resistance. Conjugation of FDI6 to gold nanoparticles is intended to improve drug stability, increase intracellular delivery, and reduce systemic toxicity. To achieve selective targeting, the nanoparticles are functionalized with anti-EGFR antibodies, promoting receptor-mediated transport across the BBB and preferential uptake by EGFR-overexpressing glioblastoma cells. Following cellular internalization, FDI6 inhibits FOXM1 signaling to suppress tumor growth and enhance therapeutic response. The plasmonic properties of gold nanoparticles further enable surface-enhanced Raman spectroscopy (SERS) for noninvasive monitoring of nanoparticle localization and treatment response. By integrating antibody-mediated targeting, FOXM1 inhibition, and molecular imaging within a single nanoplatform, this approach offers a promising theranostic strategy for the treatment of glioblastoma and highlights the potential of targeted gold nanomedicine for brain cancer.

MWRM 2026 MW94

Gold nanospheres as a novel drug delivery method for placenta

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Placental dysfunction remains one of the most prolific and difficult to treat conditions affecting women worldwide, primarily due to the maternal-fetal interface. Through traditional methods, any treatment given to the mother will also affect the fetus, causing damage and further complication to the pregnancy. Nanoparticle technology is a cutting-edge technique that shows great promise in this regard. Nanoparticles can be used as a vehicle to deliver drugs and can be tagged with peptides to specifically target the placenta and avoid affecting the fetus. In this experiment, the nanoparticles that were used were gold nanospheres.
Gold nanospheres (AuNS) were conjugated with PEG (a non-specific conjugate) and iRGD (a peptide that specifically targets placental cells) and left to incubate in the presence of HTR-8 placenta cells. After 24 hours, the survival of the cells was analyzed using MTT assay. By the end, gold nanospheres exhibited excellent targeting to HTR-8 cells while only displaying minor toxicity.

MWRM 2026 MW398

Graph theory analysis of DNA adsorption mediated by alkaline earth metal ions

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Divalent metal ions such as Mg^{2+}, Ca^{2+}, Sr^{2+}, and Ba^{2+} readily adsorb DNA to anionic surfaces in aqueous solution. This phenomenon is relevant to the adsorption and self-assembly of DNA-based nanoscale materials due to the ion-specific effects observed experimentally. However, the mechanism through which these metal ions induce DNA adsorption and the origin of their ion-specific effects are unclear. One hurdle for improving our understanding of this process is quantitative analysis of how the network of divalent metal ion contacts evolves over time. To address this issue, we use ChemNetworks to extract atomic coordinates from classical molecular dynamics simulations and construct time-dependent graphs of metal ions and their contacts. We define the graph nodes and edges in a variety of ways to assess the relevance of correlated ion motion versus site-specific ion binding. Graph theory analysis, such as node centrality, can reveal physical insight to this complex adsorption process. From this work, we aim to identify the mechanism of alkaline earth metal ion induced DNA adsorption and the origin of its ion-specific effects. This knowledge may be used to tune DNA adsorption and self-assembly in future nanoscale material applications.

MWRM 2026 MW332

Ground state destabilization as a means to access transformable poly(acrylamides)

***Alexis Redwine**, aredwine@ku.edu, Aaron Teator. Chemistry, University of Kansas, Lawrence, Kansas, United States*

Within the realm of polymer science, routes to new synthetic polymers are often limited by functional group tolerance as well as monomer selection. As new advanced materials are sought after, the need for new functional synthetic polymers continues to increase. Ground state destabilization of amides can be afforded through introduction of bulky substituents onto the nitrogen, resulting in increased electrophilicity at the carbon center. This study leverages one such approach, featuring the design and synthesis of novel monomers with an activated amide pendant that, after polymerization, can undergo subsequent modification in near to quantitative yield as determined by ^{1}H NMR spectroscopy and size exclusion chromatography (SEC).

MWRM 2026 MW332

Ground state destabilization as a means to access transformable poly(acrylamides)

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MWRM 2026 MW426 - Withdrawn

MWRM 2026 MW357

Hierarchical bimodal nanoporous gold-enhanced molecularly imprinted polymer sensor for point of care real-time monitoring of salivary cortisol

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The stress hormone cortisol is a primary steroid hormone that serves as a critical biomarker for diagnosis of chronic stress and cardiovascular diseases. Developing smart devices for rapid, point-of-care, and real-time cortisol detection is significant for early diagnosis and mental health management. We present an electrochemical sensor utilizing a molecularly imprinted polymer (MIP) integrated with a hierarchical bimodal nanoporous gold (hb-NPG) monolith on a disposable screen-printed carbon electrode (SPCE). The MIP is formed by electropolymerization of o-phenylenediamine during cyclic voltammetry sweeps in the presence of a cortisol template. The hb-NPG framework provides enhanced conductivity with a high surface area where bigger pores help in mass transport and smaller pores help in adsorption, resulting in a limit of detection of 1 nM
and a linear range from 1 nM to 70 nM. Differential pulse voltammetry using 2-ferrocenemethanol as the redox probe is used to detect cortisol binding into MIP cavities after removal of the cortisol template. The device exhibits robust reusability, maintaining stability over five regeneration cycles and reproducibility with an RSD of 5.04% and 4.54%, respectively. Furthermore, the sensor also demonstrates superior selectivity, with over 100-fold of common interferents in saliva, including uric acid, ascorbic acid, urea, glucose, and dopamine. This electrochemical sensor also detected cortisol in spiked artificial saliva within the normal range. Hence, our sensor offers sensitive, selective, and potential point-of-care diagnostics for personalized and real-time stress-related disorders.

MWRM 2026 MW72

High-capacity lithium-oxygen batteries enabled by electrolyte engineering

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Lithium-oxygen (Li-O_2) batteries offer theoretical energy densities exceeding 3,500 Wh/kg, but practical implementations have struggled due to poor mass transfer, electrolyte instability, and low electrode utilization. This talk demonstrates Li-O_2 batteries with extremely high energy density (>1,000 Wh/kg) and our approaches to extend battery cycle life.
Conventional Li-O_2 batteries rely on slow O_2 diffusion through stagnant electrolyte, restricting achievable capacities. By designing flow battery architectures that actively circulate O_2-saturated electrolyte through the porous positive electrode, forced

convection becomes the dominant transport mechanism. This concept enables thick electrodes (~50 mg/cm^2) and thick lithium metal (~0.5 mm) to achieve near-theoretical utilization. Using commercially available materials, this design achieved areal capacities >100 mAh/cm^2 and cell-level specific energy > 1,000 Wh/kg. With the well-engineered electrode and electrolyte designs, pumping power to flow the electrolyte is negligible (~1% of discharged energy).
Meanwhile, we address electrolyte instability under superoxide chemistry. Conventional dilute electrolytes (1M LiTFSI in TEGDME or 1M LiTFSI in DMSO) suffer from parasitic superoxide attack, limiting cycle life. We developed both ionic liquids (ILs) and solvate ionic liquids (SILs) as advanced electrolytes. SILs based on equimolar glyme-LiTFSI mixtures (e.g. Li(G_4)TFSI at 2.75M) achieve near-complete coordination of solvent molecules to Li ion, leaving only 5-6% free glyme for parasitic reactions (vs. 87% in dilute electrolytes). Elevated temperature (up to 60°C) can significantly reduces viscosity 3-4 fold while preserving the protective coordination shell. Meanwhile, the LiF/Li_2S-rich SEI formation enabled both ILs and SILs to maintain 100% charging efficiency through more cycles than dilute electrolytes.
These advances demonstrate that Li-O_2 batteries can achieve practical energy densities exceeding 1,000 Wh/kg while maintaining competitive cycle life. The discoveries from this study can benefit many other rechargeable batteries, such as metal-air, metal-ion batteries as well as supercapacitors.

MWRM 2026 MW436

High-resolution lipidomic profiling identifies distinct metabolic dysregulation following traumatic brain injury in a mouse model

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Traumatic Brain Injury (TBI) can lead to long-term damage to the brain through the disruption of neuronal membranes, triggers neuroinflammation, and changes the lipid metabolism. While omega-3 polyunsaturated fatty acid (PUFA) is known to promote brain health, the specific lipid alteration associated with omega-3 mediated neuroprotection post TBI is limited. We used a Fat-1 transgenic mouse model to examine whether endogenous omega-3 enrichment alters the brain lipid response following mild TBI. Lipids were extracted from brain tissue of WT Sham, WT Blast, Fat-1 Sham, and Fat-1 Blast mice and analyzed by LC-QToF-MS in both positive and negative ion mode. Data were processed for feature extraction and analyzed using PLS-DA, volcano plots, and lipid class–based functional analysis.
PLS-DA analysis reveals the clear separation between WT Sham and WT Blast groups demonstrates that blast injury induces substantial remodeling of the brain lipidome. The continued separation observed between Fat-1 Sham and Fat-1 Blast groups indicates that, despite omega-3 enrichment, Blast exposure causes lipidomic perturbation. Lipid profile of Fat-1 Blast mice was significantly different from WT Blast mice, indicating a different post-injury lipid response. Functional analysis highlighted biologically relevant lipid classes associated with membrane support, cell-survival signaling, mitochondrial

resilience and inflammation resolution, including glycerophosphoserines (PS) and glycerophosphoethanolamine (PE) lipid class. Overall, the findings suggest that the omega-3 enrichment may alter the post-injury brain lipidome toward a more neuroprotective condition. This exploratory lipidomic study provides a foundation for future targeted lipid validation and the identification of candidate biomarkers for traumatic brain injury (TBI)–associated neuroprotection.

MWRM 2026 MW109

High-throughput analysis of purine riboswitch tertiary contact formation

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Non-coding RNAs are functional RNA molecules that play essential roles in cellular processes by folding into complex three-dimensional structures. They are stabilized by tertiary interactions between secondary structural elements that are critical for RNA stability and function. One common but understudied tertiary interaction is the loop-loop contact, in which two hairpin loops interact to stabilize RNA structure and regulate ligand binding and catalytic activity. Despite their importance, the thermodynamic properties and sequence requirements remain poorly understood. To address this gap, we used the adenine riboswitch from *Vibrio vulnificus,* a purine riboswitch whose loop-loop tertiary contact is directly coupled to ligand binding, as a model system. This contact comprises two canonical and three non-canonical base pairs. Although previous studies have examined mutations in these regions, a comprehensive and systematic analysis of sequence constraints and cooperative interactions within the loop-loop contact has been lacking. We developed a high-throughput mutational strategy combined with DMS chemical mapping to characterize these interactions. We designed a library of 6,500 wild-type adenine riboswitch variants with systematic loop mutations. We performed adenine ligand titrations to measure ligand binding and magnesium titrations to probe tertiary contact formation. Our results showed that disrupting the canonical tertiary contact was generally not tolerated, highlighting its essential role in RNA structure. Most compensatory mutations retained ligand binding, whereas some restored the tertiary contact upon ligand binding, suggesting cooperativity between ligand binding and tertiary contact formation. Non-canonical pairs showed limited sequence flexibility, while non-interacting nucleotides were the most flexible. Overall, our findings agree with the evolutionary conservation model of purine riboswitches and provide quantitative insights into sequence rules governing loop-loop interactions. Ultimately, we aim to develop a predictive model of sequence preferences for tertiary contact formation in purine riboswitches and extend this framework to other RNA systems, providing insights into RNA structure and function.

MWRM 2026 MW292

High-throughput microwave synthesis and machine-learning optimization of covalent organic framework (COFs)

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Covalent organic frameworks (COFs) are crystalline porous materials whose confined pore environments support applications in gas storage, atmospheric water harvesting, catalysis, and energy storage. However, COF discovery often relies on labor-intensive trial-and-error synthesis followed by endpoint characterization, providing limited insight into the transient processes that govern crystallization. Microwave synthesis offers a promising platform for accelerating discovery because reaction temperature and power can be rapidly adjusted while synthesis progress is monitored in real time.
We present the microwave-assisted synthesis of a dual-knot, single-linker COF through 144 experimental reactions conducted across a defined range of synthetic conditions. Product crystallinity was evaluated by powder X-ray diffraction, and a crystallinity index was calculated as the ratio of the intensity of the primary diffraction peak to its full width at half-maximum. Each reaction was continuously recorded to monitor changes in color, turbidity, and particle formation during synthesis. The resulting dataset was used to implement Bayesian optimization and predict conditions that maximize COF crystallinity. Integrating reaction parameters with time-resolved video data also provides a foundation for identifying pathway-defining intermediate states and enabling adaptive synthesis control. Future incorporation of synchronized infrared spectroscopy, video imaging, temperature histories, and programmable microwave actuation could support a digital twin capable of detecting nucleation onset and recommending mid-reaction changes in temperature or microwave power. This framework combines high-throughput synthesis, machine learning, and real-time reaction monitoring to accelerate COF discovery and advance trajectory-controlled autonomous synthesis.

MWRM 2026 MW14

HPLC-UV analysis of hemp-derived cannabinoids in honey bee tissues

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Honey bees (*Apis mellifera*) are essential agricultural pollinators, but managed colonies continue to experience severe losses due to multiple stressors, including pesticide exposure. As industrial hemp (*Cannabis sativa* L., <0.3% THC) expands in Kansas, there is growing interest in whether hemp-derived phytocannabinoids may contribute to pollinator health through antioxidant-related pathways. In this study, a high-performance liquid chromatography with UV detection (HPLC-UV) method was used to detect and quantify phytocannabinoids in honey bee foragers collected from hives placed near

industrial hemp. Bee abdominal tissues were extracted and analyzed for several target cannabinoids, including cannabidiol (CBD), cannabichromene (CBC), cannabigerol (CBG), delta9-THC, delta8-THCA, and cannabidiol hydroxyquinone (CBDHQ). Five phytocannabinoids were detected at measurable levels in bee samples, with concentrations ranging from 8.4 to 119 ng per bee, while CBDHQ was not detected. These results provide direct analytical evidence that honey bees foraging on hemp can acquire and accumulate hemp-derived phytocannabinoids in their tissues. This work establishes a foundation for future studies examining cannabinoid uptake, metabolism, and possible protective effects against pesticide-induced oxidative stress in pollinators.

MWRM 2026 MW270

Hybrid MXene and metal organic framework for electrochemical nitrate sensing

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Molecular sensing of nitrates has widespread importance in food, agriculture, and the environment, such as water for a sustainable world. Yet a fundamental, stable, reliable, and direct point-of-care sensing platform for nitrate environmental monitoring is still under consideration. Furthermore, complex problems such as soil health and water quality monitoring for precision agriculture require reliable engineered materials for fundamental sensing studies. In such environments, both excess and deficiency of nitrate ions pose risks such as impaired plant growth and increased disease susceptibility, while excessive nitrogen fertilization drives nitrate leaching into groundwater, eutrophication of surface waters, and microbially mediated nitrous oxide emissions, a potent greenhouse gas. Continuous nitrate monitoring is therefore essential for environmental protection and agricultural sustainability. However, conventional detection methods (chromatography, electrophoresis, luminescence-based assays) remain slow, labor-intensive, and impractical for field deployment, motivating growing interest in optical, colorimetric, electrochemical, and spectral sensing platforms. The present work introduces a dual transition-metal MXene, molybdenum titanium carbide ($Mo_2TiC_2T_x$), integrated with copper-based metal-organic frameworks to exploit copper's intrinsic electrocatalytic activity toward nitrate molecules. The resulting hybrid MXene and copper metal-organic framework nanocomposite promotes efficient charge transfer, elevated active-site density, and enhanced analyte adsorption, enabling a nanomolar-level nitrate detection plausibility. The validation using real water samples from the environment confirmed the development of potential practical on-site applicability of the developed sensors. This work establishes a robust foundation for trace-level nitrate monitoring, with strong potential for expansion toward broader macronutrient detection across complex food, soil, and water matrices.

MWRM 2026 MW183

Hydrogen vs halogen bonding: The competition effect on thermal expansion in multicomponent solids

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Thermal expansion (TE) describes the behavior a material demonstrates due to changes in temperature. TE is largely affected by the types of interactions (e.g. hydrogen and halogen bonding, π-π stacking, etc.) present in the material. Additionally, there is a growing interest in the thermal behavior of multicomponent solids, as the inclusion of a second component allows for tunability of solid-state properties such as TE. We were interested in investigating solids that are sustained by multiple types of intermolecular interactions and determining the impact of interaction type on TE behavior. Thus, we designed compounds containing both hydrogen- and halogen-bond donating moieties and prepared cocrystals using molecules with hydrogen/halogen-bond acceptor groups. Here, we will describe the propensity to form hydrogen and halogen bonds when in competition and the impact of interaction type on TE behavior. Moreover, one system exhibits unexpected solid-state behavior in response to temperature. This study aims to contribute to the overall understanding of the influence of intermolecular interactions on the thermal behavior of multicomponent solids.

MWRM 2026 MW18

Identification of *Citrus bergamia* flavonoids responsible for HMG-CoA reductase inhibition

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Citrus bergamia (bergamot), a citrus fruit widely recognized for its use in health supplements and Earl Grey tea, has recently attracted scientific interest for its effects on cholesterol levels. This study aimed to identify which out of five bergamot flavanoids (neoeriocitrin, naringin, neohesperidin, melitidin, and brutieridin) interact with and inhibit the 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMG-CoA reductase) enzyme. HMG-CoA plays a key role in the synthesis of cholesterol, and is the target of statins, the class of medication that is prescribed to lower cholesterol levels. The enzyme was successfully purified via nickel-affinity chromatography, and purity was confirmed with an SDS-PAGE gel. The five bergamot compounds and several dietary bergamot supplements were separated and characterized with high-performance liquid chromatography (HPLC), which was followed by liquid chromatography-mass spectroscopy (LC-MS) to analyze and verify the compounds. UV-visible spectrophotometry was used to observe changes in absorbance over time to measure

the enzymatic activity of HMG-CoA reductase and the effectiveness of each potential inhibitor. These results suggest that melitidin is the strongest inhibitor of HMG-CoA reductase.

MWRM 2026 MW407

Identification of potential PDGFRA-targeting therapeutics for glioblastoma using diffusion and structure-based drug discovery

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Glioblastoma is an aggressive brain cancer with limited treatment options and poor patient outcomes. Overactivation of the Platelet-Derived Growth Factor Receptor Alpha (PDGFRA) pathway contributes to uncontrolled tumor growth, making it a promising therapeutic target. This study used an artificial intelligence-driven drug discovery pipeline to identify potential PDGFRA inhibitors for glioblastoma treatment. Protein sequences were obtained from UniProt and modeled using AlphaFold 3. Potential binding sites were predicted using P2Rank, and chemically diverse compounds from the ZINC20 database were screened using DiffDock, a diffusion-based molecular docking platform. Drug-likeness and pharmacokinetic properties were evaluated using SwissADME and ADMET prediction tools. Several compounds demonstrated favorable binding affinities to PDGFRA, with the strongest candidate exhibiting a predicted binding energy of -7.04 kcal/mol. The top compounds also showed acceptable pharmacokinetic profiles and compliance with Lipinski's Rule of Five. These findings highlight the potential of artificial intelligence and structure-based drug discovery to accelerate the identification of novel therapeutic candidates for glioblastoma. Further experimental studies are needed to validate the efficacy of these compounds.

MWRM 2026 MW156

Identifying key mechanisms for inhibiting calcium carbonate nucleation in reverse osmosis concentrate

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Calcium carbonate ($CaCO_3$) scaling is a major challenge in desalination systems. However, elucidating the *in situ* interactions between antiscalants and $CaCO_3$ during the earliest stage of scale formation, namely nucleation, remains difficult because the initial nuclei are nanoscale in size. Furthermore, the mechanisms governing antiscalant performance in suppressing $CaCO_3$ during homogeneous and heterogeneous nucleation are not yet fully understood. In this study, we used synchrotron-based X-ray scattering techniques to investigate time-resolved $CaCO_3$ nucleation in the presence of

diethylenetriamine penta-methylene phosphonic acid (DTPMP) and polyacrylic acid (PAA). DTPMP contains five phosphonate groups with strong Ca^{2+} chelation capability, whereas PAA is a polymeric antiscalant rich in carboxylate groups. X-ray scattering results showed that DTPMP inhibited homogeneous nucleation more effectively than PAA by prolonging the induction time, as evidenced by *ex situ* small angle X-ray scattering (SAXS) measurement. In contrast, *in situ* grazing incidence small angle X-ray scattering (GISAXS) measurements informed that PAA more effectively suppressed heterogeneous nucleation, reducing the nucleation rate by a factor of 303. Combined microscopic and spectroscopic analyses revealed that suppression of homogeneous nucleation was primarily governed by Ca^{2+} chelation, while inhibition of heterogeneous nucleation was dominated by formation of a hydration layer on the substrate surface. These findings provide valuable mechanistic insights into antiscalant-scale interactions and offer design principles for developing antiscalants tailored to control mineral scale formation.

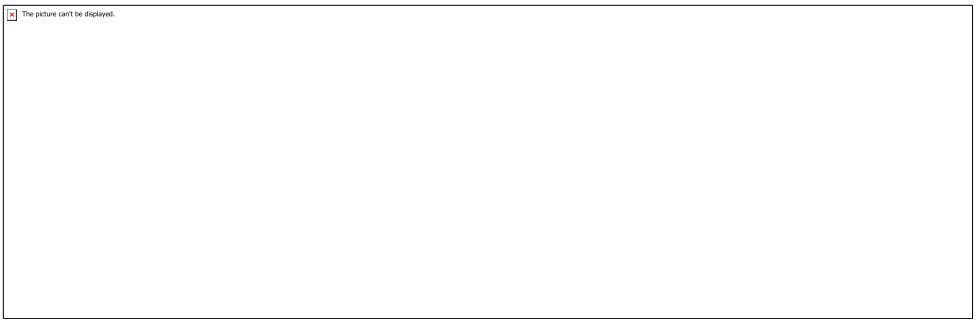
MWRM 2026 MW303

Imidazolium salts from renewable sources for antibacterial applications

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Bacterial infections and bacterial contamination of food is a growing concern with the rise of antibiotic resistance bacteria. Several approaches such as antimicrobial peptides, silver nanoparticles, or carbohydrate polymers have shown promise in combating bacteria. Another approach which has received considerable attention is the use of imidazolium salts. Imidazolium salts are known to disrupt the cell wall of the bacteria causing death. Here, we report the incorporation of imidazolium salts into epoxidized soybean oil (ESBO). ESBO is made from a renewable resource, in addition to being inexpensive and readily available.

The synthesis of these materials was a straightforward two-step process. ESBO was reacted with imidazole in refluxing IPA overnight. The resulting imidazole containing ESBO was then reacted with an alkyl halide (butyl, hexyl, or octyl). These imidazolium or benzimidazolium containing materials were characterized by IR and H-NMR spectroscopy. In addition, the testing of these materials in antibacterial applications with gram-positive and gram-negative bacteria will also be reported.



MWRM 2026 MW373

Impact of nanoconfined water upon irradiation of metal-organic nanotubes

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Hybrid porous materials, such as metal-organic frameworks (MOFs), are emerging as materials for high radiation fields, including nuclear waste remediation and radiation detection, because of their capacity to capture hazardous radionuclides or scintillation capabilities. Within the pore spaces, these materials often contain solvent molecules that may undergo radiolysis to form highly reactive free radical species, resulting in degradation of the structural linker or other decomposition processes. Radiolysis of bulk solvents has been explored, but much less is known about radiolysis effects within confined regimes. In the current work, we explored the impact of gamma radiation on a metal-organic nanotube (UMONT) in both a hydrated and dehydrated form. The presence of free radicals within both the pre- and post-irradiated samples was examined using electron paramagnetic resonance (EPR) spectroscopy. Structural changes were monitored via powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), and Fourier transform infrared (FTIR) spectroscopy. Structural characterization confirms that the crystalline framework and the confined water network remain intact even after γ irradiation doses up to 20 kGy, demonstrating the stability of the UMONT. EPR spectroscopy measurements reveal the formation of oxygen-centered radicals localized on the organic linker, which arise from defect sites generated during thermal dehydration of the nanotube. Surprisingly, the presence of nanoconfined water did not induce the formation of water radiolysis products that were previously observed in bulk liquids or hydrated solid-state materials. This suggests that the degree of water ordering related to the confinement effect may influence radical recombination or diffusion within porous solid materials.

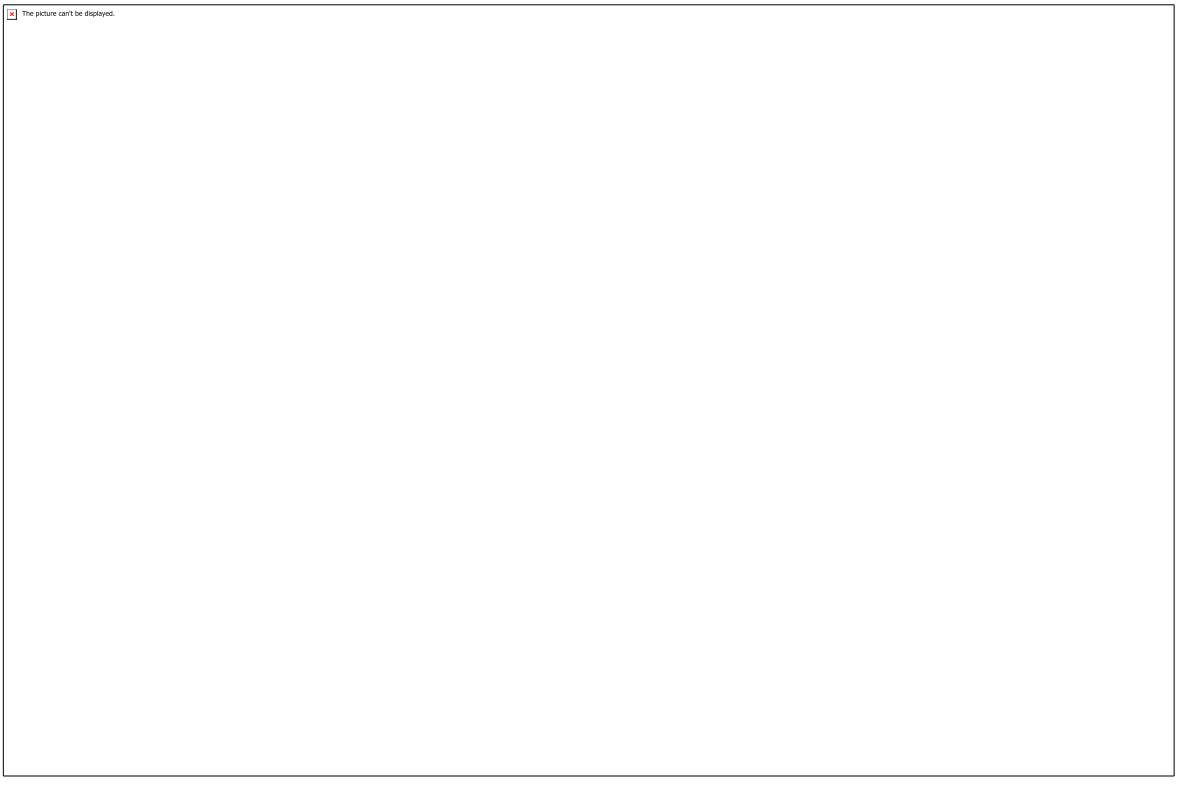
MWRM 2026 MW01

Implications for dual-pathway course design in general chemistry

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Addressing the needs of all students in an academically-diverse class is a problem facing many introductory STEM courses due to the varying levels of preparation in math, chemistry, and physics. Facing an ever-widening achievement gap in later courses, several years ago Washington University in St. Louis (WashU) changed from a single-track option for general chemistry to two parallel tracks, which differed in pace and depth, that allowed students to enter at an appropriate level while still ensuring an

equitable exit and adequate preparation for the following single-track organic chemistry experience. A placement exam (scored from 0-27), in addition to available standardized test scores, was used to determine incoming readiness and suggest a non-binding placement into the appropriate course sequence – Chem 1601 (Principles of General Chemistry) or Chem 1701 (General Chemistry); grades in organic chemistry were used to evaluate the effectiveness the two courses. An unconditional comparison of the organic chemistry GPA for students matriculating from Chem 1601 versus Chem 1701 suggests that Chem 1701 students earn a noticeably higher grade (B+, 3.4, SD = 0.7) than Chem 1601 students (B, 3.0, SD = 0.8). In order to control for selection bias, this study compares two groups of students, one on each side of the placement “cut-off” region. Results for Group A (diagnostic score of 11-14) showed that there was no statistically significant difference in organic chemistry GPA for students matriculating from Chem 1601 versus Chem 1701 (GPA = 2.99 with SD of 0.71 for Chem 1601 compared to GPA = 3.03 with SD of 0.70 for Chem 1701). Similar results were obtained for students in Group B with diagnostic scores of 17-20 indicating that, compared to the single-track approach, this dual-path model can better prepare our academically-diverse students, offering both challenge when appropriate and foundational skills when needed.



Chem 2601 and Chem 2602 GPA comparison for students matriculating from Chem 1601 vs. Chem 1701 in two diagnostic score ranges.

MWRM 2026 MW354

Improved in-channel microchip electrophoresis with electrochemical detection for catecholamine analysis

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Altered catecholamine metabolism and oxidative stress are hallmarks of neurodegenerative diseases, yet understanding their complex interplay requires analytical platforms capable of simultaneously monitoring multiple with high sensitivity, selectivity, and temporal resolution. Despite advances in electrochemical sensing, the simultaneous detection of neurotransmitters, their metabolites, and oxidation products in complex biological systems remains a significant analytical challenge. To address this need, our laboratory is developing a microdialysis-coupled microchip electrophoresis with electrochemical detection (MD-ME-EC) platform for continuous in vivo monitoring of neurotransmitters. The previous system employed pyrolyzed photoresist film (PPF) electrodes as working electrodes in the near in-channel configuration or the ME-EC analysis. However, the limits of detection of the resulting system are not low enough to detect endogenous concentrations of catecholamines due to the noise produced by the separation voltage and post-separation band broadening. To overcome these limitations, we redesigned the system using a true in-channel configuration incorporating a palladium (Pd) decoupler. This eliminates the separation-field interference while still maintaining efficient electrophoretic separation. Selection of the working electrode material was guided by cyclic voltammetry, which compared platinum (Pt) and palladium electrodes for dopamine oxidation. Platinum exhibited faster heterogeneous electron-transfer kinetics and lower oxidation overpotentials than palladium, demonstrating superior electrochemical performance. Based on these results, a substrate containing a Pt working electrode and a Pd decoupler were fabricated on soda-lime glass substrates using photolithography and metal sputtering. The resulting ME-EC device was evaluated using a simple-T PDMS separation channel with a background electrolyte consisting of 25 mM boric acid and 4 mM SDS. Baseline separation of dopamine, epinephrine, norepinephrine, serotonin, and L-DOPA was achieved, while the Pd decoupler effectively grounded the electrophoretic field and absorbed hydrogen generated during electrolysis, enabling stable in-channel electrochemical detection. This platform provides a foundation for fabricating microelectrode arrays that will enable simultaneous electrochemical detection of neurochemicals and facilitate integration with online microdialysis for continuous neurochemical monitoring.

MWRM 2026 MW102

Improvement of copper and zinc affinity of thermostable green protein (TGP-E) by TGP-E E144H and TGP-E E144H A164H

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Thermostable green fluorescent protein (TGP-E) is a fluorescent protein known for its increased thermal stability and bright green hue. Fluorescent proteins are widely used tagging tools in molecular biology, and their unique binding affinities allow them to target specific intracellular structures or organelles with high specificity. Two mutants were made to incorporate improved sensitivity for copper and aluminum for use as a metal sensor. The first mutation adds E144H to have two histidine residues compose a potential metal binding site with the native 172H residue. The second mutation started with the E144H mutant and added A164H which should make a three-histidine binding site for metal ions. Both mutations were introduced with site-directed mutagenesis performed PCR and were subsequently transformed into XL10-Gold Ultracompetent cells. Mutations were verified with DNA sequencing. The mutant plasmid was transformed into BL21 cells, growths were scaled up in 2L of LB media with added IPTG to induce protein production. Cells were grown for two days, centrifuged and resuspended in buffer for harvesting, then lysed by sonication. After removing insoluble debris through centrifugation, TGP-E E144H and TGP-E E144H A164H were both purified using a nickel affinity column with Tris buffers. A microplate reader was utilized to measure the effects of varying copper and zinc concentrations on TGP-E E144H and TGP-E E144H A164H fluorescence.

MWRM 2026 MW376

Improving fast-charging performance and durability of graphite anodes for lithium-ion battery

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Graphite is widely used as an anode material in lithium-ion batteries; however, its limited fast-charging capability remains a challenge for applications such as electric vehicles. Conductive carbon black improves electrode conductivity and rate performance, but excessive addition reduces the active graphite content. In this study, graphite anodes containing 5–35 wt% carbon black were evaluated while maintaining a constant binder content. An optimized carbon-black concentration improved capacity retention during high-rate charge–discharge cycling by enhancing electronic transport within the electrode. To address mechanical degradation caused by repeated lithium insertion and extraction, a ceramic-based coating was also introduced to reinforce the graphite anode. This combined approach provides a practical strategy for improving

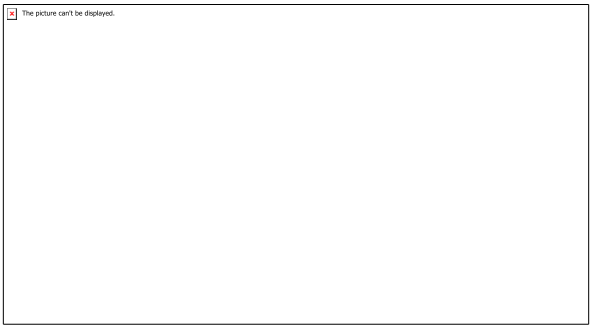
both the fast-charging performance and long-term stability of graphite-based lithium-ion battery anodes.

MWRM 2026 MW247

Improving Li-S battery performance by incorporating a set of MoS_x/rGO electrocatalysts in the S/C cathode and interlayer

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Lithium-Sulfur battery (LSB) is an attractive emerging battery for electrical energy storage due to its high specific capacity, high energy density and materials sustainability. However, the development of LSB is hindered by many technical challenges, including so-called “polysulfide shuttle effect” due to formation of highly soluble lithium polysulfides (LPSs) intermediates (Li_2S_n, with n = 8, 6, 4, 3 and 2) during the charge-discharge processes. Here we report an approach to mitigate this with two electrocatalysis approaches. Firstly, a family of molybdenum sulfides (MoS_x) anchored on reduced graphene oxide (rGO) nanosheets have been synthesized with tunable structures and electrocatalytic properties, from 1D amorphous MoS_3/rGO to 2D crystalline MoS_2 nano-patches. After being directly incorporated in the S/C cathode, the amorphous 1D MoS_3/rGO catalyst demonstrates the highest specific capacity of about 1,300 mAh/g at 0.1C while the 2D crystalline MoS_2/rGO catalyst shows the highest stability and a high Coulombic efficiency of 97% at a 1C rate, which correlates well with the adsorption capacity and electrocatalytic conversion efficiencies of various LPSs by both experimental studies and DFT calculations. The tunable catalytic properties provide a way to achieve the best Li-S performance by combining catalysts optimal for different LPS conversion steps. Secondly, we demonstrate that a dual-catalyst strategy can further enhance the LPS conversion kinetics, specific capacity, and long-term cycling stability compared to using only one type of electrocatalyst. To achieve this, we employ a thin catalyst coating on top of the S/C cathode as a catalytic interlayer while a second catalyst is directly mixed in the S/C cathode. When combining 2D crystalline MoS_2/rGO in the S/C cathode and 1D amorphous MoS_3/rGO in the interlayer, the synergistic effect leads to a remarkable initial specific capacity of ~ 1,417 mAh/g at 0.1C and ~1,000 mAh/g at 1C, with a good capacity retention over 500 cycles.



Dual MoS_x/rGO Electrocatalysts incorporated in the S/C Cathode and Interlayer

MWRM 2026 MW112

Improving the sensitivity of DNBS-based fluorescent sensors for hydrogen sulfide detection in aqueous media

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2,4-Dinitrobenzenesulfonate (DNBS)-based fluorescent sensors are widely used for hydrogen sulfide (H_2S) detection due to their high selectivity. However, their application in aqueous media is often limited by the hydrophobic nature of DNBS, which typically requires a high proportion of organic co-solvents, such as DMSO. In water-rich environments, DNBS hydrophobicity reduces its effective reaction with H_2S, leading to decreased sensor sensitivity. In this work, a supramolecular additive was used to improve H_2S detection in aqueous media. As a result, the sensitivity of DNBS-based fluorescent sensors was significantly improved in aqueous solutions. This approach provides an effective strategy to enhance the performance of DNBS-based H_2S sensors under aqueous conditions.

MWRM 2026 MW249

Influence of groundwater contaminates on electrocatalytic nitrate reduction

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Nitrate contamination is a major environmental and public health concern worldwide. Electrocatalytic nitrate reduction offers a sustainable approach for both nitrate remediation and ammonia production using renewable electricity. However, its practical application is limited because real groundwater contains diverse ions and contaminants that compete for catalyst active sites, alter interfacial electron transfer, and modify the local reaction environment. These interactions influence catalyst activity, reaction kinetics, product selectivity, and long-term stability.
This study investigates catalyst deactivation mechanisms associated with common groundwater ions, including surface passivation, corrosion, and competitive adsorption. It examines how these contaminants affect catalyst activity, selectivity, and efficiency for the nitrate reduction reaction. To investigate these mechanisms, surface-enhanced Raman spectroscopy (SERS) is employed to monitor surface intermediates during electrocatalytic nitrate reduction on copper (Cu) electrodes under varying potentials and groundwater contaminant like Cl^-, Mg_2^+, and SO_4^{2-}. SERS enables highly sensitive detection of surface species through localized surface plasmon resonance (LSPR)-induced electromagnetic enhancement on nanostructured Cu surfaces. Bulk electrolysis experiments are conducted to quantify gaseous and liquid products using gas chromatography (GC) and ultraviolet–visible (UV–Vis) spectroscopy, respectively.

Catalyst stability and structural changes before and after electrolysis are further characterized using X-ray fluorescence (XRF) and X-ray diffraction (XRD).
The study also explores optimization of catalyst design and operating conditions, including applied potential and pulsed electrolysis, to improve active-site accessibility, minimize competitive adsorption, and reduce catalyst deactivation under realistic groundwater conditions. The findings are expected to advance the development of contaminant-tolerant electrocatalysts and help bridge the gap between laboratory-scale studies and practical groundwater treatment. Ultimately, this work aims to support scalable electrocatalytic technologies for decentralized water treatment, sustainable ammonia production, and nitrogen resource recovery. Future studies will evaluate catalyst performance in more complex groundwater systems and develop mitigation strategies to further improve activity, selectivity, and long-term stability.

MWRM 2026 MW439

Influence of substrate elasticity on vapor-deposited stable glasses

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Organic stable glasses prepared by physical vapor deposition (PVD) exhibit enhanced thermodynamic and kinetic stability compared with ordinary glasses. They are of interest for applications in organic electronics and advanced functional materials. While stable glasses have been extensively studied on rigid substrates, relatively little is known about how compliant substrates influence their formation and stability. Understanding these effects is important for extending stable glass technology to more organic molecules for different uses.

Typically, PVD is performed onto rigid substrates, where the role of the substrate elasticity in stability is not well understood. In this research project, thin films of N,N′-Bis(3-methylphenyl)-N,N′-diphenylbenzidine (TPD) and 4,4′-Bis(N-carbazolyl)-1,1′-biphenyl (CBP) were deposited by physical vapor deposition onto soft polydimethylsiloxane (PDMS) substrates of varying thickness. Films were prepared over a range of deposition temperatures to investigate conditions favorable for stable glass formation. Ellipsometry and Atomic Force Microscopy were used to evaluate film thickness, optical properties, and to monitor changes associated with glass formation and crystallization.

Preliminary results indicate differences in film behavior on soft PDMS substrates compared with conventional rigid substrates. Initial TPD and CBP films exhibited evidence of substrate-dependent structural behavior. However, some samples did not undergo the expected transformation to stable glasses, suggesting that substrate properties or deposition conditions may significantly influence the formation process.

Ongoing work includes repeat deposition of TPD and CBP on 5 nm and 13 nm PDMS substrates to improve reproducibility and further investigate the relationship between substrate compliance and stable glass formation.

These results will provide insight into the role of soft substrates in vapor-deposited stable glasses and may inform the design of flexible organic electronic materials and devices.

MWRM 2026 MW262

Infrared quantification of siloxanes in synthetic biogas in the presence of carbon dioxide

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Biogas, an emerging renewable energy alternative to natural gas, often contains siloxanes when collected from post-consumer landfills and/or wastewater treatment facilities. When upgraded biogas undergoes combustion for energy production, the siloxanes can form abrasive silicon dioxide particles that, even in trace amounts, cause significant damage to the combustion turbines and engine parts. Siloxanes are typically removed by activated carbon filters as part of the biogas upgrading process. However, there is no standard on-line method for assessing filter saturation. Thus, undetected breakthrough events often occur. Gas chromatographic methods are utilized for low-level siloxane detection in upgraded biogas, yet their operational cost and complexity are not suitable for routine measurement. Fourier-transform infrared spectrometry (FTIR) gas analyzers provide real- to near-real-time analysis of many process streams, but siloxane quantification often suffers due to the appearance of spectral interferents in the “fingerprint region”, such as carbon dioxide. Carbon dioxide is typically present at 100,000 parts-per-*million* levels in biogas, while siloxanes are present at single parts-per-*billion* levels. Moreover, their concentrations may vary greatly from source to source and over time for individual sources. Therefore, a robust analysis method is needed to monitor trace amounts of siloxanes in the presence of significant and variable spectral interferents.
A gas stream modification process is presented and employed with a gas phase FTIR instrument for determination of siloxanes in biogas. Near-real-time siloxane quantification is demonstrated for an in-lab synthetic biogas mixture consisting of 25% carbon dioxide, 10% methane, and 65% nitrogen with low ppb_v levels of siloxanes. The siloxane concentrations quantified were at 100s of ppb_v levels, with spectral interferent carbon dioxide present at > 10^7 higher concentrations. The method demonstrated in this work will facilitate the development of simple, inexpensive IR-based devices for on-line and near-real-time monitoring of siloxanes in biogas.

MWRM 2026 MW286

Infrared study of partially hydrated lithium thiocyanate salts: Insight into hydration structure and geometry

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Hydrated lithium thiocyanate is an attractive system both for studying lithium ion transport phenomena and as a model system for exploring molecular pair interactions. In this work, infrared studies of the water stretching fundamentals in the solid phase are reported. Hydrates containing H_2O, along with its isotopic variations (D_2O and HOD) are examined. These measurements supplement previous studies of simultaneous vibrational transitions (molecular pair combination bands) in the solid. Partially hydrated salts are observed both via the dehydration of the hydrated salt and the hydration of the dehydrated salt. In the latter case, the evolution of the anhydrous salt into a hydrated state can be studied in real time. This in turn is useful in assessing the structure and geometry of the mono- and di-hydrate of lithium thiocyanate. Absorptions attributable to the mono-hydrate are consistent with spectra previously published, while absorptions ascribed to the di-hydrate contain distinct peaks not previously observed in the infrared spectrum of the compound. Published x-ray crystal structures are employed to compute, via VPT2 and VSCF electronic structure calculations, the predicted infrared absorptions for the mono- and di-hydrates. The results obtained support the proposed vibrational assignments. It is also found that the observed solid phase transition frequencies can be used to successfully fit the absorption profile of water in aqueous lithium thiocyanate, thus providing insight into the structure of the liquid solution. Finally, possible reasons for the failure to previously observe the di-hydrate peaks reported in this study, along with an explanation for the narrower absorption profile found for HOD as compared to H_2O and D_2O in the crystals are discussed.

MWRM 2026 MW314

Injectable microgels for wound healing applications

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Chronic wounds remain a significant healthcare challenge due to delayed healing, persistent inflammation, and recurring bacterial infections. Injectable hydrogels have emerged as promising biomaterials for wound healing because they can conform to irregular wound geometries while providing a supportive environment for tissue regeneration. In this project, we are developing injectable, biodegradable microgels that combine the biological properties of gelatin and chitosan with polymeric crosslinkers. Gelatin promotes cell adhesion and tissue regeneration, while chitosan provides inherent antimicrobial activity through disruption of bacterial membranes. Initial microgel formulations were prepared using bifunctional poly(ethylene glycol) (PEG) crosslinkers

to investigate the effects of crosslinker composition on swelling, injectability, and mechanical properties. Building on these results, thermoresponsive polymeric crosslinkers containing *N*-isopropylacrylamide (NIPAM) are being synthesized by reversible addition–fragmentation chain-transfer (RAFT) polymerization to enable temperature-responsive gelation. Microgels are prepared through bulk crosslinking, followed by lyophilization and milling to generate injectable microparticles. Rheological characterization demonstrated that increasing chitosan incorporation enhances microgel stiffness while maintaining injectability. Antimicrobial testing further showed that chitosan-containing microgels effectively inhibit bacterial growth, confirming that the incorporation of chitosan provides antimicrobial functionality in addition to improving mechanical properties. Ongoing work focuses on evaluating the thermoresponsive behavior of the RAFT-derived crosslinkers and optimizing the microgels for wound healing applications. This work establishes a versatile injectable microgel platform that combines biodegradability, antimicrobial activity, tunable mechanical properties, and the potential for temperature-responsive gelation.

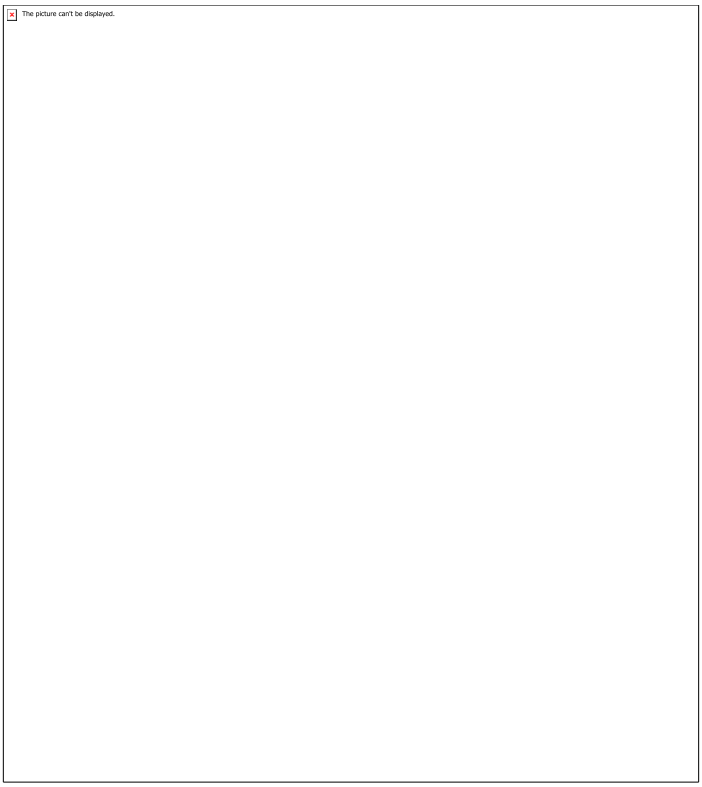
MWRM 2026 MW298

Inositol-derived stiff methacrylates for sustainable high-temperature polymer applications

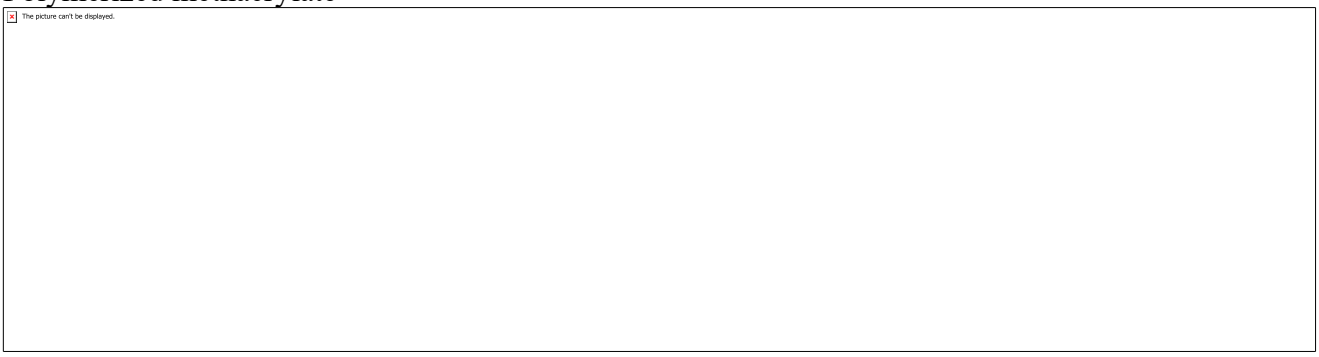
Tyler Schepanski*, tylerschepanski@gmail.com, Dhananjay Dileep, Eric W. Cochran, Thi Pham, William Teggatz, Katherine Bessie, Lilly Harris, Samuel Chambers, Aaron Bal, Kyle Tsujimoto, Kenneth Strezo. Chemical and Biological Engineering, Iowa State University of Science and Technology, Ames, Iowa, United States*

High-performance polymers for extreme environments, i.e., elevated temperatures and pressures, are mostly petroderived, thereby lacking sustainability. To address this issue, we synthesized a bio-derived polymer using myo-inositol sourced from waste corn steep liquor, a non-food-competitive feedstock. Inspired by the rigid diamondoid scaffold provided by adamantane, myo-inositol is ketalized to form a rigid condensate called “bananin,” producing a route to rigid processable biobased thermoplastics. We demonstrated scaled-up synthesis of the monomer with yield exceeding 85% followed by regioselective acylation using differing functional groups to access a broad property space culminating in the installation of the polymerizable methacrylic handle. These monomers were then polymerized using free- and controlled-radical polymerization to control monomer architecture and properties. The polymer's glass transition temperature exceeded 100 °C despite an octanoyl spacer, illustrating the rigidity instilled by the inositol core. Reversible addition-fragmentation chain transfer (RAFT) polymerization also enabled the synthesis of hard-soft diblocks by combining rigid and rubbery segments, resulting in durable and tunable materials. The preserved ketal linkages also allow for facile post-polymerization functionalization to modulate the surface hydrophilicity and enable self-healability. This combination of bio-renewable origin, competitive thermal performance, and multimodal post-polymerization positions bananin methacrylates as a versatile platform for high-performance coatings,

thermoplastic elastomers, and surface-active materials where sustainability and performance find consensus.



Polymerized methacrylate



Post-polymerization functionalization

MWRM 2026 MW375

Insights into metal-organic framework and polymer infiltration for membrane applications

*Colton Rhoads, Noah Nawracaj, Milana Rasin, **Angela Devlin**, angeladevlin@creighton.edu. Chemistry and Biochemistry, Creighton University, Omaha, Nebraska, United States*

Polymer membranes with metal-organic framework (MOF) fillers have demonstrated promise in separation applications, exhibiting enhanced membrane selectivity and permeability compared to polymer-only membranes, due to the high internal surface area and discrete pore sizes of MOFs. However, many polymers can infiltrate MOFs, which is detrimental to membrane performance, as the internal porosity can become blocked. This work aims to probe the role of polymer polarity and polymer chain length on pore infiltration in a family of zirconium-based MOFs. Polymer infiltration into UiO-MOFs is monitored over time via ^{1}H NMR. This work may provide guiding principles for compatible MOF–polymer pairs for informed membrane design.

MWRM 2026 MW428

Integrated filtration and analytical evaluation of multi-mixed matrix membranes for water purification

***May Moe Thu Han**, mhan24@ole.augie.edu, Mara Skogen, Cyndey Johnson-Edler. Chemistry & Biochemistry, Augustana University, Sioux Falls, South Dakota, United States*

Most industrial water filtration membranes cannot effectively capture environmental contaminants from pesticides and fertilizers, including glyphosate, atrazine, 2,4-D and nitrates. Metal Organic Frameworks (MOFs) are incorporated into polyethersulfone (PES)/polyvinylpyrrolidone (PVP) membranes to develop a Mixed Matrix Membrane (MMM) and Multi-Mixed Matrix Membrane (M4) targeting the aforementioned contaminants. MMMs are prepared by incorporating a single MOF (ZIF-8 or UiO-67) into the PES/PVP casting solution, while M4 incorporates both MOFs into the same membrane. Membranes then undergo phase inversion followed by solvent exchange and are analyzed using cross-flow filtration. 2,4-D water samples at varying concentrations are analyzed via HPLC, and contaminant concentrations in synthetic contaminated water are compared with those in environmental water samples. MOFs and membranes are characterized using SEM, NMR, FTIR/ATR, PXRD, and contact angle (membranes only). The MOFs fall within the nanometer range, ZIF-8 (~400 nm) and UiO-67 (~600 nm), which increases surface area and active sites, while being evenly embedded within the PES/PVP membrane pores. It is hypothesized that MOF incorporation will improve pesticide- and fertilizer-derived contaminant capture compared to unmodified PES/PVP membranes.

MWRM 2026 MW226

Integration in upper-division chemistry laboratories: Synthesis and characterization of oxovanadyl(IV) compounds

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The current interest in the biological chemistry of vanadium is due to the insulin - mimicking properties of oxo-vanadyl complexes. We have developed an upper-division synthesis and characterization laboratory based on vanadium(IV) complexes of *acac salen*, citric, picolinic and tartaric acid. The vanadium(IV) compounds were prepared in acid medium by reduction of V(V)/ligand exchange or oxidation of V(III) (*acac*)$_3$ (in the presence of O_2) and ligand exchange. The oxo-vanadyl(IV) complexes were characterized by UV-Vis., EPR, FT-IR (V=O stretch), EPR , ^{1}H-NMR (Evan's method for magnetic susceptibility) and by cyclic voltammetry. In the case of tartaric acid, we isolated both monomeric (IV) and bi-metallic tartarate complexes that show the expected 8-line EPR spectra for V(IV) and a complex EPR for the bi-metallic compound. In solution, vanadyl (IV) ion coordinates with tartrate anion to give different complexes depending upon the pH and the ratio of vanadyl to tartarate

MWRM 2026 MW251

Integration of thermoelectric generators and solid oxide electrolysis cells for efficient waste heat recovery in green hydrogen production

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Green hydrogen production relies on high-performance and sustainable technologies that enhance energy efficiency while reducing carbon emissions. This study proposes an innovative thermoelectrochemical cycle that exploits the recovery of residual heat from industrial and tertiary sectors by integrating thermoelectric generators (TEG) and solid oxide electrolysis cells (SOEC).
TEGs convert dissipated thermal energy into electricity, directly powering the SOEC, which performs high-temperature steam electrolysis (700-900°C). This process significantly reduces electrical consumption compared to conventional alkaline or PEM electrolyzers and improves overall system efficiency. Additionally, recovered heat helps stabilize SOEC operation and minimizes energy losses, thereby optimizing hydrogen production.
This approach is particularly suited for industrial sites generating significant thermal flows, but it also holds great potential for the tertiary sector, including data centers, hospitals, and commercial infrastructures, where substantial amounts of thermal energy remain underutilized. The integration of the TEG-SOEC system in these environments enables decentralized and low-carbon hydrogen production, supporting the energy

transition and reducing CO2 emissions.
The main challenges of this technology include optimizing thermoelectric materials, enhancing SOEC durability, and assessing the techno-economic feasibility of the integrated system. Current research focuses on improving TEG efficiency, developing advanced ceramic materials for SOEC electrodes, and optimizing operating conditions to maximize performance and economic viability. This study aims to establish a scientific and technological framework for more efficient and sustainable hydrogen production by fully harnessing available thermal energy sources.

MWRM 2026 MW229

Interpretation of the electronic structure from experimental X-ray absorption spectra (XAS) using computational methods

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X-ray Absorption Spectroscopy (XAS) is a powerful characterization technique for studying the electronic structure and local atomic environment of materials. It has element specificity, adapts to all types of systems including crystalline and amorphous materials, and is widely applied across multiple fields such as chemistry, materials science, and physics. However, its spectra are disturbed by interference from multi-electron effects and complex structural factors, making them extremely difficult to interpret. This review analyzes the interpretive support that four categories of computational methods provide for experimental data, namely density functional theory (DFT), time-dependent density functional theory (TD-DFT), ab initio methods, and machine learning. It sorts out their core application scenarios, the latest cross-field advances, as well as current challenges, technical trends, and future directions. Through a reliable framework that integrates experimentation and computation, this work aims to support electronic structure research and the design of advanced functional materials.

MWRM 2026 MW229

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MWRM 2026 MW348

Investigating bulk graphite crystal growth through silicon doping and isotope enrichment

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Graphite is extensively known for its electronic and thermal applications because of its unique properties. In this study, high-quality graphite single crystals were grown by precipitation from a molten iron-carbon solution under controlled cooling conditions. This work aims to improve our understanding of graphite crystal growth and guide the design of high-quality graphite through compositional engineering. Silicon doping has been hypothesized to enhance crystal size, morphology, and growth yield; therefore, silicon was added to the melt to investigate its influence on crystal growth. The influence of carbon isotope composition on graphite formation was also explored. Although carbon isotopes exhibit nearly identical chemical behavior, they have shown preferences in bonding. This study explores the potential clumping of heavier isotopes and the influence of isotope composition on graphite crystal formation. Using a combination of X-ray diffraction (XRD) and Raman spectroscopy, isotope distribution and crystal quality are correlated with key process parameters, specifically temperature and composition.

MWRM 2026 MW16

Investigating evolutionary conservation of 7SK stem-loop 3 RNA structural dynamics

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7SK RNA is a highly conserved non-coding RNA that plays a key role in regulating transcription elongation in vertebrates. 7SK RNA assembles with proteins to form the 7SK ribonucleoprotein complex. This complex acts as a switch controlling the release of positive transcription elongation factor b (P-TEFb), thereby regulating transcription

elongation. Structurally, 7SK RNA contains four main stem-loops (SL): 1, 2, 3, and 4. SL3 plays a role in restoring transcription elongation by recruiting proteins that lead to P-TEFb release. In *Homo sapiens* (Humans), SL3 exchanges between two states, SL3e and SL3a, as a conformational ensemble. This exchange is predicted to be evolutionarily conserved indicating functional significance. However, it is not clear how sequence differences within the two-state ensemble impact functional dynamics. Computational predictions depict vertebrate organisms to express conformations varying from SL3e, SL3a, or both. *Danio rerio* (Zebrafish) has been predicted and experimentally determined by chemical mapping to exhibit the SL3e-state. *Xenopus laevis* (African Clawed Frog) is predicted to form both the SL3e-state and SL3a-state but experimentally exhibits the SL3a-state. This project utilizes the atomic-level details of Nuclear Magnetic Resonance (NMR) analysis to examine the structural dynamic variations of 7SK SL3. SL3 domain constructs of *Danio rerio* and *Xenopus laevis* were designed, synthesized by in-vitro transcription, and purified. Constructs were structurally characterized via 2D ^{1}H-^{1}H Nuclear Overhauser Effect Spectroscopy (NOESY) and Heteronuclear Single Quantum Coherence (HSQC). A comparative analysis with *Homo sapiens*, locked constructs, and additional vertebrates confirmed *Danio rerio* has characteristic resonances specific for the SL3e-state. Furthermore, *Xenopus laevis* demonstrates characteristic resonances for the SL3a-state, thus experimentally exhibiting the absence of the two-state conformational ensemble. By understanding the SL3 two-state dynamics among vertebrates, this study provides insights into transcription elongation regulation throughout evolution.

MWRM 2026 MW113

Investigating intermolecular interactions via cocrystal synthesis between amidobenzoic acids and various pharmaceutical agents

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Cocrystals are formed when two different molecules assemble through intermolecular forces, primarily hydrogen bonds, creating new solid materials with properties that can differ from those of the individual components. Because these interactions can improve characteristics such as stability, solubility, and drug performance, cocrystals are of growing interest in pharmaceutical research. In this study, several amidobenzoic acids—molecules found in a variety of antiviral and anti-allergy medications—were combined with common pharmaceutical compounds to investigate their ability to form cocrystals. The compounds were mixed by solvent-assisted grinding with a small amount of methanol and analyzed using infrared (IR) spectroscopy and differential scanning calorimetry (DSC) to detect cocrystal formation. Slow solvent evaporation was also used in an attempt to grow single crystals for further study. The results showed that Aspirin readily forms cocrystals with amidobenzoic acids, and that subtle differences in the structure of the amidobenzoic acid strongly influence both the success of cocrystal formation and the melting point of the resulting material.

MWRM 2026 MW17

Investigating landfill and soil communities for potential rubber-degrading abilities

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Since the rise of the automobile industry in the late 19th century, the commercial use of natural rubber (NR) as a production material across numerous markets has skyrocketed. Consequently, rubber has become a widespread environmental contaminant, prompting the need for bioremediation strategies. To investigate the potential for strains of soil and landfill bacteria to degrade rubber, adaptive laboratory evolution (ALE) experiments by successive passaging were conducted using four different rubber substrates and one copolymer as a carbon source. To test for rubber biodegradation activity, Schiff's fuchsin-sulfite reagent was added to plated cultures and selectively stained rubber biodegradation products. We hypothesized that cis-1,4-polyisoprene and polybutadiene, the only liquid substrates tested, will allow more surface area for bacteria to utilize for growth and will thus experience accelerated biodegradation compared to other substrates. We further predicted that polystyrene-block-polybutadiene, the only copolymer tested, will exhibit the slowest, if any, biodegradation by bacteria, as polystyrene undergoes different biodegradation pathways than rubber. Initial trials displayed evidence of landfill community rubber biodegradation as detected by turbidity in growth tubes containing cis-1,4-polyisoprene. Improved rubber biodegradation identified in this study shows promise for the use of ALE to improve the rubber degradation abilities of bacteria. Furthermore, successful strains from this study will be used in future work characterizing rubber biodegradation mechanisms.

MWRM 2026 MW326

Investigating the effect of polymer composition on metal chelation thermodynamics

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Metal-chelating polymers have important applications in targeted radionuclide delivery, environmental remediation, and critical metal recovery. However, it is not well understood how polymer composition influences metal binding. While increasing the number of chelating groups is often expected to improve metal binding, high concentrations of these groups may instead reduce binding because of steric crowding or other unfavorable interactions. Likewise, non-chelating hydrophilic repeat units may influence polymer solubility and chain conformation, affecting the accessibility of chelating groups to metal ions. This project investigates how the ratio of chelating and

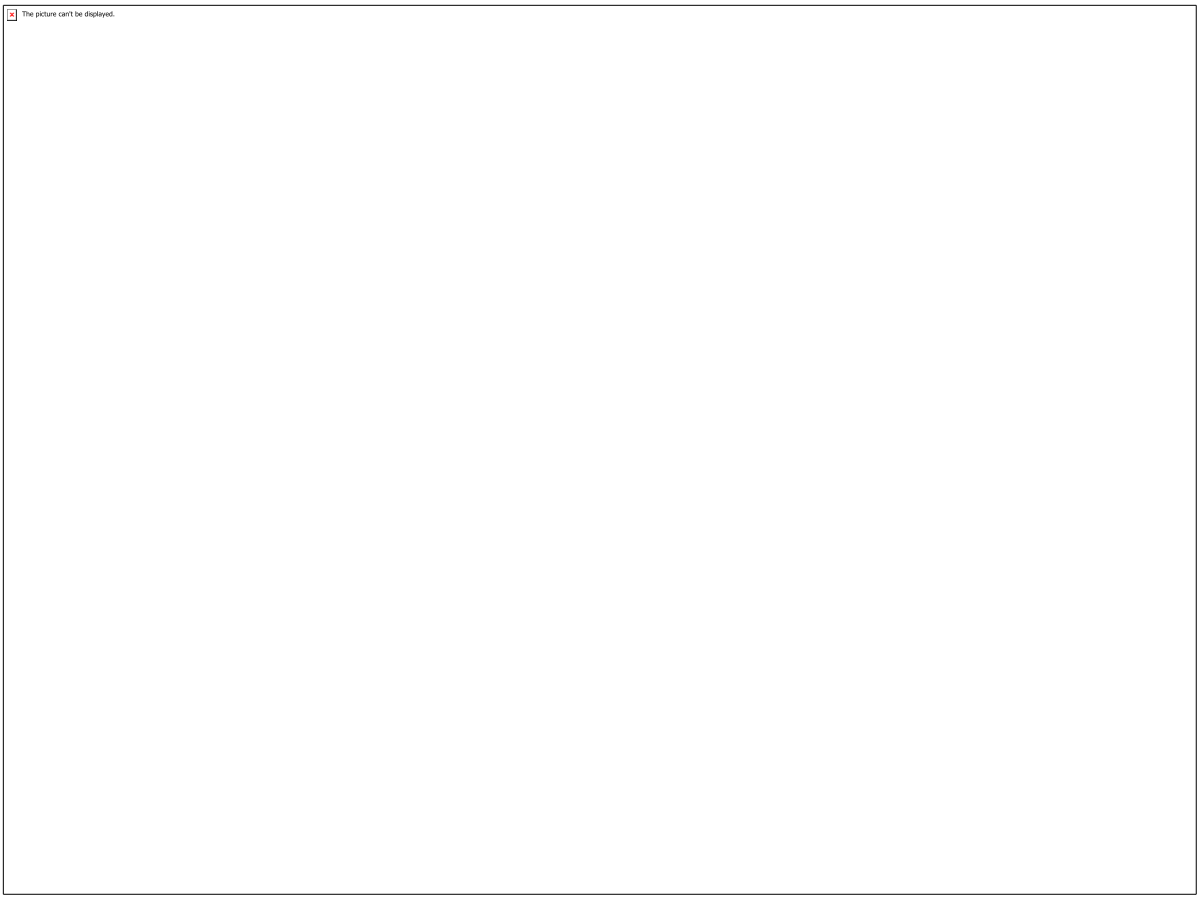
non-chelating hydrophilic repeat units influences metal-binding affinity and chelation thermodynamics in a series of random copolymers synthesized by reversible addition–fragmentation chain-transfer (RAFT) polymerization. Copolymers of acrylic acid (chelating) and N,N-dimethylacrylamide (non-chelating) were synthesized in a series of different molar ratios. The copolymers are characterized by NMR to determine conversion and composition, size exclusion chromatography (SEC) to determine molecular weight, and dynamic light scattering (DLS) to determine solution size and zeta potential. A complete thermodynamic profile of metal chelation is obtained using isothermal titration calorimetry (ITC). This work aims to establish composition–property relationships to guide the design of polymeric chelators for radionuclide delivery.

MWRM 2026 MW125

Investigating the importance of flexibility in antimicrobial quaternary ammonium surfactants using alkyne hydrogenation

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Antimicrobial resistance (AMR) is a problem that is estimated to have caused 1.27 million global deaths in 2019 by the World Health Organization. Our group is interested in making quaternary ammonium compound (QACs) surfactants, which are broad-spectrum bactericides and an important tool in the toolbox of combating AMR.
Most, if not all, commercial antimicrobial surfactants are structurally flexible, typically with long hydrocarbon chains, which contribute to their effectiveness in disrupting bacterial cell membranes. However, our group has synthesized *rigid* antimicrobial surfactants that are more effective at killing bacteria than the commercial surfactants by recent MIC data.
A series of symmetric diarylacetylene quaternary ammonium compounds (QACs) have been synthesized with varying hydrophilicities using click chemistry, Pd-catalyzed Stille cross-coupling, and classic S_N2 chemistry.
To test the effectiveness of rigid vs. flexible surfactants, the rigid acetylenes were partially hydrogenated to alkenes and completely hydrogenated to the alkane using classic organic chemistry textbook reactions (Fig. 1). Hydrogenation of the rigid QAC acetylene with an alkali metal in liquid ammonia to make a *trans*-alkene, Lindlar's catalyst to make a *cis*-alkene, and Pd on carbon to make an alkane were attempted. Results about this chemistry will be discussed and MIC values will be investigated later.



MWRM 2026 MW333

Investigation of adsorption of naphthalene and pyrene by pentafluorostyrene-based homopolymer, copolymers, and nanoparticles

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Polycyclic aromatic hydrocarbons (PAHs) are persistent organic contaminants that frequently accumulate in aquatic environments. Naphthalene and pyrene, with their π-conjugated aromatic structures, serve as representative PAHs for investigating the adsorption performance of fluorinated polymeric materials. The electron-deficient aromatic rings of pentafluorostyrene (PFS), resulting from fluorine atoms, are expected to interact favorably with the electron-rich π-systems of PAHs through donor–acceptor π–π interactions. This work evaluates PFS-containing polymers as adsorbents for the removal of naphthalene and pyrene from aqueous solutions. To improve adsorption efficiency, polymer nanoparticles with higher surface areas were also prepared. PFS homopolymers and PFS-co-*tert*-butyl acrylate copolymers were prepared by atom transfer radical polymerization (ATRP), and nanoparticles were subsequently produced

through chain collapse of linear polymer, using thermal crosslinking of benzocyclobutene (BCB) groups. Batch adsorption experiments were performed using aqueous solutions of naphthalene and pyrene at ppm and ppb concentrations, and their adsorption was evaluated by UV–Vis and fluorescence spectroscopies, respectively. Both naphthalene and pyrene exhibited measurable decreases in solution concentration after incubation with the polymer materials, demonstrating effective adsorption.

MWRM 2026 MW180

Investigation of a Tandem Indole 3-Sulfenylation/C2-C2' Coupling Reaction

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As part of a program directed toward the synthesis of 3-sulfenylindoles, we have observed an unanticipated tandem indole 3-sulfenylation/C2-C2'-coupling reaction. Given the spectrum of bioactive properties of 2,2'-biindoles, we have directed efforts toward investigation of the scope and limitations of the indole-indole coupling transformation. Experimental protocols will be described for indole-indole coupling as well as efforts toward further manipulation of the bi-indole core.

MWRM 2026 MW267

Investigation of electrodeposited Cu-MOF for enzyme immobilization at electrode interfaces

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Metal organic frameworks (MOFs) are highly porous coordination polymers with tunable structures often used in biological applications from gas capture to drug delivery. However, conventional MOF synthesis often requires high temperature, high pressure, or organic solvents that can limit use in biological applications. In contrast, electrodeposition provides a mild, and reproducible approach with high control for fabricating MOF thin films directly on electrode surfaces under aqueous conditions.Enzymes have been used in biosensors for their selectivity and sensitivity, but their instability and loss of activity remain significant challenges. Enzyme immobilization while retaining activity remains a challenge, but our previous work has demonstrated the aqueous synthesis of the MOF, Cu-BPDC, along with successful enzyme encapsulation with retained enzymatic activity. We have also demonstrated investigation of enzyme orientation of enzymes immobilized within MOFs using electron paramagnetic resonance spectroscopy (EPR). In this work, we investigate electrochemical synthesis of Cu-BPDC for immobilization of enzymes on electrode interfaces. Cu-BPDC was electrodeposited anodically and characterized by SEM and XRD. The well-studied redox enzyme glucose oxidase and spin-labeled T4 lysozyme were studied for immobilization in Cu-BPDC. These immobilized enzymes were

characterized electrochemically using cyclic voltammetry and the orientation of enzymes was characterized using EPR.

MWRM 2026 MW252

Investigation of low-dimensional materials as potential Li-ion anode materials: A case study of quasi-1D $NbTe_4$

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Low-dimensional materials refer to materials where one or more physical dimensions are reduced to a very small scale, usually on the nanoscale. Low-dimensional materials are attractive as anode materials for rechargeable batteries due to unique chemical features such as large surface area, enhanced electronic conductivity, short ion diffusion pathways, and good thermal stability, which are absent in bulk materials. Compared with two-dimensional (2D) materials, one-dimensional (1D) materials have attracted growing interest for their emerging properties. 1D materials possess greater chemical flexibility than 2D materials and might host more Li ions. In this work, we report the study of quasi-1D niobium tetratelluride ($NbTe_4$) and determine its potential for use as an anode material in lithium-ion batteries. The first-cycle discharge capacity of $NbTe_4$ was found to be 407.7 mAh/g, which is comparable to graphite (~370 mAh/g). With further cycling, the capacity was found to drop to below 100 mAh/g by the 100th cycle, which indicates low cycling stability and that $NbTe_4$ would not be an improvement over graphite. Starting from $NbTe_4$, moving to more earth-abundant NbS_4, the research is still ongoing.

MWRM 2026 MW433

Investigation of pH and metal coordination effects on natural phenolic compounds using UV-visible spectroscopy

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Natural phenolic compounds are widely distributed in plants and are recognized for their antioxidant activity and ability to coordinate with metal ions. These interactions can influence the chemical stability, antioxidant properties, and bioavailability of phenolic compounds, making them important in food, environmental, and medicinal chemistry. The objective of this study was to investigate the effects of pH and metal ion concentration on the coordination behavior of naturally occurring phenolic compounds using ultraviolet-visible (UV-Vis) spectroscopy. Phenolic extracts were prepared from blueberries, green tea, and spinach and reacted with copper(II) sulfate, iron(III) chloride hexahydrate, and aluminum nitrate at varying concentrations and pH values. Changes in absorbance were monitored at the wavelength of maximum absorbance (λmax) to

evaluate metal–phenolic complex formation and solution stability. Preliminary results indicate that metal ion concentration and pH significantly influence the spectroscopic response of the phenolic extracts. In general, decreasing metal ion concentration produced lower absorbance values, suggesting reduced metal–phenolic complex formation, while differences among the plant extracts indicate that phenolic composition affects metal-binding behavior. These findings improve the understanding of metal coordination in naturally occurring phenolic compounds and provide a foundation for future studies on their antioxidant properties and potential applications in food chemistry, environmental remediation, and medicinal chemistry.

MWRM 2026 MW308

Investigation of structure and performance in alginate–hemp composite films for sustainable packaging

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Persistent plastic packaging waste has increased interest in renewable films that combine useful mechanical and surface properties with improved end-of-life potential. Alginate–hemp composite films were prepared using alginate as the film-forming matrix and hemp-derived material as a renewable reinforcement. The study examined how formulation influences molecular interactions, morphology, wettability, and mechanical behavior. Fourier-transform infrared spectroscopy was used to characterize functional groups and interactions within the composite matrix. Tensile testing evaluated mechanical response, while water contact-angle measurements assessed surface wettability. Scanning electron microscopy characterized film morphology and hemp dispersion, and energy-dispersive X-ray spectroscopy examined elemental composition and distribution. Comparative characterization revealed formulation-dependent differences in tensile behavior, wettability, and microstructure, while spectroscopic and elemental measurements provided complementary insight into the organization of the composite matrix. Together, the results connect composition and structure with packaging-relevant performance and provide a basis for optimizing alginate–hemp films for sustainable packaging applications.

MWRM 2026 MW254 - Withdrawn

MWRM 2026 MW71

Ionic liquids for electrochemical gas sensing

***Xiangqun Zeng**, xzr5w@missouri.edu. Chemistry, Chemical and Biomedical Engineering, University of Missouri System, Columbia, Missouri, United States*

Chemicals and materials with active ionic species are widely employed in various chemical and electrochemical applications such as solvents, catalysts, sensors, fuel

cells, batteries, atomic switches, etc. Ionic liquids (IL) are liquids often composed of bulky organic cations or anions whereas conductive polymers are solids with dopant ions in a rigid organic framework. In this presentation, we will discuss the fundamental research of ionic liquid interface electrochemistry for gas sensor applications. Being composed entirely of ions and with a broad structural and functional diversity i.e., bifunctional (organic/inorganic), biphasic (solid/liquid), and biproperty (solvent/electrolyte) materials, ionic liquids have the complementing attributes and the required variability to allow a systematic design process across many components to enhance sensing capability for miniaturized gas sensor system implementation. The simplicity of the demonstrated detection principles could yield forward-thinking solutions to many sensors challenges, especially miniaturization and robustness that is essential for their integration with engineering advancements such as portable electronics, networked sensing and next-generation monolithic implementation of autonomous sensors with the performance, cost, power, and operational lifetime characteristics to suit a broad range of applications.

MWRM 2026 MW400

Ion pairing in confined aqueous electrolytes

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Understanding how ion–ion association evolves under nanoscale confinement is a central challenge in physical chemistry, with implications for nanofluidics, energy storage, and selective separations. As aqueous electrolytes transition from bulk environments to quasi-two-dimensional graphene slits and quasi-one-dimensional carbon nanotubes, the reduction in accessible configurational space fundamentally alters solvation structure, dielectric screening, and the balance between ion pairing and dissociation. Experimental characterization of these effects remains difficult, while conventional simulations either lack chemical accuracy or are computationally prohibitive.

Here, we develop a graph neural network–based machine-learning potential trained on accurate DC-SCAN based electronic structure theory data to achieve near chemical accuracy at large scales. An active learning strategy efficiently samples configurations spanning bulk solution, graphene slit pores, and carbon nanotubes, enabling a unified description across confinement regimes. Using this framework, we systematically investigate lithium halide aqueous systems and demonstrate how reduced dimensionality impacts ion–ion association, modifies hydration structure, and shifts the equilibrium between contact, solvent-shared, and solvent-separated ion pairs. Confinement and interfacial curvature are shown to promote preferential localization and anisotropic solvation environments that are absent in bulk solution.

These results reveal how dimensional reduction governs electrolyte structure at the

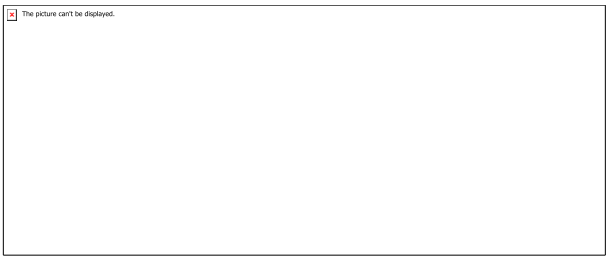
molecular level, providing fundamental insight into ion behavior in nanoconfined water and providing predictive simulations of confined aqueous systems.

MWRM 2026 MW67

Is current always proportional to surface? Consequences in catalysis

***Christophe Renault**, crenault@luc.edu. Chemistry and Biochemistry, Loyola University Chicago, Chicago, Illinois, United States*

Benchmarking electrocatalytic-nanoparticles typically assumes a current proportional to the surface of active material. In other words when the surface of catalyst is doubled so is the electro-catalytic current. In this work we will challenge this dogma. We theoretically and experimentally demonstrate using numerical simulations and hydrazine oxidation on gold nanoparticles that only a limited range of active material coverage obeys this assumption. We provide guidelines to correctly assess electrocatalytic acitvity of dispersed materials.



MWRM 2026 MW217

Key role of students metacognitivie skills in learning organic chemistry

***Helena Malinakova**, hmalina@ku.edu. Department of Chemistry, The University of Kansas, Lawrence, Kansas, United States*

Students in organic chemistry courses are encouraged devote a significant portion of their study time to problem-solving practice. Despite the best efforts of both students and the instructors, not all the students who follow this advice succeed in this challenging class. Herein, we report on a study aimed at identifying which aspects of the problem-solving practice are most critical to students' success in the Organic Chemistry I course. The study participants responded to six questions (using the 1-5 Likert scale: strongly agree to strongly disagree) that explored students' study habits prior to a problem-solving session, the depth of their understanding of the problem-solving methodologies, and the nature of their response to situations when they failed to arrive at the correct answer. The data analysis sought to identify correlations between the key

characteristics of students' problem-solving practice and their dominant learning approach (Deep vs Surface learning) as assessed by the OCH-Adjusted M-ASSIST instrument, as well as their achievement level (final grade) in the Organic Chemistry I class. Remarkably, student's ability to employ metacognitive analysis of their own weaknesses and deficiencies was identified as the aspect of the problem-solving practice that positively correlated with a high statistical significance with students' Deep learning approaches (meaningful learning) as well as high levels of achievement in the class (final grade). Conclusions of this study can be leveraged to effectively coach students through the problem-solving practice to maximize their success in Organic Chemistry courses.

MWRM 2026 MW31

Kinetic analysis of intramolecular cyclization in aryl diazonium-containing peptides with tyrosine and histidine residues

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Cyclic peptides have been gaining popularity in therapeutic development for their enhanced metabolic stability and have increased binding affinity when compared to their linear counterparts. These qualities stem from their constrained, rigid conformations that improve resistance to degradation and reduce the entropic cost of target engagement. Traditional cyclization methods involve strong nucleophilic residues such as lysine or cysteine, but more recent studies have shown success using proximity-driven reactivity to achieve site-selective azo coupling between tyrosine/histidine and aryl diazonium moieties. This study aims to expand on this approach by investigating the kinetics of the chemoselective intramolecular cyclization by examining the distance between the reactive groups necessary for cyclization. We also seek to determine the pH levels at which such interactions are favorable in order to help predict their formation in vivo. Peptides with varying distances between the two reactive groups were constructed using Fmoc solid-phase peptide synthesis and tested for cyclization at various pH levels. Peptide purification was performed using high-performance liquid chromatography (HPLC) and the cyclization progress was monitored using mass spectrometry and UV-Vis spectroscopy to detect new azo bond formation. Understanding the factors that influence these cyclization reactions will help expand the breadth of peptide signaling processes that can be mimicked or antagonized in the development of novel drug therapies.

MWRM 2026 MW350

Label-free detection and identification of epitranscriptomic modifications using XToF nanofluidic device

***Minaza Yahiya**, minaza.yahiya@ku.edu, Steven A. Soper. Chemistry, University of Kansas, Lawrence, Kansas, United States*

Epitranscriptomic modifications are diverse post-transcriptional alterations found in cellular RNA, with over 170 distinct types identified to date. These modifications influence RNA structure, catalysis, and gene expression, playing vital roles in both normal physiology and disease, including tumor development. Dysregulation of RNA modifications has been observed across multiple cancers, highlighting their potential as diagnostic biomarkers and therapeutic targets.However, current detection methods such as miCLIP (m6A individual-nucleotide resolution crosslinking immunoprecipitation) face limitations ; notably dependence on highly specific antibodies and amplification bias. To address these challenges, we introduce a novel label-free identification approach utilizing the Exonuclease Time-of-Flight (X-ToF) device.This dual in-plane nanopore sensor fabricated using nano-injection molding to create structures in Cyclic Olefin Polymer (COP) with a Cyclic Olefin Copolymer (COC) cover plate enclosing the fluidic network was primarily designed to sequentially cleave single nucleotides from intact RNA/DNA molecules using an immobilized processive exonuclease enzyme and to electrokinetically propel the resulting single molecule through the nanopore, generating current transient signals. Hence this device consists of three main components: an input/output network with pores for RNA/DNA entry, a nanoscale enzymatic bioreactor housing surface-immobilized enzymes, and a nano-flight tube for single-molecule electrophoresis and sensing. Modified rNMPs are electrokinetically translocated through the nanofluidic network using 1XNE buffer with KCl. Using our novel approach utilizing solid state nanopores, which integrates Nano-electrochromatography and Resistive Pulse Sensing (RPS) technology, we were able to successfully differentiate m6A, Inosine and Pseudouridine from rAMP , rCMP , rUMP , and rGMP based on their time-of-flight which reflects each nucleotides apparent mobility, the dwell time and the peak amplitude. Machine learning achieved 97.13% accuracy in identifying canonical and modified classes using X-TOF’s multidimensional molecular fingerprinting.
Future work aims to extend this platform for direct RNA sequencing with embedded epitranscriptomic modifications, enabling both short- and long-read analyses.

MWRM 2026 MW350

Label-free detection and identification of epitranscriptomic modifications using XToF nanofluidic device

***Minaza Yahiya**, minaza.yahiya@ku.edu, Steven A. Soper. Chemistry, University of Kansas, Lawrence, Kansas, United States*

Epitranscriptomic modifications are diverse post-transcriptional alterations found in cellular RNA, with over 170 distinct types identified to date. These modifications influence RNA structure, catalysis, and gene expression, playing vital roles in both normal physiology and disease, including tumor development. Dysregulation of RNA modifications has been observed across multiple cancers, highlighting their potential as diagnostic biomarkers and therapeutic targets.However, current detection methods such as miCLIP (m6A individual-nucleotide resolution crosslinking immunoprecipitation) face limitations ; notably dependence on highly specific antibodies and amplification bias. To address these challenges, we introduce a novel label-free identification approach utilizing the Exonuclease Time-of-Flight (X-ToF) device.This dual in-plane nanopore sensor fabricated using nano-injection molding to create structures in Cyclic Olefin Polymer (COP) with a Cyclic Olefin Copolymer (COC) cover plate enclosing the fluidic network was primarily designed to sequentially cleave single nucleotides from intact RNA/DNA molecules using an immobilized processive exonuclease enzyme and to electrokinetically propel the resulting single molecule through the nanopore, generating current transient signals. Hence this device consists of three main components: an input/output network with pores for RNA/DNA entry, a nanoscale enzymatic bioreactor housing surface-immobilized enzymes, and a nano-flight tube for single-molecule electrophoresis and sensing. Modified rNMPs are electrokinetically translocated through the nanofluidic network using 1XNE buffer with KCl. Using our novel approach utilizing solid state nanopores, which integrates Nano-electrochromatography and Resistive Pulse Sensing (RPS) technology, we were able to successfully differentiate m6A, Inosine and Pseudouridine from rAMP , rCMP , rUMP , and rGMP based on their time-of-flight which reflects each nucleotides apparent mobility, the dwell time and the peak amplitude. Machine learning achieved 97.13% accuracy in identifying canonical and modified classes using X-TOF’s multidimensional molecular fingerprinting.
Future work aims to extend this platform for direct RNA sequencing with embedded epitranscriptomic modifications, enabling both short- and long-read analyses.

MWRM 2026 MW140

Label-free single-molecule detection and machine learning classification of amino acids using a solid-state in-plane nanopore platform

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Direct, single-molecule protein sequencing holds transformative potential for proteomics, biomarker discovery, and personalized medicine by offering insights into low-abundance proteins that bulk-averaged techniques cannot resolve. Unlike nucleic acids, proteins lack an amplification strategy and exhibit immense sequence diversity, making single-molecule approaches essential. However, a persistent technical bottleneck is the reliable, label-free identification of individual amino acids. Existing approaches typically require chemical derivatization or fluorescent tagging, which increases complexity, alters analyte behavior, and limits scalability. Furthermore, the native physicochemical differences among unmodified amino acids are often too subtle to resolve using single-parameter sensing methods.

To address this challenge, we developed a solid-state nanopore sensing platform for the direct, label-free classification of underivatized amino acids. The devices were fabricated utilizing a cyclic olefin polymer (COP) substrate and cyclic olefin copolymer (COC) cover plate, which were subjected to a 10-minute ultraviolet surface treatment to optimize sensor performance and surface properties. Individual translocation events were monitored using Resistive Pulse Sensing (RPS). We successfully characterized eight amino acids (Arginine, Aspartic acid, Cysteine, Serine, Leucine, Isoleucine, Proline, and Tryptophan) by extracting three complementary electrical signatures per event (current blockade amplitude, dwell time, and Time-of-Flight (ToF)).

Because subtle structural differences among unmodified amino acids produce overlapping signal distributions, a Random Forest machine learning classifier was applied to the combined multidimensional dataset. The model successfully differentiated the analytes, achieving an overall classification accuracy of 92%. This high-accuracy discrimination establishes a scalable strategy for label-free amino acid identification, overcoming key detection limitations and providing a critical foundation for future solid-state nanopore platforms in single-molecule peptide fingerprinting.

MWRM 2026 MW404

Leucine-rich arrestin loop and receptor phosphosite spacing modulate membrane engagement in ACKR3–arrestin2/3 molecular dynamics simulations

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Arrestins are essential regulators of GPCR-mediated signal transduction. Arrestin binding to a receptor, primarily through the receptor's phosphorylated C-terminal tail, can terminate GPCR signaling by blocking G protein-dependent pathways, promote receptor-mediated internalization, or activate arrestin-dependent signaling pathways. GPCR–arrestin complexes assemble at lipid membranes. An important unresolved question is how membrane engagement contributes to arrestin activation and how this process depends on different receptor phosphotail binding and arrestin isoform chemistry. To address this question, we used all-atom molecular dynamics simulations of ACKR3–arrestin2/3 complexes to test how sequence differences in a membrane-facing C-lobe arrestin loop and the spacing between receptor phosphosites and the end of transmembrane helix 7 influence lipid contacts and activation-related interdomain motions. Specifically, we compared arrestin2, which has a longer leucine-rich C-lobe loop, and arrestin3, which has a much shorter C-lobe loop, both complexed with wild-type ACKR3, as well as arrestin2 complexed with an ACKR3 variant containing a poly-glycine insertion in the C-tail before the phosphosites to increase spacing.

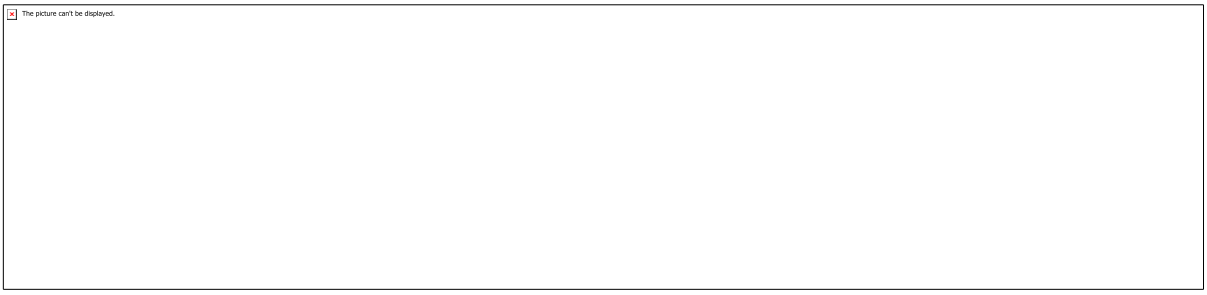
Our analyses indicate that, in all cases, arrestin showed strong engagement with the phosphorylated receptor tail, consistent with this region serving as the primary receptor-arrestin interaction site. For arrestin2, the leucine-rich loop formed broad membrane contacts, whereas for arrestin3 membrane contacts are more concentrated and less frequent. The GPCR–arrestin variants exhibited distinct lipid-contact patterns, suggesting that loop chemistry and receptor phosphosite organization can modulate membrane engagement. Whole-arrestin contact maps further indicate that membrane interactions are distributed across multiple surface regions. Overall, these results suggest that arrestin isoform identity and the receptor C-tail phosphorylation pattern influence arrestin dynamics that may lead to distinct downstream signaling outcomes, although the relationship between lipid contacts and activation-related interdomain motions appears to be complex.

MWRM 2026 MW261

Leveraging multi-component reactions toward xylochemical decarboxylative functionalization

***Jon A. Tunge**, tunge@ku.edu. Chemistry, The University of Kansas, Lawrence, Kansas, United States*

New decarboxylative functionalizations that leverage xylochemistry will be discussed. Metallaphotoredox/cobalt-catalyzed decarboxylative elimination chemistries enable new cross-coupling variants that are poised to utilize biorenewable feedstocks rather than conventional petroleum-based reactants. The utility of products as bioisosteres and as potential reagents for bioorthogonal chemistry will be demonstrated through subsequent cycloaddition chemistries. Furthermore, experiments will be presented to highlight the mechanistic underpinnings of cobalt-catalyzed decarboxylative eliminations as well as the underlying photochemistry. For example, Stern-Volmer quenching indicates reaction initiation through oxidative quenching by cobaloxime catalysts. Competition experiments suggest that the reduced cobaloxime catalyst facilitates decarboxylative elimination through rapid HAT (ca. 10^8 $M^{-1}s^{-1}$) from radical intermediates. Finally, studies of the photocatalytic decarboxylation suggest that back electron transfer rates may be important in limiting rates of decarboxylation.



MWRM 2026 MW149

Lewis acid effects on the reduction of a monometallic vanadyl complex

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Vanadyl complexes with Schiff-base and salen ligands are well documented, and previous studies have shown that Lewis acids can tune the electrochemical properties of the vanadyl ion in heterobimetallic species. However, little work has been done to elucidate the thermodynamic and kinetic effects of Lewis acid adducts on the one-

electron reduction of monometallic vanadyl complexes in non-aqueous media. Here, the synthesis and spectroscopic studies of a monometallic Schiff-base salen-type vanadyl complex, denoted $[VO]L^4$, are described. Cyclic voltammetry was used to estimate thermodynamic and kinetic parameters associated with electrochemical reduction of vanadium from its +4 to +3 oxidation state (V^{IV} to V^{III}), and time-resolved pulse radiolysis (TRPR) studies were performed at the Laser Electron Accelerator Facility (LEAF) at Brookhaven National Laboratory to explore the kinetics of the reduction reaction. Aided by findings from the electrochemical and TRPR techniques, the influence of the Lewis acidic sodium cation on the $V^{IV/III}$ couple has thus been studied.

MWRM 2026 MW363 - Withdrawn

MWRM 2026 MW228

Lipid oxidation and effect of antioxidants in food matrices of varying water activity level: A model for food chemical education

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Lipid oxidation is a critical factor studied by the food industry that influences the quality, safety, and shelf-life of food products. Water activity (aw) is a measurement describing the amount of water in a food available to participate in chemical reactions (e.g., lipid oxidation). This correlation is seen in Labuza's Food Stability Map. Manufacturers typically control lipid oxidation by adding antioxidants, synthetic or natural, to their formulations. Some synthetic antioxidants may introduce health concerns for humans.

While building fundamental laboratory skills such as micropipetting, reagent preparation, and quantitative analysis, students can explore natural antioxidant alternatives in response to more consumers advocating for natural ingredients in their food. Antioxidant efficacy was investigated in a range of aw foods, including commercial crackers, lab-made crackers, date cookies, and raisin bread, using the thiobarbituric acid reactive substances (TBARS) assay - a well-established method for assessing lipid oxidation by measuring malondialdehyde (MDA) levels, which is a secondary product of lipid oxidation. The antioxidants investigated were synthetic (butylated hydroxytoluene) and natural (eugenol and the amino acids, methionine and proline).

By utilizing entry-level laboratory techniques and tools throughout the procedure, this study demonstrates how this research can be incorporated into the preparatory and/or collegiate curriculum to deepen understanding of basic lab techniques, food chemistry, oxidation mechanisms, and experimental design while fostering student engagement through hands-on scientific inquiry.

MWRM 2026 MW22

Liquid chromatography-mass spectrometry lipidomic characterization for pulmonary arterial hypertension (PAH)

Ella J. Simmons[1]*, ella.simmons@jacks.sdstate.edu, Sanjida Afroz Mitu*[1]*, Nashrifa Israt Khanom*[1]*, Aminul Islam*[1]*, M. Nurul Islam*[1]*, Taslim A. Al-Hilal*[2]*. (1) Chemistry, Biochemistry, and Physics, South Dakota State University College of Natural Sciences, Brookings, South Dakota, United States(2) Molecular Pharmaceutics and Biomedical Engineering, The University of Utah College of Pharmacy, Salt Lake City, Utah, United States*

Pulmonary arterial hypertension (PAH) is a progressive cardiopulmonary disease characterized by pulmonary vascular remodeling, increased pulmonary vascular resistance, and right ventricular dysfunction. Despite treatment advances, PAH remains associated with substantial morbidity and mortality, and its underlying mechanisms are incompletely understood. Emerging evidence suggests that altered lipid metabolism may contribute to disease development and progression. This study therefore aimed to characterize plasma lipid profiles in a PAH model using untargeted liquid chromatography–mass spectrometry (LC–MS).
Previously prepared plasma extracts from low-risk PAH patients, moderate-risk PAH patients, and control groups were analyzed by LC–MS in positive- and negative-ionization modes. Raw data were processed using Agilent MassHunter Qualitative Analysis and MZmine through mass detection, chromatogram construction, peak resolution, deisotoping, feature alignment, and gap filling. Processed feature lists were evaluated for reproducible differences in mass-to-charge ratio, retention time, and signal intensity, followed by statistical analysis in MetaboAnalyst.
Ongoing analysis will determine whether PAH and control samples exhibit distinct plasma lipid profiles and identify features for targeted follow-up. Characterizing PAH-associated lipid alterations may clarify disease-related metabolic remodeling and reveal possible lipid markers for future validation and clinical investigation.

MWRM 2026 MW101

Liquid chromatography-mass spectrometry lipidomic characterization for pulmonary arterial hypertension (PAH)

Ella J. Simmons[1]*, ella.simmons@jacks.sdstate.edu, Sanjida Afroz Mitu*[1]*, Nashrifa Israt Khanom*[1]*, Aminul Islam*[1]*, M. Nurul Islam*[1]*, Taslim A. Al-Hilal*[2]*. (1) Chemistry, Biochemistry, and Physics, South Dakota State University College of Natural Sciences, Brookings, South Dakota, United States(2) Molecular Pharmaceutics and Biomedical Engineering, The University of Utah College of Pharmacy, Salt Lake City, Utah, United States*

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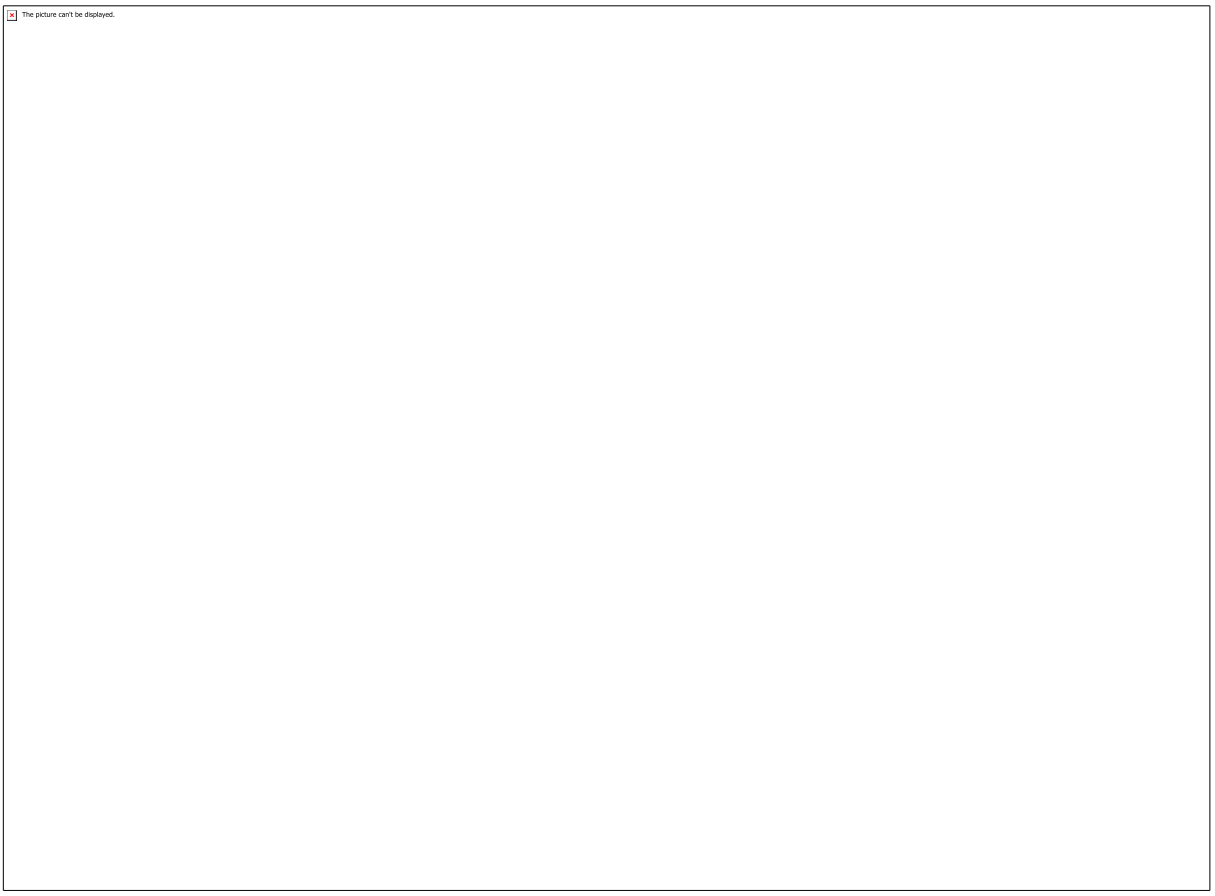
MWRM 2026 MW07

Machine learning guided discovery of isoform selective HDAC8 inhibitors through virtual screening and generative design

Bennett Garfinkel[1]*, bgarfinkel74@claytonschools.net, Talin Bhatt*[1]*, David Wharton*[1]*, Henry Politte*[2]*, Taraman Kadayat*[3]*. (1) Clayton High School, Clayton, Missouri, United States(2) Saint Louis University, St. Louis, Missouri, United States(3) Larkin University College of Pharmacy, Miami, Florida, United States*

Histone deacetylases (HDACs) are enzymes that remove acetyl groups from histones, repressing gene expression and regulating cell division. HDAC8 is a class I HDAC whose overexpression is linked to various tumors and cancers. Selective HDAC8 inhibitors could enable treatment of cancers and parasites such as Schistosoma mansoni. However, achieving HDAC8 selectivity is challenging due to high structural homology among HDAC isoforms. L-shaped ligands have shown potential for achieving this selectivity.
A warhead is the inhibitor component that chelates zinc in the HDAC8 active site. Hydroxamic acid is the most prominent warhead and typically achieves low-nanomolar IC50 values, but its chemical structure contributes to off-target effects and poor pharmacokinetics. Many ligands also lack sufficient HDAC8 affinity, resulting in cross-reactivity that limits therapeutic potential. This project aims to streamline discovery of potent, non-hydroxamate HDAC8-selective inhibitors by integrating machine learning with virtual screening and generative design. We implemented an eight-island evolutionary computational pipeline utilizing an audited, eight-chemotype Zinc Binding Group (ZBG) whitelist. Machine learning models were trained on a merged dataset of ~73,000 entries from BindingDB, ChEMBL, and internal data. A Tier-1 hard-gate system filtered non-hydroxamate molecules while excluding metabolic liabilities. NSGA-II

Pareto optimization prioritized candidates using predicted pIC50, selectivity profiles, and docking scores from HDAC1, HDAC6, and HDAC8. Lineage tracking maintained chemotype diversity, while drift filtering preserved ZBG integrity throughout the process, producing a refined pool of selective inhibitor candidates.
This approach advances computational drug discovery by enabling rapid targeting of challenging enzymes. By filtering metabolic risks and prioritizing isoform selectivity through cross-target data, this framework provides a foundation for developing safer, more effective cancer therapeutics.



MWRM 2026 MW07

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MWRM 2026 MW50

Machine learning interatomic potentials for liquid alloy catalysts

***Yao Du**, yaodu@ksu.edu. Kansas State University, Manhattan, Kansas, United States*

Machine learning interatomic potentials (MLIPs) have emerged as a powerful tool for probing compositionally and configurationally complex systems, offering near-DFT accuracy at low computational cost. The Ga-Ni-Fe-Si liquid alloy system was chosen because this mixture has been used successfully to grow diamond crystals under atmospheric pressure. However, the chemical role of each elemental species and the crystal growth pathways remain unclear. The vast configurational possibilities for this multi-component system make standard quantum mechanical methods costly and inefficient.
In this work, we used the Allegro package to develop an MLIP. Allegro employs an E(3)-equivariant convolution for interactions among geometric tensors, enabling training on more information-rich and faithful representations of atomic environments. The potential is trained on DFT data generated from ab initio molecular dynamics simulations of both pure liquid Ga and various binary, ternary, and quaternary Ga-Ni-Fe-Si alloy structures. The validated MLIP reproduces key liquid structural properties, including radial distribution functions for atomic pairs and the local coordination environment. The MLIP also remains stable during large-scale molecular dynamics simulations that are impractical with direct DFT calculations.
Using this MLIP, we investigated the atomic-scale roles of individual alloying elements in the liquid catalyst. The simulations show that Ga serves as the liquid-state solvent for the transition-metal species. Fe atoms strongly tend to form short-range clusters, whereas Ni atoms remain dispersed throughout the liquid alloy. These distinct local environments shape the distribution and mobility of catalytic sites. Simulations of methane decomposition further indicate that Ni provides the preferred active sites for C-H bond activation, supplying carbon species for subsequent diamond nucleation. In addition, Si atoms stabilize the initial sp3 carbon configurations during the early stage of diamond-like bonding in the liquid alloy catalyst.
The developed MLIP extends molecular dynamics simulations to larger system sizes and longer time scales, enabling systematic investigation of the roles of individual alloying elements and laying the groundwork for future studies of diamond nucleation.

MWRM 2026 MW193

Mapping molecular heterogeneity and interfacial anisotropy in biomolecular condensates using single-fluorogen imaging

***Matthew D. Lew**, mdlew@wustl.edu. Electrical & Systems Engineering, Washington University in St Louis, St. Louis, Missouri, United States*

The material properties and biological functions of biomolecular condensates emerge from collective molecular interactions that create heterogeneous and anisotropic

organization at the nanoscale. We combine environmentally sensitive fluorogens with single-molecule tracking, super-resolution imaging, and orientation-sensitive microscopy to visualize the local environments, structures, and dynamics hidden within protein- and RNA-based condensates.

In condensates formed by intrinsically disordered proteins, freely diffusing fluorogens transiently illuminate distinct molecular environments without requiring covalent labels. Single-fluorogen localization and tracking reveal slow-moving nanoscale clusters surrounded by faster dispersed molecules. Measurements using solvatochromic probes further show that these clusters are more hydrophobic than the surrounding condensate interior, providing direct experimental support for describing condensates as spatially heterogeneous network fluids.

At the interfaces of RNA-based condensates, fluorogenic probes reveal direction-dependent molecular motion. Purine-rich scaffold RNAs drive phase separation, whereas more weakly interacting pyrimidine-rich RNAs adsorb to and wet condensate interfaces. Single-molecule trajectories show faster motion parallel to the interface than perpendicular to it, linking differential molecular interactions to interfacial anisotropy.

Together, these studies demonstrate how single fluorogens can serve as nanoscale reporters of chemical environment, translational dynamics, and molecular organization. Our imaging approaches expose structural and dynamical features that are obscured by ensemble measurements, offering new tools for connecting molecular interactions to the mesoscale properties of biomolecular condensates.

MWRM 2026 MW154

Measuring and understanding how organic electrolytes impact molecular europium redox chemistry

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Organic electrolytes are useful for studying redox chemistry, but understanding the influence of electrolyte properties on the electroanalytical data that result from measurements of molecular redox chemistry has not received the attention it deserves. In this presentation, the results of a joint experimental-theoretical study of the conductivities of acetonitrile-solvent-based organic electrolytes will be discussed. Measurements of conductivity have been carried out with a calibrated Jones-geometry device on the following supporting-electrolyte salts of tetrabutylammonium ($NBu4^+$, TBA^+): hexaflurophosphate (PF_6^-), trifluoromethanesulfonate ($CF_3SO_3^-$, OTf^-), bis(trifluoromethanesulfonyl)imide ($N(SO_2CF_3)_2^-$, $TFSI^-$), and tetrakis[3,5-bis(trifluoromethyl)phenyl]borate ($BArF_{24}^-$). The results show that the identity of the anion impacts the conductivity (measured in S cm^{-1}) of the electrolyte, as does the concentration of the individual electrolytes. Measurements of conductivity carried out

upon dilution of standard solutions with more-polar acetonitrile and less-polar diethyl ether have been used to interrogate the behaviors in different solvent dielectric environments. Results from computational molecular dynamics afford mechanistic insights into the specific role of the structures of the anions in driving interactions with cations and the solution environment. Predictive relationships are being sought in order to facilitate design of improved (higher conductivity) electrolytes as well. Our latest results will be discussed, including application of the studied electrolytes to electroanalytical characterization of europium triflate ($Eu(OTf)_3$), an effort aimed at interrogating how the electrolytes impact Eu(III)/Eu(II) redox cycling. Taken together, the results described here offer insights into how seemingly similar electrolytes behave in varying environments and drive unique solution properties.

MWRM 2026 MW232

Measuring Hammett substituent constants with a sensitive organometallic ^{13}C NMR reporter

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Hammett parameters (σ constants) provide the most widely used quantitative measure of substituent electronic effects in aromatic compounds. Originally developed to describe the influence of *meta*- and *para*-substituents on the ionization equilibria of benzoic acids, they continue to serve as a fundamental framework for understanding structure–property relationships. Recent experimental and computational studies have renewed interest in refining these parameters, yet significant ambiguities persist. For example, reported σ_p values for the $–NMe_2$ substituent range from −0.21 to −1.05. Moreover, the most authoritative experimental compilation assigns σ_p values of −0.83 for $–NMe_2$ and −0.72 for $–NEt_2$, an ordering that is chemically counterintuitive, whereas a recent machine-learning approach assigned an identical σ_p value of −0.75 to both substituents. In this poster, we report the synthesis and characterization of a series of new azulenes bearing –NHMe, $–NMe_2$, or $–NEt_2$ substituents at the 6-position and a [$–NCCr(CO)_5$] spectroscopic handle at the 2-position of the azulenic scaffold. The [$–NCCr(CO)_5$] moiety serves as a remarkably sensitive ^{13}C NMR reporter through its $\delta(^{13}CO)$ and $\delta(^{13}CN)$ chemical shifts, thus enabling not only quantitative measurement of electronic communication across the 2,6-azulenic π-system but also extraction of effective Hammett constants for dialkylamino and other substituents. The resulting σ_{eff} values resolve the long-standing discrepancies surrounding dialkylamino substituents. In contrast to both previous experimental assignments and the machine-learning model, our ^{13}C NMR reporter unambiguously differentiates $–NMe_2$ and $–NEt_2$ on the basis of their net electron-donating abilities and places them on the conventional Hammett scale in a manner consistent with chemical intuition.

MWRM 2026 MW202

Mechanically transparent seams and coatings: A solvent-free dual-network approach

***Gabriela Moreira Lana**, gmoreiralana@mst.edu. Chemical and biochemical Engineering, Missouri University of Science and Technology, Rolla, Missouri, United States*

Soft and stretchable materials are widely used in textiles, wearable devices, and protective systems, but bonding and adding functionality to these materials without altering their native mechanical response remains a central challenge. Conventional seams, adhesives, and coatings often introduce stiff or poorly integrated interfacial layers that create stress concentrations, reduce stretchability, or require solvent-intensive processing. Here, we present a solvent-free dual-network elastomer design strategy for creating functional soft interfaces that mechanically match the underlying material while adding targeted properties, creating a “mechanically transparent” interface. This approach combines self-assembled ABA triblock copolymers, which provide physically associated hard domains, with an in situ photopolymerized secondary network formed from a reactive diluent. In mechanically transparent seam systems, this architecture enables stretchable adherends to be joined while preserving their nonlinear deformation response and adding sealing behavior and resistance to environmental exposure. We further extend the same framework to solvent-free protective coatings using a bio-based material that generates hydrophobic surfaces with tunable mechanical properties. Together, these studies establish a modular route to solvent-free seams and coatings that preserve the mechanics of soft substrates while adding functionality such as sealing, environmental resistance, and hydrophobicity.

MWRM 2026 MW393

Mechanistic study of propene metathesis on heterogenous catalyst

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The growing scarcity of propene, a critical feedstock in the petrochemical and polymer industries, has spurred interest in its production via olefin metathesis, a reaction mechanistically opposite to the Phillips Triolefin Process. An important issue that hinders progress in this direction is the limited understanding of the reaction mechanism by the tungsten oxide ($W(=O)_2$) on silica catalyst, due to the structural complexity of the amorphous support, which correlates with the activity of the sites. In this work, we employ density functional theory (DFT) calculations on cluster models of WO_2-doped amorphous silica to elucidate the complete mechanism of propene metathesis and provide structures and energetics of transition states and metallacyclobutane intermediates. We focus first on the activation stage, where the $W(=O)_2$ site reacts with 2-butene via a [2+2] cycloaddition to form a metallacyclobutane intermediate. This

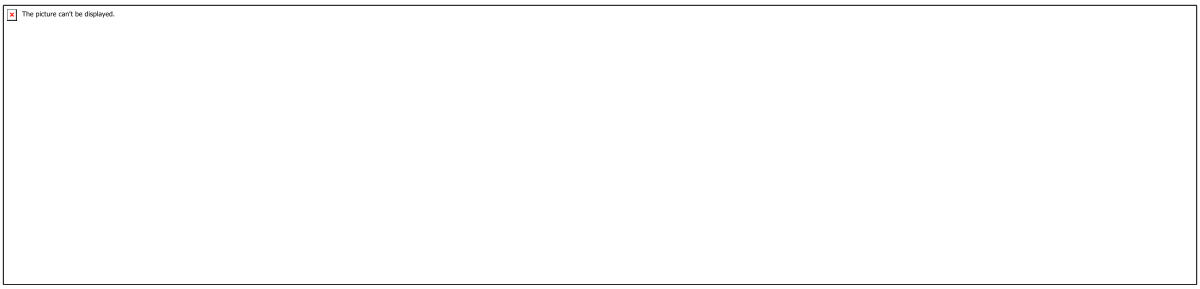
intermediate subsequently undergoes cycloreversion to generate a catalytically active tungsten-carbene species which has energy higher than that of the starting materials. This is consistent with the experimental data that the active metal-carbene is transient and readily proceeds into the propagation stage. Furthermore, we investigate the energy barriers of the propagation cycle to form propene. The results show that the propagation cycle proceeds kinetically faster than the activation stage and follows the Herrison and Chauvin metathesis mechanism. We also want to design potentially better catalysts than the original WO_2 - silica catalyst by introducing activity promoters. Ongoing work is focused on elucidating the same reaction mechanism on realistic models of the amorphous support, and extending these studies to bimetallic systems to evaluate the role of the secondary metal in the enhancement of the catalytic activity.

MWRM 2026 MW122

Mechanochemical control of divergent carboxylic acid activation: Selective formation of N-acylsuccinimides and anhydrides

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Mechanochemical synthesis can promote reactions with improved sustainability profiles while simultaneously providing reaction environments that are difficult to reproduce under conventional solution-phase conditions. Beyond accelerating known reactions, variation of milling parameters can redirect reaction pathways and provide an unusual means of controlling product selectivity.
Here, we report the phosphonium-mediated mechanochemical activation of carboxylic acids through a divergent process that selectively affords either N-acylsuccinimides through C–N bond formation or symmetrical anhydrides through C–O bond formation. Both product classes are useful activated carboxylic acid derivatives that can serve as intermediates or acyl-transfer reagents in subsequent synthetic transformations. Remarkably, the reaction outcome can be redirected simply by changing the number and size of the grinding balls under otherwise identical conditions. These observations illustrate how mechanochemical parameters can influence competing reaction pathways and reveal reactivity that is not readily accessible under conventional conditions. Control experiments were conducted to investigate the origins of this divergence and to distinguish the effects of reagent composition, mixing, milling time, and mechanical energy input on product formation. The observed selectivity is also being compared with calculated reaction energetics to determine whether the divergent outcome arises from product thermodynamics, kinetic differences between competing pathways, or changes in the formation and reactivity of activated acyl intermediates. Overall, this study demonstrates that milling parameters can provide a practical means of controlling C–N versus C–O bond formation from a common carboxylic acid precursor and may offer broader design principles for divergent mechanochemical synthesis.



MWRM 2026 MW273

Mesopore-confinement enhances selective polyolefin hydrogenolysis

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Catalytic hydrogenolysis offers a promising route for converting waste polyolefins into valuable hydrocarbon products. However, conventional Ru catalysts often produce substantial amounts of methane, reducing carbon efficiency and limiting selectivity toward liquid products. We developed a mesopore-confined Ru catalyst comprising ruthenium nanoparticles confined within a mesoporous silica framework supported on reduced graphene oxide. The confined catalyst exhibits significantly enhanced performance in polyethylene hydrogenolysis, providing substantially higher wax production rates while suppressing methane formation compared to non-confined Ru catalysts. Kinetic studies reveal that mesopore confinement alters the hydrogen-pressure dependence of the reaction and promotes selective mid-chain C–C bond cleavage. In addition, decreasing pore diameter further improves wax selectivity and reduces methane yield. These results demonstrate that catalyst architecture and nanoscale confinement can strongly influence both the activity and selectivity of polyolefin hydrogenolysis. Mesoporous confinement provides an effective strategy for improving the conversion of waste plastics into liquid hydrocarbon products while minimizing undesired gas formation.

MWRM 2026 MW362

Metabolism-guided design of integrated electro-biomanufacturing systems

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The integration of electrocatalysis with microbial metabolism offers a promising strategy for converting renewable electricity and captured carbon into sustainable fuels and

materials. While significant effort has focused on improving electrocatalytic carbon conversion, comparatively little attention has been devoted to understanding how electrochemically generated substrates influence intracellular metabolism and ultimately determine the performance of integrated electro-biological systems. We hypothesize that cellular metabolism should be regarded not merely as the downstream consumer of electrochemical products, but as a guiding principle for the design of electro-biomanufacturing platforms.
To explore this concept, we developed integrated electro-biological systems that couple CO_2 electroreduction with engineered microbial production of polyhydroxyalkanoate bioplastics and diesel-range lipids. Systems-level metabolic analyses revealed that electrochemically generated C2 intermediates reshape cellular physiology beyond serving as carbon sources, influencing ATP homeostasis, intracellular redox balance, carbon partitioning, and acid stress. These insights identified the fundamental metabolic constraints governing efficient utilization of electrochemical products and guided metabolic engineering strategies to improve carbon conversion. In parallel, electrocatalyst compositions were optimized to generate product distributions that better matched microbial metabolic capabilities, enabling synergistic co-design of catalyst performance and cellular metabolism.
Together, these studies suggest that the success of integrated electro-biomanufacturing depends on understanding how microbial metabolism responds to electrochemically generated chemical environments. Rather than independently optimizing electrocatalysis and biocatalysis, a metabolism-guided design framework provides a foundation for engineering more efficient electro-biological systems and expands opportunities to translate renewable electricity and captured CO2 into a broad range of sustainable fuels and materials.

MWRM 2026 MW380

Metal-doped semiconducting polymer nanoparticles for bioanalysis and cancer treatment

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Semiconducting polymer nanoparticles, commonly referred to as polymer dots (Pdots), possess high fluorescence brightness, excellent photostability, tunable optical properties, and readily modifiable surfaces. Incorporating metal ions into Pdots further expands their functionality by introducing metal-dependent optical, mass-spectrometric, and catalytic properties. In this work, we present a versatile strategy for preparing metal-doped or metal-coordinated Pdots and demonstrate their applications in chemical sensing, cellular analysis, and cancer therapy.

MWRM 2026 MW420

Metal ion-induced large fragment deactivation: A new strategy for site-selective fluorination in complex molecules

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Complex natural product functionalizations generally involve the use of highly engineered reagents, catalysts, or enzymes to react exclusively at a desired site through lowering of a select transition state energy. In this presentation, we report a complementary strategy in which all transition states representing undesirable sites in complex substrates are simultaneously energetically increased through the chelation of a metal ion to the fragment we wish to neutralize. In the case of electrophilic, radical-based fluorination reactions, charge repulsion, induced steric effects, and electron withdrawal provide the necessary deactivation and proof of principle. Ionophoric antibiotics of topical interest, including monensin, maduramicin, and salinomycin proved to be attractive targets through highly selective reactions that yield products of pharmaceutical, biochemical, and physical organic interest.



MWRM 2026 MW39

Metal-metal bonded vanadium, chromium, and molybdenum complexes supported by redox-active tetradentate ligands

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In this talk, I will describe our recent efforts to develop metal-metal bonded complexes using a series of acyclic and triaryl tetradentate ligands derived from *o*-phenylenediamide. These ligands are dianionic in their fully reduced form, but we have

demonstrated previously how the *o*-phenylenediamide subunit can undergo sequential one-electron oxidations when bound to metals like Ni and Ru. The goal of this work is to determine if similar ligand-centered redox activity is accessible in metal-metal bonded complexes with group 5 and 6 transition metals. I will show how variations to the L-type flanking donor groups (*e.g.*, NMe_2, SMe, OMe) impact the nuclearity and structures of divalent complexes prepared with vanadium and chromium. I will also show how metal-metal bonded divanadium complexes can activate dinitrogen and cleave strong N-N bonds in other nitrogen-containing substrates like azobenzene. Preliminary efforts aimed at preparing low-valent dimolybdenum complexes will also be presented along with supporting crystal structures, spectroscopic data, and theoretical calculations.

MWRM 2026 MW438

Method-dependent variability in µ-FTIR microplastic analysis: Effects of scan area, spectral resolution, and library composition

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Micro-Fourier transform infrared (µ-FTIR) spectroscopy is widely used for microplastic analysis, yet differences in mapping design, spectral acquisition, and reference-library composition can limit comparability among studies. This study evaluates how mapped section size, spectral resolution, and library composition affect particle detection, size representation, and polymer identification in environmental samples. The study design includes the analysis of field samples and lab-generated samples on anodisc filters in transmission mode to assess the effects of these operational parameters. A comparison of the selection of scan areas of 2 and 4-mm^2 sections to cover 20% area of the filter at spectral resolutions of 4 and 8 cm^{-1}, with counts normalized to the actual analyzed area was performed. Spectra are matched at a 70% threshold against commercial library and in-house generated libraries that included Pristine, UV-aged and chemically treated polymer spectra to represent the effects of environmental weathering and sample treatment approaches used in microplastic studies on polymer identification. Preliminary results demonstrate clear method sensitivity. The 2-mm^2 design detected 7.06 particles mm^{-2} compared with 3.68 particles mm^{-2} for 4-mm^2 sections, a 92% increase after area normalization and represented a greater proportion of 50-100 µm particles. Library expansion also substantially changed identification outcomes. Compared with commercial library alone, the extended library newly identified 12-46 particles and reassigned 3-17 previously identified particles across acquisition conditions. Adding pristine spectra produced 0-22 new identifications and 0-10 reassignments; UV-aged spectra produced 8-20 and 1-6, respectively; and chemically treated spectra produced 2-8 and 1-2. These findings indicate that both acquisition design and inclusion of environmentally altered polymer spectra affect apparent microplastic abundance and assigned polymer identity. The completed study will support standardized µ-FTIR analysis, library construction, and transparent reporting for microplastics.

MWRM 2026 MW158

Microbial and electro-microbial design for efficient carbon utilization

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Sustainability and climate change are major challenges facing our generation. Algal carbon capture and utilization offer a potential solution, but algal bioproduction has been hindered by low light penetration and high harvesting and production costs. We addressed these challenges by integrating artificial intelligence and synthetic biology, using two machine learning models to predict light penetration and growth rate. Integrating these models allowed us to predict maximized growth at the optimal density, guiding development of a semi-continuous cultivation (SAC) system that substantially improved cell growth rate. We also engineered a rapidly growing strain, *Synechococcus elongatus* UTEX 2973, enabling low-cost harvest and continuous cultivation. This semi-continuous cultivation approach unleashed cyanobacterial growth and carbon utilization potential, achieving 0.1 g/L/hour biomass productivity and 0.2 mg/L/hour limonene productivity in photobioreactors. Reconfiguring this system in an outdoor pond achieved a record 43.3 g/m2/day biomass yield, translating to a minimum biomass selling price of $281/ton, making algal carbon utilization economically viable.
While cyanobacteria are among the most efficient carbon utilization platforms, photosynthesis inefficiency still limits their potential. Our recent work shows that electrocatalytic CO2 reduction (CO2RR), coupled to bioconversion, can substantially improve solar-to-molecule conversion. We designed electrocatalysis, the chem-bio interface, and microorganisms together to enable efficient electro-microbial conversion using C2 intermediates (EMC2). Soluble C2 intermediates enable rapid mass transfer, readily enter primary metabolism, carry more energy and electrons, and serve as better molecular building blocks. This EMC2 design achieved 6x and 8x increases in microbial biomass productivity compared to C1-intermediate and hydrogen-driven routes, respectively, and enabled integrated, continuous, rapid biomass and PHA production from CO2 at record productivity. Building upon this success, we also co-designed electrocatalysis and bioconversion to build an electrobiodiesel route, achieving a record CO2-to-fatty-acid yield (1,840.2±3.3 g/L/day) and 4.4% solar-energy-to-molecule conversion efficiency for CO2-to-lipid conversion, using 45x less land than soybean biodiesel with competitive economics and substantial emissions reduction.

MWRM 2026 MW389

Microfluidic mixing of the high viscosity urethane forming reaction of PTMEG and H12-MDI

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The challenges associated with processing highly viscous reactive mixtures in microfluidic systems were investigated using the synthesis of an industrially relevant polyurethane prepolymer from PTMEG-2000 and H12-MDI as a model reaction. Continuous experiments conducted in a quartz microfluidic reactor chip with passive serpentine mixing geometry exhibited substantial deviations in both viscosity evolution and kinetic behavior relative to well-mixed batch operations. Visibly separate layers in the effluent comprised different NCO compositions, indicating inadequate homogenization within the microfluidic system, consistent with low Reynolds and Dean numbers. Although mixing of the effluent, before further reaction, restored kinetic behavior comparable to batch experiments, viscosity differences persisted, suggesting structural differences in the resulting polymer products. GPC analysis supported this hypothesis by revealing that higher viscosities did not correlate with elevated molecular weights. These results demonstrate that passive microfluidic mixing strategies commonly employed for low-viscosity systems may be inadequate for highly viscous polymerizing systems.

MWRM 2026 MW70

Microscale surface ion conduction: Expanding the capabilities of porous biosensors

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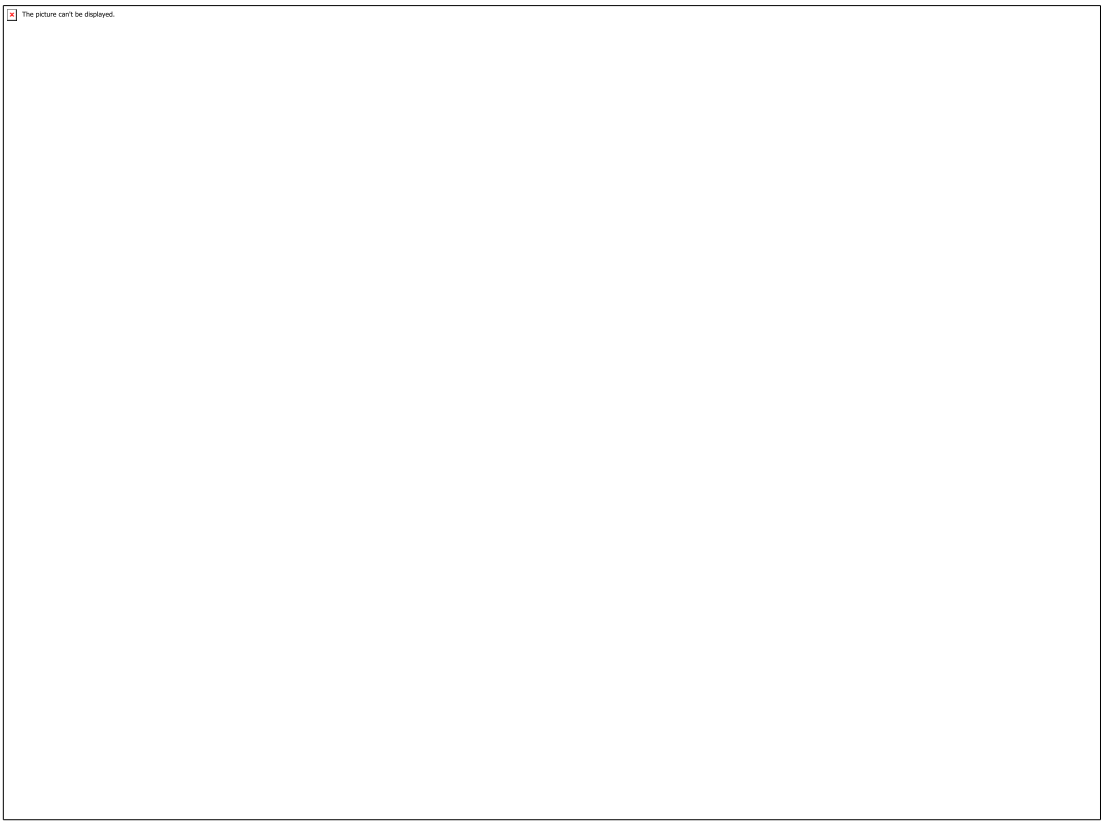
Surface ion conduction provides a label-free electrical transduction mechanism in which analyte binding perturbs ionic transport at a charged interface. Conventional ion-conduction sensors are typically confined to nanopores. We have developed microscale surface ion conduction (μSIC), which leverages microporous sensing elements to unlock sensing capabilities inaccessible to nanopore-based sensors while maintaining sensitive detection.

Using probe-functionalized packed beds of microparticles, μSIC has enabled label-free detection of single-stranded DNA, viral RNA, antibodies, and whole virions in undiluted

saliva. This principle was extended to the detection of per- and polyfluoroalkyl substances (PFASs) in tap water using chromatographic media as the sensing element, demonstrating that μSIC can exploit established partitioning interactions for sensing. Taking advantage of the ability of the micropores to accommodate thick coatings and microscale targets, we incorporated bacterially imprinted polymer-coated beads to sense *Escherichia coli*. These findings reveal that nanoscale confinement is not required for sensitive surface ion conduction sensing and that large analytes can generate strong signals despite residing well beyond the electrical double layer.

The flow-through architecture of μSIC also enables integration with electrokinetic enrichment. Faradaic ion concentration polarization (fICP) concentrates analytes within the sensing bed by several hundred-fold, whereas ICP has produced >1000-fold enrichment, yielding femtomolar detection of ssDNA. Unlike fICP, ICP is applicable to a broad range of electrolytes, including environmental waters and biofluids.

Finally, we are investigating how porous architecture governs μSIC. Preliminary studies in additional microporous materials examine the effects of pore size, network organization, and nanoscale constrictions on surface ion conduction. These studies aim to establish governing principles for rationally tailoring porous sensing substrates to specific analytes, sample matrices, and applications.



MWRM 2026 MW296

Microstructural diversity through Brook rearrangement polymerization

***Alec Lininger**, aleclininger428@hotmail.com, Aaron Teator. Chemistry, The University of Kansas, Lawrence, Kansas, United States*

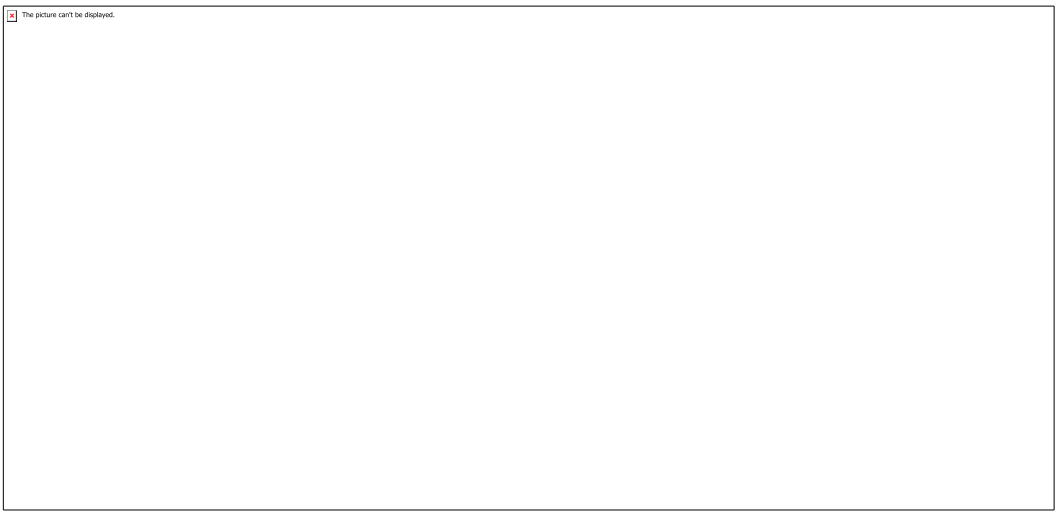
Modern polymerization techniques often require an olefin within the starting monomer for initiation and propagation to occur. While efficient, these techniques limit the microstructure to only certain functionalities and a two-carbon backbone repeating unit. To access a greater number of polymer microstructures in order to produce polymers with different functionalities, a novel method must be accessed. “Through-space” anion relay chemistry via Brook Rearrangement is a method that would allow access to a range of microstructures when used for polymerization that could not be accessed through different means, including variation of carbon number in the backbone as well as tolerance toward various functional groups. This unique application of rearrangement chemistry for propagation has allowed access to novel polymer structures, expanding upon known polymer functionalities and thermal properties.

MWRM 2026 MW174

Modulating hole transport properties in PAHs: Substitution-driven optoelectronic tuning

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The efficiency of perovskite solar cells hinges on the development of advanced materials capable of facile charge transport. Polycyclic aromatic hydrocarbons (PAHs) are promising materials for hole transport layers (HTLs) due to their planarity, extended π-conjugation, and thermal and chemical stability. However, the relationship between subtle structural variations and charge transport efficiency remains poorly understood. This research details the synthesis and characterization of two regioisomeric PAH derivatives designed for initial investigation into the impact of changes in molecular geometry on optoelectronic properties. A Diels-Alder cycloaddition reaction was employed to extend an acenaphthene dimer core, which was previously synthesized by our group and demonstrated to be a high-efficiency HTL candidate. Subsequent functionalization via a Buchwald-Hartwig amination was utilized to introduce alkoxydiarylamino moieties for improved solubility and optimized frontier molecular orbital alignment. Density functional theory (DFT) calculations were used to model the optimized geometries and predict the HOMO-LUMO energy levels. Spectroscopic methods were used to determine the UV-Visible absorption, fluorescence, and optical band gap of the synthetic products. This study establishes the utility of precise molecular design in modulating the optoelectronic properties of HTLs, providing a framework for the future development of high-efficiency perovskite solar cells.



Structures of regioisomeric products 1 and 2.

MWRM 2026 MW414

Molecular dynamics modeling of concentrated aqueous solutions at salt surfaces: The role of explicit polarizability

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Prior work in our group has shown the impact of ionic crystal surfaces on electrolyte structure and dynamics using pairwise potentials in classical molecular dynamics simulations. While believed to be accurate for structural studies, such models are known to be inaccurate in predicting ion transport properties. To quantify these discrepancies at interfaces relevant to energy storage technologies, we explore both polarizable and non-polarizable solvent models for the well-studied system of water with monatomic salts at crystal interfaces. Popular water models used in molecular dynamics simulations give each atom a fixed charge, but real ions and water molecules can shift their electron clouds in response to nearby charges, a property called polarizability. In this work, we compare two non-polarizable water models, SPC/E and TIP4P, with the SWM4-NDP Drude model to study how Li^+ and Cl^- ions arrange at the salt interface and at graphite. LiCl solutions are prepared across a wide range of concentrations, from dilute conditions to much higher concentrations. This work explores whether polarizability leads to a more accurate description of Li^+ and Cl^- ion behavior at the interface and connections with current experiments on highly concentrated aqueous solutions for energy storage.

MWRM 2026 MW131

Molecular probes for decoding NTMT1 biology: From substrate discovery to real-time targeted protein degradation

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NTMT1 methylates protein N-termini and regulates mitosis, chromatin interactions, DNA repair, and genome stability. Although dysregulated in cancer, its substrates and cellular functions remain incompletely defined. We combined molecular probes to discover NTMT1 substrates, selectively deplete the enzyme, define proteome-wide responses, and measure degradation in living cells. An improved synthesis of the clickable cofactor analogue Hey-SAM achieved approximately 98% conversion from S-adenosyl-L-homocysteine (SAH). Chemical proteomics of Hey-SAM profiling identified 72 putative substrates, among which CRISPR-Cas9 knockout controls and mass spectrometry established Obg-like ATPase 1 (OLA1) as an NTMT1 substrate in cells. Converting an NTMT1 inhibitor into a VHL-recruiting proteolysis-targeting chimera (PROTAC) produced the first-in-class NTMT1 degrader, reducing NTMT1 selectively in time- and dose-dependent manners in HCT116 and HT29 colorectal carcinoma cells and reaching a DC_{50} of 7.53 μM and > 90% maximal degradation in HCT116 cells. Compared with an inhibitor control, label-free quantitative global proteomics detected changes in over 1,800 proteins after degrader treatment. Calreticulin, an immunogenic cell-death signal, increased by approximately 50% and was confirmed by immunoblotting, providing a systems-level view of the response to NTMT1 depletion. Finally, CRISPR knock-in of HiBiT at the endogenous NTMT1, paired with transient LgBiT expression, enabled continuous NanoBiT monitoring in live HCT116 cells. The system preserved NTMT1 function, resolved concentration-dependent degradation over 24 hours, and revealed high-concentration signal artifacts from degrader precipitation. Together, these platforms connect substrate mapping, selective perturbation, proteomic mechanism discovery, and real-time pharmacodynamic measurement to advance NTMT1-directed probes and potential therapeutics.

MWRM 2026 MW259

Molecules, molecular diagnostics, and the interplay between organic synthesis and functionalized electrodes

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Electrochemistry has long held potential as a tool for constructing a wide variety of organic molecules, and the organic chemistry community is both recognizing and impressively exploiting that potential with increasing regularity. Those efforts have taught us a great deal about how to think about electrochemical reactions and how to

use the technique to accomplish new transformations that enrich the synthetic enterprise.

The relationship between organic synthesis and electrochemistry can also be viewed in the opposite direction with the new synthetic chemistry being developed in order to facilitate exciting opportunities to expand the scope of electrochemical experiments. For example, new synthetic methods that allow for the site-selective generation of chemical reagents and catalysts have enabled the construction of complex molecular surfaces on addressable microelectrode arrays. These efforts have set the stage for developing the microelectrode arrays as analytical devices for rapidly screening the binding behavior of small molecule libraries with biological targets and developing rapid "point-of-care" diagnostics.

The exploration of these new electrochemical tools is beginning to “give back” to the synthetic arena. A number of preparative scale synthetic applications have now arisen based on the concept of site-selective reagent generation. These applications range from the use of paired electrochemical reactions for more sustainable reagent generation to the recent discovery that chemical reagents can be confined to specific regions within a preparative reaction; a development that offers a new strategy for controlling the selectivity of chemical transformations.

In the talk to be given, the interplay between organic synthesis and electrochemistry will be highlighted with an emphasis on lessons learned and challenges being undertaken.

MWRM 2026 MW365

Monomeric antigen-CD22l conjugates temporarily deplete cognate B cell subsets

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Autoantigen-reactive B cells are pathogenic in multiple autoimmune diseases, and restoring self-tolerance to this population is essential to prevent disease progression. Accomplishing this in a selective manner has been challenging, as many antigen-specific B cell tolerization
approaches have limited efficacy. In efforts to overcome this challenge, we have identified that conjugation of one or more sialic-acid derived, high-affinity CD22 ligands to a small protein antigen, proinsulin(F25D), temporarily depletes several insulin-binding B cell subsets in a murine model of type 1 diabetes where B cells function as pathogenic antigen-presenting cells. The impact of the conjugates’ architecture on binding and activity in vitro will be discussed along with the PK/PD profiles following single injections in transgenic NOD mice. Beyond supporting the development of

antigen-specific treatments for autoimmune disease, the activity of monomeric antigen-CD22L conjugates grants insights as to how the presence of native CD22 ligands on protein antigens may affect B cell responses in health and disease.

MWRM 2026 MW391

Multicomponent constrained nuclear-electronic orbital wavefunction methods: Development and applications of CNEO-MP2 and CNEO-CCSD

***Gabrielle B. Tucker**, gabriellebrieanna@gmail.com, Kurt Brorsen. Chemistry, University of Missouri, Columbia, Missouri, United States*

Molecular geometries and properties can be influenced significantly by nuclear quantum effects like vibrational averaging, zero-point energy, and isotopic substitution. As experimentally measured properties inherently include these and other important nuclear quantum effects, it is desirable to develop electronic structure methods capable of including these effects to facilitate more direct comparison between experiment and theory. One class of electronic structure methods capable of incorporating these effects is that of multicomponent methods, in which more than one component of the system can be treated at the same level quantum mechanically. Both density functional theory and wave-function based multicomponent methods have been introduced in a variety of multicomponent frameworks in recent years. Here we detail the development and application of our recently developed second order Møller-Plesset perturbation theory method within the constrained nuclear-electronic orbital multicomponent framework, and its preliminary extension to the coupled cluster singles and doubles level. We also present recent work in applying constrained nuclear-electronic orbital methods to homogenous and heterogenous hydrogen and halogen bonded dimer systems.

MWRM 2026 MW351

Multi-field spin-matrix workflow for measuring and interpreting carbohydrate ^{1}H NMR spectra

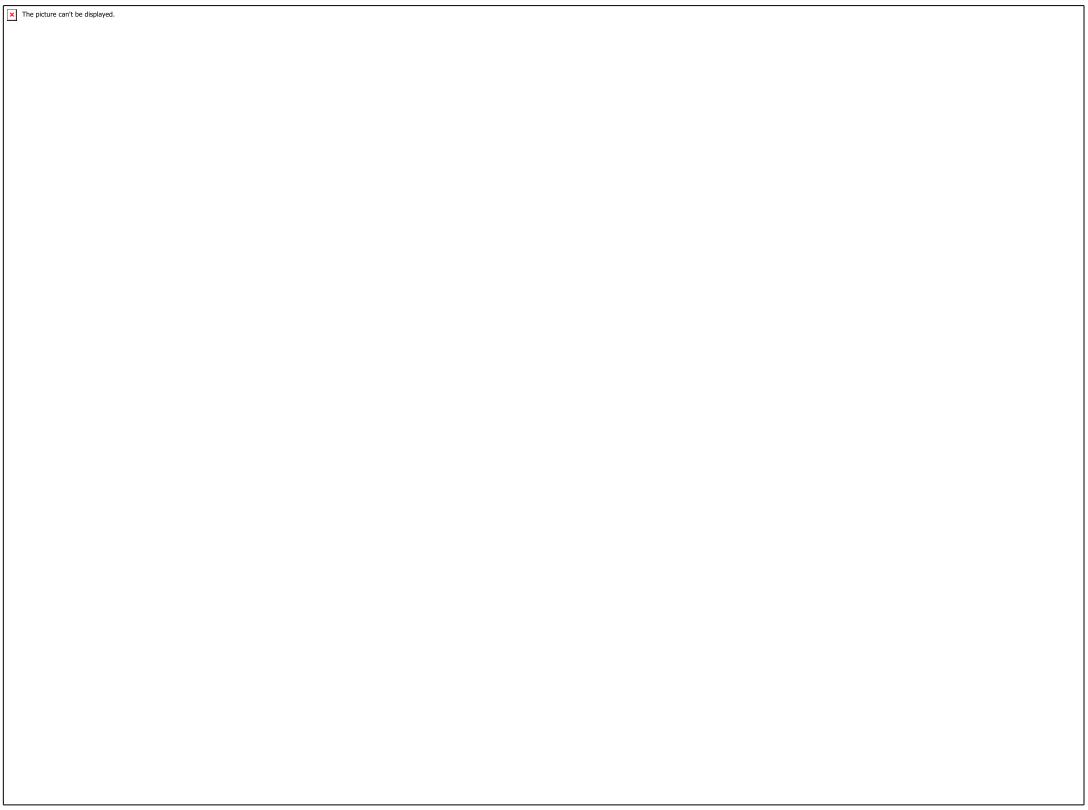
***Ceceilia Hedrick**[1,2,3], cecehedrick@gmail.com, Stephanann Costello[4,3], Arthur S. Edison[4,3]. (1) Chemistry, University of Nebraska Omaha, Omaha, Nebraska, United States(2) Bioinformatics, University of Georgia, Athens, Georgia, United States(3) University of Georgia Complex Carbohydrate Research Center, Athens, Georgia, United States(4) Biochemistry and Molecular Biology, University of Georgia, Athens, Georgia, United States*

Carbohydrate ^{1}H NMR spectra contain extensive peak overlap, multiple anomeric forms, and acquisition-dependent line shapes that complicate quantitative interpretation. We developed a reproducible workflow combining DSS-referenced spectra, parameterized quantum-mechanical spin matrices, and independent spectral simulations to evaluate carbohydrate measurements across magnetic fields.

Alanine was first used as a controlled AX_3 calibration system. Its known four-spin topology, Hα and methyl chemical shifts, and approximately 7.2-Hz Hα–CH_3 coupling provided an analytical doublet/quartet benchmark. At 600 and 900 MHz, both direct Spinach FID-to-FFT simulations and analytical AX_3 theory agreed with reference spectra with correlations near 0.97. This validated field referencing, Hz-to-ppm conversion, linewidth and phase handling, and field transfer before analyzing more complex carbohydrates.

For sucrose, a deposited 14-spin GISSMO/BMRB matrix was refined using 600- and 900-MHz spectra and tested blindly at 800 and 1100 MHz. The refined model gave correlations of 0.9957 and 0.9945 for the training fields and 0.9428 and 0.9794 for the held-out fields.
The workflow was also applied to two unidentified samples. Mystery Sugar 1 was consistent with a two-component D-xylose model, with correlations of 0.9249, 0.9159, and 0.9007 at 600, 900, and 1100 MHz, respectively. Mystery Sugar 2 was consistent with a two-anomer mannose model, but this result remains provisional because its atom assignments and coupling constants require additional validation.

This workflow provides a transparent strategy for measuring, validating, and improving carbohydrate spin matrices across NMR field strengths.



Sucrose ^{1}H spectra at 600, 800, 900, and 1100 MHz shown on a common DSS-referenced axis. Experimental spectra (olive), refined Spinach fits (red dashed), and published GISSMO simulations (blue dotted) are compared.

MWRM 2026 MW76

Multifunctional alginate-corn starch hydrogel beads for enhanced soil water retention and delivery of bioinoculants in agricultural soils

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Soil evaporative water loss and limited soil water holding capacity reduce agricultural water use efficiency by decreasing the period during which moisture remains available to plant roots, thereby constraining crop productivity under drought-stressed conditions. This research develops a shelf-stable, rehydratable alginate-based hydrogel bead that is optimized for water retention in the soil. The bead was designed to provide repeated water uptake after drying, extend soil moisture availability, while creating a protected, nutrient-rich microenvironment that supports the survival and activity of encapsulated microbial inoculants that further improve soil health. Beads were produced by ionic gelation of sodium alginate with calcium chloride to form a crosslinked calcium–alginate hydrogel network. Corn starch was incorporated to improve water uptake and address the poor rehydration commonly observed in dried calcium–alginate materials. Glycerol was added as a plasticizer to reduce brittleness and maintain bead integrity during drying and rewetting, while tryptic soy broth served as an internal nutrient source to support bacterial survival and growth after rehydration in the soil. The effects of corn starch concentration, glycerol concentration, calcium chloride concentration, and crosslinking time on bead rehydration were evaluated. Hydration performance was systematically tuned through formulation and crosslinking conditions. When applied to soil at 5% (w/w), the optimized formulation increased maximum soil moisture-holding capacity, extended the falling-rate drying period, and delayed the onset of the plant wilting-point moisture region. Encapsulated Bacillus subtilis remained viable after drying and rehydration and also produced soil-wetting metabolites in a simulated soil chemical environment. Overall, the beads integrate soil moisture retention, microbial delivery, and localized nutrient support within a single bio-degradable material, offering a promising soil amendment in drought stressed agricultural soils.

MWRM 2026 MW402

Multiscale modeling of the NarK nitrate/nitrite antiporter using adaptive-partitioning algorithms based on hierarchical truncated many-body expansion (PAP-HMBE)

***Julia Roma**, julia.moose@berkeley.edu, Bryce Westheimer, Emilie B. Guidez, Hai Lin. Chemistry, University of Colorado System, Denver, Colorado, United States*

The NarK antiporter operates in a wide variety of organisms by selectively transporting nitrate and nitrite ions across biological membranes in opposite directions, providing both a way for nitrogen nutrition to enter the cell and for toxic metabolites to be

expelled. Despite extensive biochemical investigations and crystal structure determinations, many details of Nark's transport mechanism remain elusive. Computer modeling can offer atom-level insights, complementing such experiments. For example, recent quantum modeling of the NarK binding sites revealed that in the R89K mutant, nitrite is trapped in the pore because it competes for a proton with the mutated lysine, disrupting the transport cycle, despite the arginine-to-lysine mutation preserving the charge. Such competition does not occur in the wild-type protein. This discovery highlights the importance of high accuracy quantum mechanical (QM) descriptions for the interactions between the ion and its surroundings. However, full high-level *ab initio* QM simulations of the protein are too computationally demanding to be feasible. In this work, we develop a novel multi-scale method to tackle this problem. We combine a recently proposed hierarchical many-body expansion (HMBE) method with the permutated adaptive-partitioning (PAP) algorithm that allows the description of atoms to be switched *on-the-fly* between different levels of theory (e.g. *ab initio* QM, semi-empirical QM, or even molecular mechanics) as needed. We present the preliminary results from our test calculations on a series of model systems. This advancement opens the door to more efficient modeling of diffusion processes in large and complex systems.

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MWRM 2026 MW329

N-acetylcysteine-modified chitosan/tannin-based coatings for titanium surface engineering

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Titanium and its alloys are widely used in biomedical implants due to their excellent mechanical properties, corrosion resistance, and biocompatibility. However, titanium surfaces do not inherently provide the biological functions required for optimal implant performance, including hemocompatibility and antimicrobial activity. Surface engineering strategies based on functional polymer coatings offer a promising approach to impart bioactivity while preserving the mechanical properties of titanium substrates. In this study, N-acetylcysteine-modified chitosan derivatives were synthesized through covalent modification of the primary amine groups of chitosan. Three derivatives with different degrees of modification (25, 31, and 45%) were obtained and characterized by nuclear magnetic resonance spectroscopy. The incorporation of N-acetylcysteine significantly improved chitosan solubility and processability while maintaining the cationic characteristics required for polyelectrolyte-based surface assembly. Based on these results, derivatives with the lowest and highest modification degrees were selected for titanium surface functionalization.
Multilayer coatings were fabricated on titanium substrates using layer-by-layer (LbL) assembly between cationic N-acetylcysteine-modified chitosan derivatives and anionic polyphenolic tannin-based polymers containing flavan-3-ol units. Titanium substrates were modified with either 5 or 15 bilayers to investigate the influence of coating thickness on surface coverage and physicochemical properties. Contact angle measurements showed a significant increase in surface wettability after coating deposition, with water contact angles decreasing from approximately 40° for unmodified and plasma-treated titanium to approximately 20 °. Energy-dispersive X-ray spectroscopy (EDS) spectra and elemental mapping confirmed the homogeneous deposition of polymeric coatings on titanium.
These results demonstrate the successful synthesis of functionalized chitosan derivatives and their application in the construction of polyphenolic-based multilayer coatings on titanium surfaces. Future studies will investigate the biological performance of these interfaces, including antimicrobial activity, protein adsorption, and hemocompatibility. This work establishes a versatile polymer-based strategy for developing multifunctional titanium interfaces for biomedical applications.

MWRM 2026 MW240 - Withdrawn

MWRM 2026 MW148

New insights into iron β-diketiminato complexes for their group transfer and multicomponent reactions

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Multicomponent reactions have great impact into building molecular complexity for their rapid implementation, atom economy, byproduct minimization, and more. Organometallic complexes with the β-diimines as ligands have supported the unique reactivity of low-valent transition metal complexes. The Neely lab has demonstrated isolable iron-imide complexes, a novel iron metallacycle, and other organoiron complexes have been implicated to have new reactivity. This work has sought to explore the reactivity of these low-valent iron complexes in the production of new organic products from a selection of unsaturated substrates. Particular focus was taken for the production of imidoyl ketenimines and their products through the selective application of a nitrogen source, an alkyne, and an isonitrile. Further insights into catalytic behavior as well as the preference for Iron to fulfill two-component coupling versus multicomponent reactions has been investigated. New routes towards multicomponent coupling have been explored while reaction conditions were optimized.

MWRM 2026 MW260

New strategies for photocatalytic bond activation of strong C-H bonds

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The activation of strong chemical bonds remains an important strategy for the conversion of abundant chemical feedstocks to value-added products. Photocatalysis continues to offer new methods for the activation of C–H, C–C and C–X bonds. We have developed photocatalytic C–H bond activation methods for the direct functionalization of hydrocarbons including adamantane and higher diamondoids, with a focus on achieving switchable regioselectivity via catalyst control. Recent advances in the regioselective functionalization of diamondoids will be described.

MWRM 2026 MW221

New training and professional development tools for bio/chemical analysis

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Over the last five years, Chemistry faculty at the University of Nebraska - Lincoln have developed several new tools and strategies for the training of STEM students and

professionals in the fields of analytical and bioanalytical chemistry. Two of these tools are coursework-based graduate certificate programs in chromatography and bioanalytical chemistry. In these programs, individuals use graduate courses in chemistry and other related fields to learn about and acquire training in key methods for chemical separations and analysis such as chromatography, mass spectrometry and NMR, in addition to training in fields such as chemical biology or materials science. These certificates, as developed in support of NSF-sponsored research in separation methods for bio/chemical analysis (CHE 2404209), have been taken by both students within chemistry as well as in other fields and by individuals in regional laboratories or industries, as is done through both in-person and remote teaching. In addition, two special lab practicums have been created to provide both coursework and hand-on training in some of these areas. One of these has a focus on liquid chromatography-mass spectrometry (LC-MS), using instrumentation recently acquired through the NSF (CHE 2447813). The second focuses on sized-based separation and analysis methods such as size-exclusion chromatography (SEC) and asymmetric flow field-flow fractionation (aFFFF) coupled with dynamic light scattering (DLS) and multiangle light scattering (MALS), as also acquired through NSF funding (CHE 2320239). All these novel education and training tools are being used to provide students and STEM workers in
STEM fields with background and working knowledge needed to apply these powerful methods for bio/chemical separations and analysis to new applications in fields ranging from material science and biomedical research to environmental studies.

MWRM 2026 MW171

Next generation of chemical screening libraries: From total synthesis of natural products to intermediate diversification: The story of Uvaretin and the Brocazine's

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Since its introduction in the 1908s, high-throughput screening (HTS) has remained a dominant force in drug discovery. The speed of automation in this process has rapidly increased the ability of researchers to identify new targets, scaffolds, and other clinically relevant materials. All HTS screens rely on one important item: the chemical screening library (CSL) being employed. Initially, these plates were populated with natural products and analogs accessed via total synthesis campaigns. Given the speed of HTS, more plates were needed, and most importantly, they needed to be populated with compounds; thus, entering the landscape of sp2-sp2 coupling resulting in flat compounds. These CSL have limited 3D structure, unlike natural products, and have led to the discovery of compounds with less cytotoxicity. Many groups have addressed this and generated new CSLs, each with multiple limitations. The most common limitation is the lack of a wide
diversity of cytotoxicity by these CSLs. Using the intermediates in our total synthesis

route, our lab has embarked on a new approach to generating CSLs. This pilot study will be presented employing our total synthesis route of uvaretin to generate a new CSL and the cytotoxicity assays from it, revealing a diverse and broad range of cytotoxicity in different cancerous cell lines. Furthermore, preliminary work will be presented on the creation of a more structurally complex CSL via our lab's efforts towards the brocazine family of natural products.

MWRM 2026 MW364

Next-generation plasmonic nanoparticles: Transforming biosensors and targeted therapeutics

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Plasmonic nanomaterials have emerged as powerful tools for bridging fundamental nanoscience with precision diagnostics and targeted therapeutics. This presentation will highlight our group's efforts to develop next generation plasmonic nanoparticles through three complementary research directions. First, we design and fabricate plasmonic nanostructures with precisely controlled structural and optical properties using advanced nanofabrication approaches supported by computational optimization. Establishing relationships between nanoparticle structure and function provides a foundation for producing reproducible, high-performance nanomaterials. Second, these engineered nanostructures are translated into plasmonic biosensing platforms for sensitive molecular detection and next-generation point-of-care diagnostics, with an emphasis on improving analytical performance and enabling rapid, reliable measurements. Finally, we apply these multifunctional nanostructures to targeted therapeutic systems that integrate molecular recognition with plasmonic functionality to improve treatment precision and therapeutic efficacy. These platforms are designed to support controlled therapeutic delivery, real-time monitoring, and enhanced treatment outcomes across a range of biomedical applications. Together, these research directions establish a unified framework that connects intelligent nanomaterial design, advanced biosensing, and targeted nanomedicine. By integrating fundamental nanoscience with translational applications, this work aims to advance plasmonic nanotechnology toward more precise, accessible, and clinically relevant diagnostic and therapeutic solutions.

MWRM 2026 MW204

Nitrogen insertion approaches to polymer backbone editing

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The development of controlled polymerization methods has broadly expanded the chemical space accessible for polymerization and enabled the production of well-

defined synthetic materials targeting numerous applications, including polyolefin thermoplastics and styrene-butadiene-styrene (SBS) rubber. These achievements represent decades of advancements in polymer technology; however, our ability to prepare materials with backbones comprised of functional groups beyond alkyl or ester chains remains limited. Novel materials featuring unique main-chain structures will be required to meet the rising demand for high-performance polymers that address contemporary challenges in materials science and sustainability. Direct macromolecular skeletal editing, or backbone editing, offers an alternative pathway to functional materials with unique molecular structure. This presentation will focus on our recent advancements in developing efficient, site-selective nitrogen insertion strategies for polymer backbone editing.

MWRM 2026 MW316

No time to waste: Rapid, selective, and mild depolymerization of poly(ethylene terephthalate)

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We demonstrate a rapid, selective in-tandem methanolytic-hydrolysis of poly(ethylene terephthalate) (PET) to monomers, dipotassium terephthalate and ethylene glycol, within 30 minutes at mild temperatures (60–70 °C) for milled, high-surface-area feedstocks; bulk articles such as injection molded bars undergo slower depolymerization, by a factor that we quantify through surface area-to-volume ratio (S/V), crystallinity, and surface reactivity effects. The augmented nucleophilicity of methoxide (CH_3O^-) in methanol-rich, water-lean conditions ($\chi_{H2O} \leq 0.23$; 0.5–1 N KOH in methanol) drives rapid surface denudation, sloughing saponified monomers, and continually exposing fresh surface for reaction. Complete depolymerization occurs in the vitreous state ($T_g \approx 60$–70 °C) despite the diminished bulk diffusivity of small molecules, likely confining reaction to the surface. Molecular dynamics simulations and experiments indicate that the CH_3O^- activates the ester carbonyls in a methanol-rich and water-lean low-dielectric environment through cooperative electrostatic effects. Increasing water content raises the dielectric constant and reduces the solution-phase diffusivity of the bulky hydrated CH_3O^-, suppressing depolymerization yields. Green chemistry metrics highlight an energy economy coefficient ($\eta = 5 \times 10^{-4}$ °C^{-1}min^{-1}) and a modified environmental energy impact factor ($\xi = 8400$ °Cmin) for 30 minutes at 60 °C, representing a 11-fold improvement in ξ over state-of-the-art methods while maintaining polyester selectivity. Mild, rapid chemical treatment confers polyester selectivity in mixed feedstocks, mitigating the sorting burden for post-consumer recyclate while producing monomers.



MWRM 2026 MW162

Novel enamine and imine analogs of 3-formylchromone and their cytotoxic effects

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3-Formylchromone is a compound that has shown anti-cancer properties in many different studies. The
mechanism behind its anti-cancer activities includes inhibiting proliferation and inducing apoptosis via the STAT3 signaling pathway. 3-formylchromone is an unstable intermediate, making it unusable to target cancer in the human body. Due to both the growing need for newer anti-cancer therapies, and the instability of 3-formylchromone, our research focuses on synthesizing new analogs of 3-formylchromone that can selectively target cancer cells.

The analog library was tested at various concentrations for anti-cancer activity using MTT assay on HT-29 colon cancer cells. Active compounds were screened for their apoptosis-inducing ability using Western blot analysis to study PARP fragmentation which is a hallmark of apoptosis. This poster will present the effect of solvent in the synthesis of the compound library and the biological evaluation of the compounds.



MWRM 2026 MW08

Novel path to clean power: Increasing electrode performance of microbial fuel cells

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This research investigated how the microstructure of the anode in a Microbial Fuel Cell (MFC) influences electricity generation. MFCs are bioelectrochemical systems that utilize naturally occurring soil microorganisms to convert organic matter into clean, renewable energy. Because the efficiency of electron and proton transfer is highly dependent on the conductivity of the anode, the study focused on optimizing the three-phase interface between Platinum (Pt), Carbon (C), and Nafion, a highly proton-conductive polymer.

The central hypothesis proposed that increasing Nafion loading on a Platinum/Carbon (Pt/C) anode would enhance electrical current generation up to an optimal threshold of 20% Nafion. Beyond this level, excessive Nafion was expected to hinder conductivity and reduce overall performance by disrupting the balance between proton transport and electron transfer pathways.

To test this hypothesis, nutrient-rich mud was collected from a local waterway and used as the microbial source for the fuel cells. MFCs were assembled using anode and cathode electrodes, with varying Nafion concentrations applied to the Pt/C anode layer. Electrical current production was monitored using a multimeter, with measurements recorded every 24 hours over a seven-day period.

The results demonstrated a strong relationship between Nafion loading and MFC performance. Anodes consisting of 5% Platinum-coated Carbon and 20% Nafion produced the highest electrical output, achieving peak currents of approximately 1,500 microamps. This finding confirms the existence of an optimal Nafion concentration that maximizes proton conductivity while maintaining accessibility to catalytic Platinum sites. When Nafion concentrations exceeded 20%, current generation declined significantly because excess Nafion coated and blocked active Platinum reaction sites, limiting electron transfer and reducing overall cell efficiency.

Overall, the study successfully identified 20% Nafion loading as the optimal composition for Pt/C anodes in Microbial Fuel Cells, providing valuable insight into electrode design

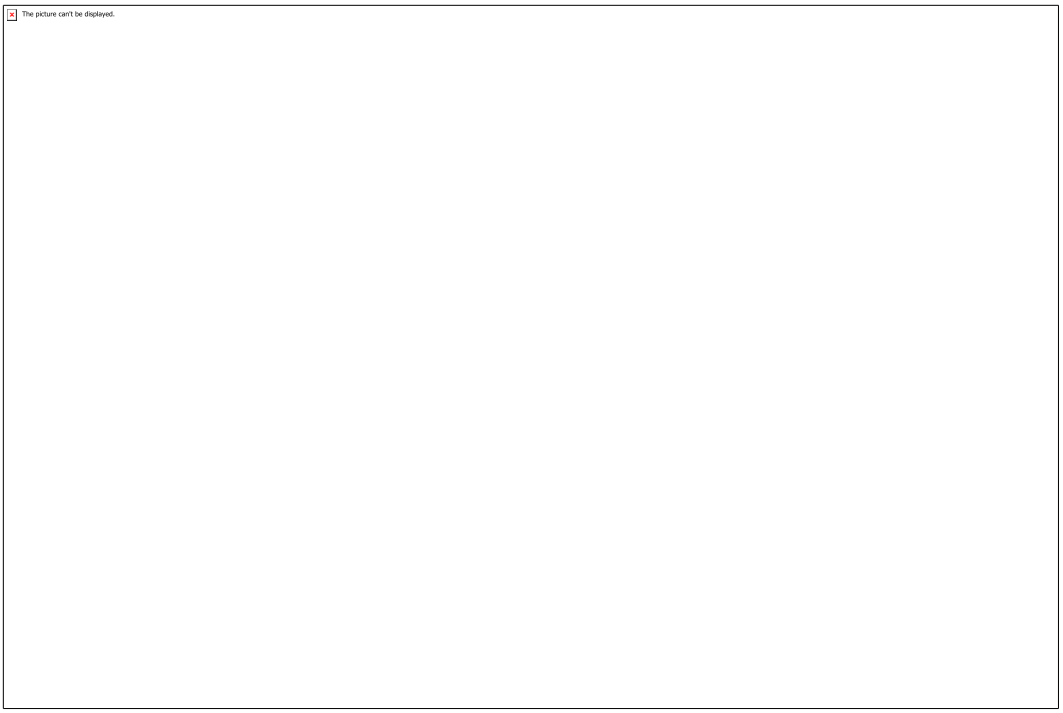
for bioenergy applications. These findings highlight the importance of carefully engineering the anode microstructure to balance proton transport, catalyst accessibility, and electrical conductivity, ultimately improving the performance and scalability of sustainable microbial energy technologies.

MWRM 2026 MW271

Occurrence, spatial distribution, and dietary risk assessment of cypermethrin and glyphosate residues in environmental matrices from agricultural settlements in southwestern Nigeria

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Pesticide contamination of agricultural ecosystems poses significant challenges to environmental sustainability and food safety. This study investigated the occurrence, spatial distribution, and dietary risk of cypermethrin and glyphosate residues in water, sediment, soil, and *Amaranthus cruentus* collected from major agricultural settlements in Oyo State, Southwestern Nigeria. A total of 120 samples were analyzed using validated chromatographic methods. Residue data were evaluated using descriptive statistics, linear mixed-effects modelling, principal component analysis (PCA), spatial autocorrelation, and deterministic and probabilistic health risk assessment.
Both pesticides were detected in all environmental matrices, with concentrations varying significantly among sample types and locations. Mixed-effects modelling showed that glyphosate concentrations were significantly higher than cypermethrin, whereas water samples contained significantly lower residue levels than soil, sediment, and vegetables. PCA distinguished contamination patterns associated with environmental partitioning, while spatial autocorrelation revealed significant positive clustering of pesticide residues (Moran's $I = 0.255$, $z = 2.91$, $p = 0.011$), indicating localized contamination hotspots linked to agricultural activities.
Estimated daily intakes and hazard quotients for adults remained below established toxicological thresholds, and Monte Carlo simulation indicated a very low probability of unacceptable non-carcinogenic risk. Nevertheless, residue concentrations in *A. cruentus* exceeded European Union maximum residue limits for both pesticides, particularly glyphosate, suggesting potential food safety concerns despite the low estimated dietary risk.
These findings demonstrate that pesticide contamination is spatially structured and influenced by environmental processes and farming practices. The study provides evidence to support risk-based pesticide management, enhanced residue monitoring, and targeted interventions to improve environmental quality and food safety in agricultural communities.



MWRM 2026 MW74

One-pot versus two-step hydrothermal synthesis of PANI-modified Ni–Co sulfide/oxide electrodes: Mass loading effects on supercapacitor performance

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Binder-free electrodes based on bimetallic Ni–Co sulfide/oxide nanostructures are promising supercapacitor materials, and conductive polymers such as polyaniline (PANI) can further enhance their charge transport. A recently reported two-step hydrothermal route produced hierarchical PANI-modified Ni_3S_2–$NiCo_2S_4$–$NiCo_2O_4$ (P-NCSO) composites on nickel foam with capacitance above 2800 F/g and a cycling stability greater than 90%. In this work, fabrication is simplified to a facile one-pot hydrothermal synthesis in which all precursors are introduced simultaneously, and the resulting electrodes are compared with two-step analogues across a range of mass loadings. Galvanostatic charge–discharge measurements in 3 M KOH reveal a pronounced loading effect: a low-loading one-pot electrode (0.67 mg/cm^2) delivers a gravimetric capacitance exceeding 10,000 F/g at 1 A/g, while comparable high loadings (~2.5 mg/cm^2) yield roughly 3,900 F/g for the two-step electrode and 2,400 F/g for the one-pot. Areal capacitance offers a more realistic comparison: the two-step electrode leads at low current density (~10 F/cm^2), yet all three electrodes converge toward 3–4 F/cm^2 at elevated rates, suggesting that electrolyte-accessible active material, rather

than synthesis route alone, governs high-rate performance. Structural characterization points to divergent physical makeup between routes: electron microscopy shows amorphous, nodular deposits from the one-pot process versus well-defined plate-like architectures from the two-step method, while elemental mapping reveals substantial nitrogen incorporation in the two-step composite that is absent in its one-pot counterpart. These results demonstrate that a simplified one-pot route yields competitive electrodes while underscoring mass loading as a dominant variable in reported performance metrics, motivating ongoing structure–property studies at matched loadings.

MWRM 2026 MW78

One-step method for the synthesis of bridged-functionalized pillararenes

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Pillararenes have emerged as an important class of macrocyclic hosts due to their pillar-shaped architectures, electron-rich cavities, and versatile host–guest recognition properties. While extensive efforts have focused on functionalization of the rim substituents, direct modification of the methylene bridges remains comparatively underexplored despite its potential to impart unique structural, electronic, and recognition properties. Developing efficient synthetic strategies to access bridge-functionalized pillararenes therefore represents an important opportunity to expand the structural diversity and functionality of this macrocyclic family. Here we report the development of a straightforward and efficient synthetic approach for the preparation of bridge-functionalized pillararenes using readily available acetal precursors. This strategy enables the direct incorporation of functional groups into the bridging positions during macrocyclization, eliminating the need for post-synthetic bridge modification. The methodology provides access to a variety of bridge-functionalized pillar[5]arenes and pillar[6]arenes. This method opens new avenues for the development of functional macrocycles with applications in molecular recognition, advanced materials, and biomedical systems.

MWRM 2026 MW124

One-step versus stepwise 2-electron electrochemical reduction of 6,6′-biazulenes

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The 6,6′-biazulenic framework consists of two azulene units, each comprising fused five- and seven-membered sp^2-carbon rings, linked through the 6-positions. Functionalized 6,6′-biazulenes combine extended π-conjugation with tunable electronic and electrochemical properties, thereby making them attractive building blocks for organic electronics, molecular electronics, and molecular sensing. Whereas the parent

(i.e., unsubstituted) 6,6′-biazulene invariably undergoes stepwise two-electron reduction regardless of the electrolyte medium, the 1,1′,3,3′-tetraethoxycarbonyl-6,6′-biazulenic scaffold exhibits concerted one-step, two-electron reduction even after further functionalization along its molecular axis. In this presentation, we examine how the substitution pattern governs switching between concerted and stepwise two-electron electrochemical reduction in 6,6′-biazulenes. To this end, we developed a regioselective double decarboxylation of 2,2′-diamino-1,1′,3,3′-tetraethoxycarbonyl-6,6′-biazulene, which provided access to a series of hitherto unknown 1,1′-diethoxycarbonyl-6,6′-biazulenes functionalized along the molecular axis. In addition to synthetic details, spectroscopic and single-crystal X-ray diffraction characterization will be presented. Electrochemical studies using cyclic and differential pulse voltammetry reveal that a single ethoxycarbonyl group on each azulene unit is sufficient to maintain concerted one-step, two-electron reduction across the 6,6′-biazulenic platform. The electronic structure origins of this behavior will also be discussed.

MWRM 2026 MW124

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MWRM 2026 MW213

On the nature of ion atmospheres and rules for their formation

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Despite the ubiquity and importance of electrolytes, our theoretical understanding of ion atmospheres still relies heavily on Poisson-Boltzmann based approaches, which are only correct at very low ionic strengths. Recently, we have used Kirkwood-Buff theory, an exact theory of solutions, together with a series of electroneutrality constraints to provide relationships between the spatial integrals over the ion-ion distributions in bulk electrolyte solutions and the surface-ion distributions in electrolyte solutions around surfaces. We have also shown that the integrals can be separated into two contributions, one resulting in charge neutralization, for which each ion contributes in proportion to its ionic strength, and the other accounting for the solution thermodynamics. Here we show that these relationships also hold for the underlying spatial distributions themselves away from a charged or uncharged surface, even over short (non-neutral) distances. A detailed analysis of the spatial nature of experimental and simulated ion atmospheres around different types of surfaces provides simple rules for the formation of all ion atmospheres. Rearrangements that promote charge neutralization conserve the number of ions associated with each formal electrolyte within a given region, whereas thermodynamic rearrangements adjust the number of neutral electrolyte “molecules” while conserving the charge of a given region. The relationships hold for atomic and molecular ions with any valency regardless of ionic strength, temperature, or pressure, in any single-phase solvent system. Together the results provide a new view of ion atmospheres that improves our understanding of simple and complex electrolyte solutions.

MWRM 2026 MW374

Optical photothermal infrared spectroscopy for quantifying ligand fractions in individual mixed-ligand metal-organic framework crystals

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Metal-organic frameworks (MOFs) are porous crystalline materials constructed from metal ions and organic ligands. One of the strategies to tailor their physicochemical properties is the mixed-ligand approach, where different types of organic ligands are coordinated to the metal ion within the same framework. As the properties of mixed-ligand MOFs are influenced by their ligand composition, a reliable quantification of the individual ligand fractions in the framework is essential. However, non-destructive determination of ligand composition, particularly at the single-crystal level, remains challenging. Here, we demonstrate a non-destructive Raman spectroscopic method for

quantifying ligand fractions in a mixed-ligand zeolitic imidazolate framework containing benzimidazolate and 2-methylimidazolate ligands. Bulk Raman spectroscopy was initially used to establish a quantitative correlation between characteristic vibrational peaks and the ligand composition of the framework. This approach is then applied to optical photothermal infrared (OPTIR) Raman spectroscopy, allowing compositional analysis of individual microcrystals with submicrometer spatial resolution. The average ligand fractions determined from bulk Raman and single-crystal OPTIR measurements agreed with values obtained using conventional solution-state ^{1}H NMR spectroscopy following complete framework dissolution, supporting the accuracy of the spectroscopic approach. OPTIR measurements also revealed substantial crystal-to-crystal variation in ligand incorporation, particularly for samples with intermediate ligand compositions, indicating compositional heterogeneity during framework formation. Furthermore, the degree of compositional variability decreased as crystal size increased, suggesting that larger crystals become more compositionally uniform during later stages of growth. Overall, this nondestructive spectroscopic approach enables quantitative determination of ligand composition at both bulk and individual-crystal levels while providing insight into crystal-to-crystal heterogeneity and growth-dependent ligand incorporation in mixed-ligand MOFs.

MWRM 2026 MW340

Optical rotation calculations on 1D periodic systems at coupled cluster with single and double excitations level

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Accurate simulations of electronic response properties for solid state materials are essential tools for technological applications in various fields. The extension of coupled cluster (CC) methods to the solid state is an important step towards high level simulations that can provide insights into the effects of electron correlation on electronic response properties of materials. In this study, we present an implementation of the linear response function for optical rotation (OR) calculations on 1D periodic systems at the coupled cluster level with single and double excitations and periodic boundary conditions (LR-CCSD-PBC). This implementation is carried out in the open-source CCResPy software that is fully based on the Python and NumPy libraries. The calculation of the Buckingham/Dunn B tensor, which describes the optical rotation of oriented chiral systems, is performed using the modified velocity gauge (MVG) and the origin invariant length gauge (LG(OI)) formalisms. We compare these two formalisms by computing the OR of periodic H_2O_2 and H_4 chains using increasing k-point mesh and basis set size. The convergence towards the thermodynamic limit is compared to reference calculations performed on long but finite molecular chains in GAUSSIAN at the CCSD level. We also study the length dependence of intermolecular interactions on the OR by increasing the distance between molecular units in the chain. LR-CCSD-PBC calculations performed with the MVG formalism typically display a faster convergence towards the thermodynamic limit with increasing k-point sampling when compared to

LG(OI). We find that the effect of intermolecular interactions are significant even up to 16 Å between molecules; furthermore, we show that point-charge embedding models are not able to reproduce this effect quantitatively, and in certain cases not even qualitatively. These insights into the optical rotation of periodic systems may allow the development of systematically improvable quantum mechanical methods for simulating optical response properties.

MWRM 2026 MW429

Optimization of acrylamide roadblocks for the recovery of high-molecular-weight DNA

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High-molecular-weight DNA is essential for accurate genome assembly and the identification of complex structural genomic variations. To improve the recovery of long DNA molecules, acrylamide roadblocks of varying concentrations were evaluated. The acrylamide roadblock slows or temporarily stops the electrokinetic migration of DNA, allowing DNA molecules to concentrate prior to recovery.
3D-printed devices containing acrylamide roadblocks of different concentrations were tested in triplicate. Following the application of the electric field, DNA was recovered and quantified. Comparison of the different acrylamide concentrations identified the conditions that produced the greatest DNA recovery. These results provide insight into optimizing acrylamide roadblock conditions for concentrating and recovering high-molecular-weight DNA for downstream genomic analyses.

MWRM 2026 MW29

Optimization of a high-throughput FRET assay for identifying cleavage-inducing ligands for the glmS riboswitch in *Staphylococcus aureus*

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The growing threat of resistance to antibiotics has made it imperative that new compounds be researched for the development of innovative antibiotics with new targets. Riboswitches are regulatory mRNA segments that bind cellular metabolites and control the expression of essential genes, serving as promising targets for antibiotic discovery. Specifically, the glmS riboswitch binds to glucosamine-6-phosphate (GlcN6P), a precursor involved in cell wall synthesis in Gram-positive bacteria, and self-cleaves as part of a negative feedback loop, effectively rendering the mRNA inactive. Unlike other known riboswitches, the glmS riboswitch requires its ligand to directly

participate in catalysis, thus functioning as both a riboswitch and a ribozyme. It is the only known riboswitch that regulates gene expression through its own catalytic activity. Identifying compounds that mimic GlcN6P and activate the self-cleavage mechanism of the glmS riboswitch may provide a valuable strategy for antibiotic development and combating antibiotic resistance in bacteria. This project investigates GlcN6P analogs capable of inducing self-cleavage of the glmS riboswitch in Staphylococcus aureus using a high-throughput FRET assay. Various GlcN6P analogs have been tested for their ability to induce self-cleavage of the glmS riboswitch. The ultimate goal is to rapidly screen large libraries of small molecules for their cleavage-inducing abilities, in an attempt to identify promising compounds for future antibiotic development.

MWRM 2026 MW25

Optimization of a high-throughput FRET assay for the self-cleavage of the *Bacillus cereus* glmS riboswitch to identify potential antibiotic compounds

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The increasing global health threat of antibiotic resistance has made it necessary to explore novel antibiotic mechanisms with distinct molecular targets. Riboswitches are non-coding regions of mRNAs that bind small metabolites and undergo conformational changes that affect downstream gene expression. The glmS riboswitch/ribozyme, present in many gram-positive bacteria including the food-borne bacterium *Bacillus cereus*, regulates the enzyme that produces glucosamine-6-phosphate (GlcN6P). The GlcN6P metabolite/ligand is a precursor to cell wall synthesis, and when it is bound to the glmS riboswitch, it triggers self-cleavage of the glmS mRNA, thereby downregulating gene expression. This riboswitch control would allow potential antibiotics to antagonize metabolic pathways that are essential to a bacteria's survival and potentially overcome current mechanisms of antibiotic resistance. The glmS riboswitch is unique in that it is the only known riboswitch that utilizes catalysis to control gene expression. Thus, the glmS riboswitch is also a ribozyme, and it is the only known ribozyme that depends on a metabolite coenzyme to activate self-cleavage. These properties of the glmS riboswitch, along with its prominence in gram-positive bacteria, make it an appealing focus for antibiotic development. This study is focused on optimizing a high-throughput fluorescence resonance energy transfer (FRET) assay for the *B. cereus* glmS ribozyme to test libraries of compounds and analogs of GlcN6P. A FAM/Cy3-labeled substrate RNA is used as a means to measure fluorescence, and the assay monitors cleavage in real time, enabling the distinction of active versus inactive ligands. The goal of this study is to establish an efficient, well-controlled, and accurate high-throughput assay capable of screening large libraries of compounds as candidate antibiotics against *B. cereus* rapidly. The results of this study could then draw further investigations of other pathogens relying on the glmS riboswitch and various other ligands for antibiotic activity.

MWRM 2026 MW130

Optimization of a small molecule inhibitor of complement protease C1s

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C1 is the initiator zymogen of the classical complement pathway (CP). In the absence of an activator, C1 circulates as an inactive complex comprised of a pattern-recognition molecule, C1q, bound to a Ca^{2+}-dependent heterotetramer of the serine protease zymogens, pro-C1r and pro-C1s. However, when C1q binds to a ligand, a conformational change occurs within the C1 complex that results in autocatalytic activation of pro-C1r. Once activated, C1r enzyme cleaves pro-C1s into its active form. Activated C1s then completes initiation of the CP by cleaving its two substrates, complement components C4 and C2. This results in the assembly of a transiently stable enzyme known as the classical pathway C3 convertase on complement-reactive surfaces. Thus, this stepwise sequence of proteolytic events represents a powerful complement initiation mechanism *in vivo*.

Despite the existence of endogenous regulatory proteins, excessive complement activity arising via the CP is a pathophysiological driver of several rare inflammatory diseases. Several of these diseases affect the hematological and renal systems, including Heparin-induced Thrombocytopenia (HIT), Cold Agglutinin Disease (CAD), and Immune Thrombocytopenic Purpura (ITP), among others. In early 2022, a C1s inhibitory monoclonal antibody known as Sutimlimab received FDA approval for treatment of CAD. Although this antibody showed a favorable safety profile in human clinical trials, its high cost and IV-only mode of administration suggest that research into alternative CP-targeted therapeutics remains a high priority. Thus, we have been focused on identifying small molecule inhibitors of C1s as a precursor to lower cost therapeutics for CP-driven diseases.

We recently reported a series of reversible, competitive inhibitors of C1s with single-digit micromolar potencies. While these molecules are a useful proof of concept that highly selective C1s inhibitors can be developed, they interact with the C1s substrate binding site (i.e., S1 pocket) via an amidine moiety, which is undesirable for synthetic and pharmacokinetic reasons. Here, we describe recent investigations of isoquinolin-1-amine and phthalazin-1-amine groups as alternatives, which are also capable of binding the S1 pocket. We will also summarize the results from a “mini fragment” library screen used to identify new chemotypes of inhibitors.

MWRM 2026 MW352

Optimization of gold nanotriangle arrays for localized surface plasmon resonance-based biosensing

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Localized surface plasmon resonance (LSPR) has emerged as a powerful sensing technique because it enables rapid, label-free detection of biomolecules. The performance of LSPR-based sensors depends on the morphology and optical properties of plasmonic nanostructures such as gold nanotriangle (AuNT) arrays, which can act as a sensing platform. In this work, AuNT arrays were fabricated by nanosphere lithography using self-assembled 500 nm and 200 nm polystyrene sphere monolayers formed at the air-water interface as templates. A 35 nm thickness of gold was thermally deposited onto the templates using a thermal evaporator under two different deposition conditions, with and without rotation of the sample mount. The resulting AuNT arrays were then characterized using atomic force microscopy (AFM) and UV-Vis spectroscopy to examine their surface morphology and LSPR response. AFM images revealed that thermal evaporation without sample mount rotation produced more uniform AuNT arrays with sharper and more distinct triangular features between the polystyrene spheres. In contrast, deposition with sample mount rotation resulted in less uniform AuNT with less well-defined triangular features. These differences in morphology were consistent with the optical measurements, where the AuNT arrays fabricated without sample mount rotation exhibited higher LSPR sensitivity than those fabricated with sample mount rotation. The optimized AuNT arrays provide a promising platform for future LSPR-based biosensing studies. Ongoing work focuses on further optimizing the nanofabrication process and evaluating the biosensing performance of AuNT arrays for LSPR-based detection of biomolecules.

MWRM 2026 MW431

Optimization of insert geometry for enhanced recovery of high-molecular-weight DNA

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High-molecular-weight DNA is essential for genomic analyses and other biomedical applications. To improve the recovery of long DNA molecules, 3D-printed devices were developed to electrokinetically elute and concentrate DNA from agarose inserts. Initial studies used large agarose inserts (2.7 × 6.6 × 7.2 mm) containing *Saccharomyces cerevisiae* chromosomes; however, a substantial fraction of the DNA remained trapped

within the insert following elution. To improve DNA recovery, smaller agarose inserts (1.6 × 5.8 × 7.0 mm) were designed and incorporated into the device using a custom holder to ensure proper positioning. DNA was eluted from the inserts into a recovery zone using pulsed electric fields. Pulse ON/OFF times, applied voltages (7.5 and 15 V), and run durations were systematically varied to identify conditions that maximize DNA recovery while minimizing the amount of DNA remaining in the insert. These studies provide insight into optimizing insert geometry and electrophoretic conditions for the efficient recovery of high-molecular-weight DNA.

MWRM 2026 MW13

Optimizing expression, purification, and crystallization conditions for FlrB 7–123 wild-type as a foundation for mutant structural studies

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Vibrio cholerae, the bacterium responsible for the disease cholera, uses sensor histidine kinases to respond to environmental changes. FlrB, one of the sensor histidine kinases, plays a major role in flagellar synthesis and motility, making it a potential target for antimicrobial therapy. This project focuses on characterizing the PAS domain as well as other adjacent regions of FlrB, corresponding to amino acid residues 7–123. We expressed the FlrB 7–123 wild-type construct, as well as mutants D76Y and L36F, in *Escherichia coli.*[3] The wild-type construct was purified using affinity and size exclusion chromatography. The resulting purified protein was concentrated and used for crystallization trials under various conditions. Crystals were obtained and harvested for X-ray diffraction analysis. One crystal yielded usable diffraction data at a resolution of 3.31 Å and the resulting structure has been solved. Establishing reliable purification and crystallization conditions for wild-type FlrB lays the groundwork for future structural analyses of the mutant constructs, which may ultimately contribute to understanding FlrB signaling mechanisms and antimicrobial target development.

MWRM 2026 MW319

Osmotically induced shape changes in membrane vesicles

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We develop a self-consistent free-energy framework in which the shape of a membrane vesicle and the osmotic pressure across it are determined simultaneously within a finite

solute reservoir, by minimizing the combined bending-elastic and solute-entropic free energy. Because the enclosed solute is conserved, the osmotic pressure becomes a thermodynamic variable that adjusts to membrane deformation rather than an externally imposed parameter, producing a nonlinear coupling between membrane mechanics and solute entropy. This coupling reframes vesicle stability: shape transitions arise from global free-energy competition rather than from the linear Helfrich criterion. Mapping the phase behavior reveals a pronounced non-monotonic boundary in the osmotic-pressure–solute-number plane, where the critical pressure for the spherical-to-deformed transition passes through an extremum as the enclosed solute number is varied, signaling reentrant stability of the spherical state. The predicted boundaries agree with coarse-grained simulations of small and large unilamellar vesicles and refine the corresponding Helfrich estimates. The framework speaks directly to biomolecular condensate confinement in crowded cellular environments, synthetic vesicles, and the design of osmotically driven encapsulation and controlled-release platforms.

MWRM 2026 MW318

Palm-reading for your phase diagram: Disentangling multi-phase effects in biomolecular condensates

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Biomolecules can have very different affinities in pairwise vs. many-body contexts. The possibility of multiple interaction affinities complicates the interpretation of experiments both in cells, where the interaction modes may represent distinct regulatory states, and in vitro, where competition between bindings states yields complex macroscopic behavior. Motivated by the phase behavior of mixtures of linker histones and DNA, we developed a thermodynamic theory to understand how multiple binding modes influence biomolecular phase diagrams. Starting from the grand partition function of the solution, we show that the phase boundary is very similar to the solubility product when expressed as a function of the monomer concentrations. However, unlike the simple salts usually described by a solubility product, biomolecular condensates do not have a fixed stoichiometry. This introduces curvature in the phase boundary when plotted on a log-log scale of monomer concentrations. Furthermore, measurement of the boundary curvature provides a quantitative prediction of the stoichiometric composition of the dense phase. A second complication that is not found in simple salts comes from the prevalence of oligomeric complexes in the dilute phase. These oligomers distort the phase boundary in the opposite direction of the stoichiometric variation and lead to effects like re-entrant transitions and “magic number” peaks. However, characterization of the oligomer association constants allows these effects to be quantitatively removed, which reveals the monomer/dense phase equilibrium. Together these findings suggest that that it is intuitively helpful to view the dilute/dense coexistence, instead, as a three-state equilibrium between monomers, dense phase, and oligomer ensemble.

MWRM 2026 MW349

Peptide identification from exopeptidase-generated amino acids

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Proteins carry out nearly every biological process, making accurate peptide and protein characterization essential for understanding biological function, identifying disease biomarkers, and developing new diagnostic technologies. Conventional protein sequencing methods, including Edman degradation and Liquid Chromatography–Mass Spectrometry (LC-MS), provide high-quality sequence information but require specialized instrumentation, extensive sample preparation, and can be limited for certain peptide analyses. To address these challenges, our laboratory is developing a peptide fingerprinting strategy that combines exopeptidase digestion with Resistive Pulse Sensing (RPS) detection of released amino acids as a foundation for future nanopore-based protein sequencing. In this approach, carboxypeptidases sequentially remove C-terminal amino acids, generating amino acid profiles that can be used for peptide identification. Carboxypeptidase Y (CPY) and Carboxypeptidase A (CPA) were evaluated using the model peptide Met-enkephalin. Digestion conditions and Fmoc-Cl amino acid derivatization were optimized, and the released amino acids were identified by HPLC and LC-MS, which served as orthogonal analytical techniques to validate the observed digestion kinetics. Under the optimized conditions, CPY demonstrated greater digestion efficiency than CPA, achieving complete cleavage of Met-enkephalin within 1 minute of digestion time, establishing an optimized solution-phase workflow that provides the foundation for future solid-phase digestion and integration into nanofluidic peptide fingerprinting platforms.

MWRM 2026 MW197

Phasor assisted photon modulation for hyperspectral single-molecule microscopy

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The development of single molecule localization based super-resolved fluorescence microscopy (SMLM) enables studies of protein assemblies down to nanometer spatial resolution. The multiplexing capability of SMLM techniques had been explored through strategies including sequential imaging of spectrally well separated fluorophores, ratiometric-, dispersive-, and excitation modulation-based spectral demixing for simultaneous imaging of spectrally overlapped fluorophores, and sequential DNA-PAINT (i.e., Exchange- and SUM-PAINT). However, the intrinsic nature of these techniques, either low signal to noise ratio (SNR), low molecular density, slow image recording rate, or sequential data acquisition, limit their throughput. In this work, we

developed a method that enables high-density single-molecule imaging with high SNR, resulting in both high throughput and large multiplexing capability of SMLM. We named it spectral phasor enabled SMLM (SP-SMLM). Applying the methodology to dSTORM imaging, we achieved up to 5-plex super-resolution imaging of proteins in fixed cells in about 1 minute. We obtained snapshots of super-resolved polarity mapping of lipid membrane with 15-sec temporal resolution in live cells, showing heterogeneity and dynamic exchanges of lipid contents in endoplasmic reticulum.

MWRM 2026 MW392

Phonon flux as a nonequilibrium mechanism for modulating biomolecular function

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Localized heating at nanoparticle–biomolecule interfaces is often interpreted using equilibrium temperature thermodynamics. Yet numerous nanoscale experiments report changes in molecular activity that are disproportionate to the measured bulk or local temperature increase. We are investigating whether these observations can be explained by a nonequilibrium phonon-flux model in which energy transferred from a nanoscale heat source initially propagates through the surrounding molecular structure as a directed vibrational energy current rather than as a fully thermalized distribution.

In this framework, molecular response depends not only on temperature, but also on the spectral phonon composition and relaxation pathways of the incoming energy flux. Thermal energy entering a protein may populate subsets of vibrational modes in non-standard distributions. Further, if these modes overlap with motions involved in substrate binding, transition-state formation, or product release, then the resulting nonequilibrium population may alter the rates of biochemical output.

We are developing an integrated approach to evaluate a phonon-flux model in dissipative systems using normal-mode analysis, molecular dynamics simulations, and nanoparticle-mediated experiments. This work aims to establish the conditions that drive systems from conventional thermal activation to phonon-flux-driven behaviors. More broadly, understanding how nanoscale energy transport across hard–soft matter interfaces may influence biomolecular dynamics and function.

MWRM 2026 MW37

Phosphenium-controlled Pt(0) catalysts for regioselective alkyne hydrosilylation

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The development of highly selective heterogeneous single-atom catalysts (SACs) remains a significant challenge, particularly for low-valent transition metals such as Pt(0), which are inherently unstable on support surfaces. Conventional oxide-supported platinum catalysts often require high metal loadings and contain a distribution of active sites, limiting the structural control necessary to establish structure-activity relationships (SARs) and achieve the high levels of selectivity observed in homogeneous systems. We have found that phosphenium ligands, chemisorbed to oxides and dissolved in solution, support highly active and moderately regioselective Pt(0) catalysts for alkyne hydrosilylation, exhibiting catalytic performance comparable to homogeneous N-heterocyclic carbene (NHC)-supported systems
Recently, we found that the Lewis acidic nature of the phosphenium ligands can be taken advantage of by coordination simple Lewis bases that increase the regioselectivity significantly and provide another means to control the SAR.
To investigate these effects, we synthesized a series of phosphenium-supported platinum complexes featuring systematically varied counter-anions, phosphenium ligands with differing steric and electronic properties, and coordinated Lewis bases. Catalytic and spectroscopic investigations have revealed that more strongly coordinating counter-anions, such as Triflate, promote increased pyramidalization at the phosphorus center, modifying the steric environment around the platinum center and leading to improved regioselectivity in alkyne hydrosilylation. In addition, the introduction of simple Lewis bases further enhances regioselectivity, in some cases matching or exceeding that of the most selective catalysts reported to date. Ongoing studies are aimed at elucidating the nature of the base-phosphenium-metal interactions and determining how these interactions influence catalyst structure and performance. These studies establish structure-activity relationships that guide the rational design of highly selective phosphenium-supported Pt(0) catalysts and future supported catalyst systems.

MWRM 2026 MW172

Photoswitch-enabled control of macrocyclic alkyne reactivity

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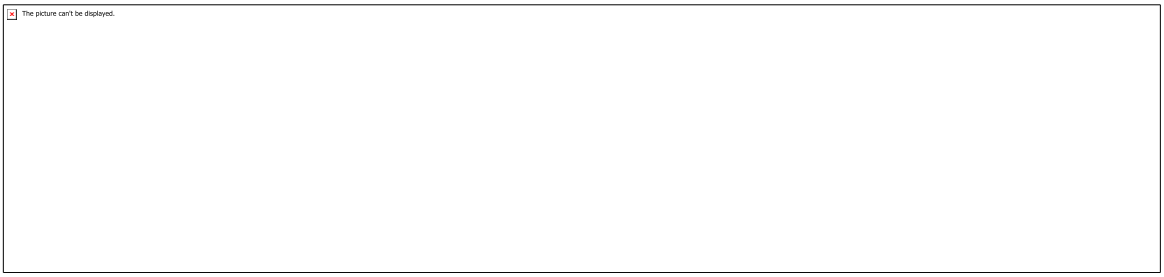
This study investigates the design and synthesis of a light-responsive macrocyclic system, where molecular strain and reactivity are induced through structural isomerization. A macrocycle incorporating a hydrazone-based molecular photoswitch was prepared and evaluated for conformational control under light irradiation. The findings suggest that hydrazones are robust switch templates that can influence a molecule's overall geometry and reactivity, underscoring the practical advantage of responsive molecular architectures.

MWRM 2026 MW182

Phthalimide-derived hemiaminals and hemiaminolates as tunable aryldifluoromethyl-transfer reagents

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Fluorine incorporation plays a central role in pharmaceutical design, where it is used to modulate metabolic stability, lipophilicity, and binding interactions. The difluoromethylene (–CF2–) unit is a valuable bioisostere of oxygen and an analog of methylene, carbonyl, and sulfonyl groups, making it widely used in drug design. Among these, the ArCF2 motif is particularly promising, creating a strong need for reliable, general, and practical methods to synthesize aryldifluoromethyl-containing molecules. Despite the potential value of the ArCF2 motif, practical methods for its installation remain limited. Currently available nucleophilic aryldifluoromethyl-transfer reagents heavily rely on ozone-depleting halogenated fluorocarbon feedstocks, which face regulatory and supply-chain concerns.
Here, we describe a new family of phthalimide-derived ArCF2-transfer reagents prepared from readily available imide scaffolds and organomagnesium reagents without using ozone-depleting fluorocarbon building blocks. The resulting difluoroalkylated hemiaminals and their corresponding hemiaminolates function as bench-stable, tunable reservoirs of nucleophilic ArCF2 equivalents. These studies establish relationships between reagent structure, fragmentation behavior, competing proton-transfer pathways, and productive ArCF2 transfer, providing a foundation for the rational design of practical difluoroalkyl-transfer reagents.



MWRM 2026 MW345

Plasma lipidomics reveals melanoma and treatment-dependent remodeling in a mouse model

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Melanoma is highly aggressive and rapidly progressive skin cancer that alter cellular metabolism to support tumor growth and has a strong propensity to metastasize to distant organs. Alterations in plasma lipids reflect the underlying tumor-driven systemic metabolism and treatment response, given the central roles of lipids in membrane structure, energy storage, and cell signaling. In this study, plasma lipid alterations in a mouse melanoma model were examined using untargeted approach using LC-QTOF-MS . Three groups were compared: control mice without tumors, untreated CD47+ B16 melanoma-bearing mice, and treated CD47-/- B16 melanoma-bearing mice receiving TA99 + MSA-IL2 therapy. Lipids were extracted from plasma using biphasic chloroform/methanol solvent system and analyzed in both positive and negative ionization modes. LC-MS data were processed using MZmine software and statistical analysis of data were conducted in MetaboAnalyst. PLS-DA reveals the clear separation among control, melanoma, and treated groups, indicating metabolic remodelling among three groups. In PLS-DA score plot reveals the pooled QC samples clustered tightly, supporting analytical reproducibility. Melanoma samples exhibited widespread lipid dysregulation, including glycerophosphocholines, glycosphingolipids, glycerophosphoethanolamines, and ceramides, when compared to controls. Although the lipid profile did not entirely restore to the control-like profile, treatment did move it away from the melanoma condition. Changes in glycosphingolipids, glycerophosphoethanolamines, sterols, and cardiolipins were also observed when the treated and melanoma groups were compared, indicating treatment-associated modification of membrane and mitochondrial lipid pathways. Overall, these results demonstrate that plasma lipidomics can identify treatment-responsive pathways for future biomarker validation and capture melanoma-associated lipid remodeling.

MWRM 2026 MW320

Polarizable constant pH molecular dynamics of proteins in aqueous and crystalline environments

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Accurate modeling of proton-coupled conformational dynamics remains a longstanding challenge in molecular simulation, particularly in highly charged and heterogeneous biomolecular environments. We applied a constant pH molecular dynamics (CpHMD) framework based on the polarizable AMOEBA force field to evaluate protonation equilibria in both solvated proteins and protein crystals. The approach combines continuous protonation-state sampling with pH replica exchange and explicit treatment of electronic polarization, enabling dynamic coupling between molecular structure and

ionization states.
Method performance was assessed using hen egg-white lysozyme (HEWL), HP36, and BBL, three benchmark systems with experimentally characterized residue pK_a values. Across 22 Asp, Glu, and His sites, predicted pK_a values exhibited a root-mean-square deviation of 0.55 pH units and a correlation coefficient of 0.92 relative to experiment. Notably, the polarizable model reproduced challenging electrostatic environments more accurately than several established fixed-charge CpHMD approaches, including the catalytic Glu35/Asp52 pair in HEWL, where large pK_a shifts arise from strong local interactions.
To examine transferability beyond aqueous solution, simulations were also performed on crystalline *Trichoderma reesei* xylanase II, for which neutron diffraction data provide residue-specific protonation information at multiple pH conditions. Simulated proton populations closely matched experimentally assigned states, yielding fractional-protonation errors of approximately 0.1-0.2 across three crystal pH values. In several cases, the simulations identified protonation assignments that prompted re-examination of the diffraction refinements and supported updated structural interpretations.
These results demonstrate that incorporating explicit polarization into CpHMD improves description of pK_a shifts and protonation behavior in diverse environments, from solvated proteins to densely packed crystals. The methodology establishes a foundation for studying proton-coupled processes in strongly electrostatic systems such as catalytic active sites, metal-binding motifs, and protein-DNA interfaces.

MWRM 2026 MW370

Polarizable Drude force field for gas adsorption

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Electronic polarization plays a critical role in governing ion-specific interactions across environments ranging from isolated ion–molecule complexes to condensed phases and confined porous materials. Developing transferable force fields that accurately describe these interactions remains a longstanding challenge for molecular simulations. The Drude polarizable force field (FF), which explicitly accounts for electronic polarization through classical Drude oscillators, provides a physically rigorous framework to address this challenge. Recent advances have established a systematic protocol for optimizing atom-pair specific Lennard-Jones (NBFIX) and through-space dipole screening (NBTHOLE) parameters using high-level gas-phase quantum mechanical (QM) interaction energies together with condensed-phase experimental thermodynamic properties. This combined strategy enables the development of transferable parameters that accurately capture both microscopic interaction energetics and macroscopic thermodynamic behavior.

MWRM 2026 MW82

Polymer architecture as a design tool for functional materials

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Polymer properties are governed not only by chemical composition but also by macromolecular architecture. Linear, branched, and hyperbranched polymers composed of identical repeat units can exhibit striking differences in solution behavior, responsiveness, molecular accessibility, and function. Our research explores polymer branching as a versatile design tool for tailoring material properties and establishing structure–property relationships across a range of functional polymer systems. Reversible addition–fragmentation chain-transfer (RAFT) polymerization provides a modular synthetic platform for preparing well-defined polymers with controlled molecular weights, compositions, and degrees of branching, enabling systematic comparisons between polymer architectures. Using this approach, we investigate how branching influences polymer behavior in diverse applications, including stimuli-responsive materials, metal-chelating polymers, and antimicrobial polymers. By comparing linear and hyperbranched architectures while independently varying polymer composition and functionality, these studies seek to understand how branching affects molecular conformation, self-assembly, accessibility of functional groups, and interactions with biological and chemical targets. Together, these efforts demonstrate that polymer architecture represents an independent design parameter that can be leveraged alongside polymer composition to tune material performance.

MWRM 2026 MW311

Polymer infiltration in UiO MOFs monitored by NMR: Exploring the role of polymer chain length

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MOF-based mixed-matrix membranes (MMMs) have demonstrated promise in separation applications, exhibiting enhanced membrane selectivity and permeability compared to polymer-only membranes. However, there is a lack of fundamental understanding regarding factors that influence a polymer’s ability to infiltrate a MOF, which is detrimental to membrane performance, as the MOF porosity becomes partially blocked. This work aims to systematically probe the role of polymer chain length on polyethylene glycol (PEG) infiltration in a family of zirconium-based MOFs. PEG infiltration into MOFs is monitored experimentally via NMR spectroscopy. This work may contribute to the development of informed membrane design approaches and provide experimental insights on guiding principles of compatible MOF–polymer pairs.

MWRM 2026 MW311

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***Colton Rhoads**, colrhoads@gmail.com, Angela Devlin, Noah Nawracaj. Chemistry and Biochemistry, Creighton University, Omaha, Nebraska, United States*

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MWRM 2026 MW195

Potential-modulated fluorescence approach for the determination of the electron transfer rate constant of electrode-tethered electroswitchable fluorophores

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In this presentation, we discuss the potential-modulated fluorescence technique as a method to assess the electron transfer rate constant (k_s) of electroswitchable fluorophores tethered to an indium tin oxide (ITO) electrode. Previously, absorption and fluorescence spectroscopic approaches based on AC potential application were demonstrated to determine k_s for electrochromic polymer films and redox-active dye molecules on ITO. In the prior studies, k_s was determined from the AC frequency dependence of the phase shift of the AC signal associated with redox-induced change in the spectroscopic properties of the polymers/dyes. In this study, we examined k_s determination from the AC frequency dependence of fluorescence intensity amplitude instead of the phase shift. Specifically, we measured the k_s of an electroswitchable fluorophore, ATTO 655, tethered to an ITO-coated coverslip at different supporting electrolyte concentrations. The k_s values were then compared with those obtained from cyclic voltammetry data using the Laviron equation. We observed a sinusoidal change in the fluorescence intensity of ITO-tethered ATTO 655 that is associated with an applied AC potential at the lower AC frequencies but did not observe such intensity changes at higher AC frequencies. Importantly, the amplitude of the sinusoidal fluorescence signal was larger at the lower AC frequency, providing a means to determine k_s. The fluorescence approach gave higher k_s values with increasing

supporting electrolyte concentration, as consistent with those obtained using the electrochemical approach. However, the fluorescence approach always gave slightly smaller k_s values. We are currently investigating the origins of this discrepancy and extending this approach to measure k_s at the single-molecule level.

MWRM 2026 MW395

Predicting $LaFeO_3$ solid-state synthesis pathways using cellular automaton simulations and first-principles thermodynamics

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Materials that are essential to the energy sector are frequently synthesized via the solid-state reaction route. However, no general model exists to predict the reaction pathways, which could impact future synthesis improvement. New computational tools have emerged that use data-driven approaches to address this problem. In this work, we use a cellular automaton simulation ReactCA, to predict the time-dependent evolution of intermediate and product phases for the synthesis of $LaFeO_3$, a perovskite oxide used as an electrode material in solid oxide fuel cells and as a catalyst for photocatalytic, sensing, and hydrocarbon upgrading applications.
The r^{2}SCAN+U level of DFT is applied to optimize the relevant phases and provide the free energies used in the simulation, offering more reliable and internally consistent thermodynamics for the La–Fe–O system than the mixed-functional data typically available from public databases. A reaction network is built from the resulting pathways, incorporating both experimentally observed phases and phases predicted only theoretically. The simulation results indicate that $LaFeO_3$ forms rapidly at higher temperatures, around 1700 K, with finer temperature discretization further promoting conversion to $LaFeO_3$ within the same overall temperature range. Precursor ratio also governs phase selectivity, i.e., the La_2O_3-rich mixtures favor formation of the secondary phase La_3FeO_6, while the Fe_2O_3-rich mixtures favor $La_3Fe_5O_{12}$, with $LaFeO_3$ remaining the dominant product in the latter case. Substituting Fe_3O_4 for Fe_2O_3 as the iron precursor introduces additional redox intermediates without changing the thermodynamically favored final product. Together, these results demonstrate a computational framework for predicting solid-state synthesis outcomes, offering a path toward rationally selecting synthesis conditions for $LaFeO_3$ and related perovskite oxides without exhaustive experimental trial and error.

MWRM 2026 MW321

Predicting oncogenic mutants of epidermal growth factor receptor in lung cancer by molecular dynamics simulation with machine learning

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The epidermal growth factor receptor (EGFR) is a frequently mutated protein kinase found in patients suffering from non-small cell lung cancer (NSCLC). Although therapeutic drugs targeting EGFR are available, not all patients respond to these drugs, and it is not yet known whether some clinically detected mutations are actionable. Although the oncogenicity of some mutants is well established, many mutants found in patients are still not yet classified or classified as Variants of Uncertain Significance. For newly discovered rare mutants, strong evidence supporting their classification into oncogenic or benign is often lacking. Under such situations, multiple pieces of evidence can still help classification, even if each individual piece of evidence is weaker. Computational predictions have been considered as supporting information by the Standard Operating Procedure (SOP) of Clinical Genome Resource/Cancer Genomics Consortium/Varant Interpretation for Cancer Consortium (ClinGen/CGC/VICC). The SOP considers predictions from multiple computational programs as providing only one piece of supporting information to avoid double counting because these programs share common approaches. A computational approach that explicitly accounts for the conformational effects of mutations via molecular dynamics (MD) simulation could add another piece of complementary supporting information. We tested the hypothesis that features of structural dynamics observed from MD simulation could help distinguish oncogenic from benign mutants. To this end, we performed MD simulations lasting a total of 3 microseconds each for wildtype EGFR and over thirty of its oncogenic or benign mutants. We found that random forest machine learning models constructed using suitable structural features were able to distinguish oncogenic and benign mutations effectively. Although we did not supply features of structural motifs commonly used by scientists to distinguish active and inactive conformations, our machine-learning approach identified and utilized some features associated with these motifs for classifying EGFR mutants.

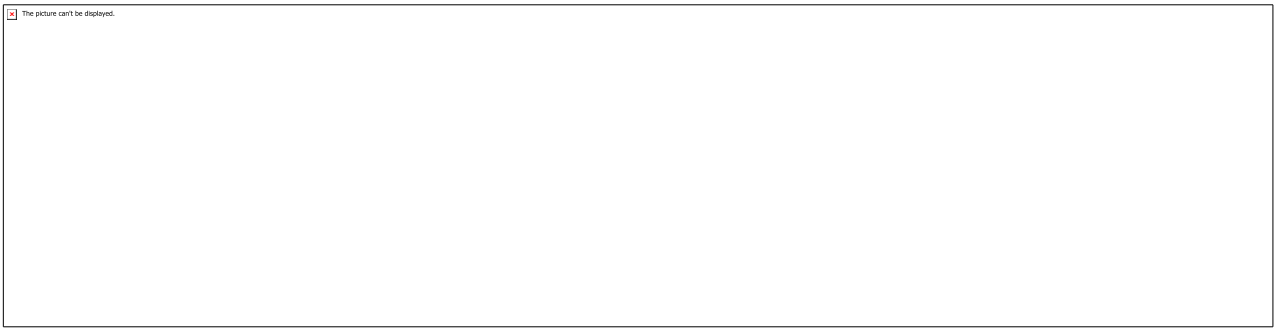
MWRM 2026 MW89

Preparation and characterization of two new cyclohexylamide-based cyanoxime ligands and their Pt(II) complexes

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Traditional Pt-based anticancer drugs are based on cisplatin forming a small family of effective compounds against human cancers with frequent G-G and G-A intra-strand base pairs. However, despite great practical results all cisplatin family drugs have

several serious drawbacks such as effectiveness of only first treatment with progressively developed tumor resistance, poor water solubility, general liver and kidney toxicity. These issues necessitate and warrant further search for other Pt-based active compounds that may exhibit different mechanism and/or kinetic of expected cytotoxicity, or lesser side effects.
Other investigations of Pt-based cytotoxic compounds are in the area of photothermal action when dark-colored compounds may absorb light and transfer it to heat, destroying cells within. In our research group we discovered six intensely colored complexes of PtL2 composition based on six different amide-cyanoximes [1,2]. These six complexes represent cytotoxic dark-green stable 1D polymers with absorption around ~700 nm. As continuation of search for new compounds, we performed synthesis and characterization of two new cyclohexylamide-based ligands which are referred to H(CACO) and H(d-CACO), and their respective two Pt-complexes as shown in Figure 1. Darker compound turned out to show dichroism, represents 1D polymer assembled by metallophilic interactions into Pt-wire and is suitable for photothermal studies. Crystal structures were determined only for two organic ligands at this time. Pt-derivatives of these new ligands will be further characterized in vitro against human cancer cell lines.



MWRM 2026 MW160

Preparation of antiseptic polyvalent triazolium salts with bridging benzyl groups

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Overuse of commercial quaternary ammonium compound (QAC) antiseptics such as benzalkonium chloride can lead to the evolution of antiseptic resistant pathogens. The development of next generation small molecule antiseptics is therefore needed to combat the potential future threat of such organisms. 1,3,4-Trisubstituted-1,2,3-triazolium salts prepared by N-benzylation of disubstituted 1,2,3-triazoles are a newly established class of QACs that display antiseptic properties. Potency for such analogs has been shown to increase with overall valency, most prominently against Gram-negative bacteria. Prior approaches to prepare such polyvalent triazolium compounds

involved the N-benzylation of reactants possessing multiple 1,2,3-triazole subunits. The goal of this study was to develop reaction conditions to efficiently prepare polyvalent triazolium salts via the joining of multiple 1,4-dialkyl-1,2,3-triazole reactants via N-benzylation with bis- and tris-(bromomethyl)arene bridging units including alpha,alpha-dibromo-meta-xylene, alpha,alpha-dibromo-para-xylene, 4,4-bis(bromomethyl)biphenyl and 1,3,5-tris(bromomethyl)benzene. Microwave irradiation was found to be more effective than thermal heating in promoting reaction completion while minimizing the amount of excess of triazole reactant used. Minimum inhibitory concentration assays were performed against Gram-positive bacteria, Gram-negative bacteria and yeast. Divalent and trivalent analogs were compared with their monovalent counterparts to identify how overall charge, bridging geometry and hydrophobicity impacted antiseptic properties. Details regarding the optimized reaction conditions for preparing such polyvalent triazolium salts, their spectroscopic characterization and the antiseptic structure-activity relationship profiling for this series of triazolium salts will be presented.

MWRM 2026 MW386

Pressure-tunable CO_2-H_2O media for enhanced hydrolytic depolymerization of polyethylene terephthalate waste

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Compressed CO_2 offers an effective reaction medium for addressing key engineering challenges in the chemical recycling of polyethylene terephthalate (PET) waste. Dissolution of CO_2 in water forms carbonic acid in situ, creating a mildly acidic environment whose acidity can be controlled through pressure. As CO_2 pressure increases, greater amounts of CO_2 dissolve in water, lowering the solution pH and promoting the hydrolytic depolymerization of PET into oligomers, terephthalic acid (TPA), and ethylene glycol (EG).
This study examines the influence of high-pressure CO_2-H_2O media on the hydrolysis of PET and PET-derived intermediates at temperatures between 180 and 220 °C and initial CO_2 pressures up to 5 MPa. Compared with hydrolysis in hot compressed water under N_2, the presence of compressed CO_2 significantly enhanced depolymerization rates. The highest performance was achieved at 180 °C with an initial CO_2 pressure of 2.8 MPa and a reaction time of 2 h, resulting in higher PET conversion and improved TPA yield. These results demonstrate that compressed CO_2 provides a dynamic and pressure-adjustable source of acidity, enabling efficient depolymerization and chemical recycling of PET waste.

MWRM 2026 MW399

Probing phase transfer catalysis with oriented external electric fields at liquid-liquid interface

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Phase transfer catalysis (PTC) involves chemical reactions across two or more phases. In PTC, the reactants are typically only soluble in the organic phase, while the catalyst is soluble in the aqueous phase. The reaction can occur at the interface, provided that the species can meet at a reasonable rate. Oriented external electric fields (OEEFs) can be used to enhance or inhibit PTC reactions by affecting the diffusion of the reagents towards or away from the interface where the reactions occur, and by directly changing the relative stability of adducts and the height of reaction barriers. In this contribution, we explore the latter effects on a test PTC reaction: the hydrogenation of acetophenone to produce an alcohol product catalyzed by a Ru complex.
We show that the direction and magnitude of the OEEF have a significant influence on this reaction. Two mechanisms are proposed: a direct one and one that includes an explicit water molecule. Then, an OEEF is aligned along two main directions: along the reaction axis (RA), with positive and negative voltage, and parallel to the dipole moment of the system, again with positive and negative voltage. Multiple values of the field magnitude are tested, but all geometries are kept frozen at the field-free structures. Aligning the field along the RA enhances the effects of the Ru-based catalyst, but the reaction is inhibited if the field points in the opposite direction. An enhancement of the reaction is also observed when the OEEF is aligned parallel to the dipole moment, and an inhibition effect is found for the field applied in the opposite direction. Future work includes a geometrical relaxation of reactant, transition state, and product adducts in the presence of the field, and the inclusion of solvation effects in mono and biphasic solutions.

MWRM 2026 MW104

Probing the thermodynamics of ligand binding and pseudoknot formation of preQ$_1$ riboswitch

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Non-coding RNAs rely on intricate three-dimensional structures, including long-range tertiary contacts, to mediate specific molecular interactions and regulate gene expression. Riboswitches, which control gene expression through ligand-induced structural rearrangements, are powerful models for studying these RNA structure-function relationships. The prequeuosine-1 (preQ$_1$) riboswitch, one of the smallest known riboswitches, undergoes a ligand-dependent transition that forms a pseudoknot tertiary contact essential for its regulatory activity. Although pseudoknot formation must

precede ligand association, the thermodynamic relationship between tertiary contact stability and ligand binding affinity remains poorly understood. We hypothesize that an optimal range of pseudoknot stability is required to support efficient ligand binding while maintaining the riboswitch's functional conformational balance. To investigate this, we generated a panel of preQ1 riboswitch mutants combining rationally designed variants and $preQ_1$-like sequences extracted from the Rfam database and measured pseudoknot formation and ligand binding affinities using Dimethyl sulfate Mutational Profiling with sequencing. Only ~6% of Rfam-derived constructs retained ligand binding activity, with binding and non-binding sequences diverging most strongly within the loop, which harbors a conserved motif required for pseudoknot formation. Rationally designed mutants supported this: poly-A tail mutations disrupted binding, stem positions proximal to the loop had to remain conserved, and binding required strong, canonical Watson-Crick pairing at each of the three pseudoknot-forming positions, though the specific base identity at each position was interchangeable among strong pairs. Together, these findings indicate that preQ1 riboswitch ligand binding is governed not by global pseudoknot stability, but by strict preservation of its base-pairing architecture, with natural sequences retaining binding only when this architecture closely matched wild-type. These results provide mechanistic insight into how tertiary contact architecture shapes ligand recognition and a framework for engineering synthetic riboswitches with tunable ligand sensitivity.

MWRM 2026 MW185

Programming molecular communication: From supramolecular design to functional materials

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Using covalent activation strategies, we show how the strength and directionality of halogen- and chalcogen-bond donors can be tuned to control molecular recognition, overcome competing intermolecular interactions, and promote predictable supramolecular assembly. A combination of crystallographic studies, computational analyses, and supramolecular synthesis establishes clear structure-property relationships that enable increasingly reliable bottom-up design of molecular solids. These design principles are then extended beyond crystal engineering to functional applications. Enhanced σ-hole activation correlates with significantly improved anticancer activity in families of organoselenium and organotellurium compounds, illustrating how intermolecular interaction design can influence biological performance. Finally, the same supramolecular concepts are applied to host-guest systems that enable the controlled encapsulation and sustained release of volatile agricultural pheromones, highlighting opportunities in sustainable crop protection.

MWRM 2026 MW107

Progress towards evaluating the modulation of receptor selectivity by amino acid isomerization across different phyla

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L- to D-amino acid isomerization is a post-translational modification which results in a change in the stereochemistry of an amino acid residue in peptides from an L- to a D-conformation. Despite the availability of methods to identify the presence of D amino acids in neuropeptides, the effects of amino acid isomerization on cellular signaling are poorly understood. Previous work using an all-L form and a corresponding D-amino acid-containing form of *Aplysia californica* allatotropin-related peptide (ATRP) showed that amino acid isomerization modulates receptor selectivity for different ATRP receptors (*ap*ATRPR1 and *ap*ATRPR2). The current work seeks to investigate the regulation of receptor selectivity by amino acid isomerization across different phyla using allatotropin peptides. In this regard, *Manduca sexta* and *Lymnaea stagnalis,* representing arthropods and mollusks respectively, were selected. Using bioinformatic analysis, we predicted four receptors (LsATRPR1A, LsATRPR1B, LsATRPR2A, and LsATRPR2B) and one new receptor (MsATR2) for ATRP diastereomers from *Lymnaea stagnalis* and *Manduca sexta*. Using cell-based secondary messenger (IP1 and cAMP) accumulation assays, we evaluated the activation of these predicted receptors by ATRP diastereomers from *Manduca sexta* and *Lymnaea stagnalis*.

We found that in *Lymnaea stagnalis*, the all-L-LsATRP is a more potent activator of LsATRPR1A and LsATRPR1B. In contrast, D2-LsATRP, containing a D-phenylalanine residue at position 2, is a more potent activator of LsATRPR2A and LsATRPR2B. Preliminary experiments show that the *Manduca sexta* allatotropin, MsAT, is a more potent activator of a newly predicted *Manduca sexta* allatotropin receptor, MsATR2, relative to other allatotropin-like peptides (MsATL-I, MsATL-II, and MsATL-III). Also, for *Manduca sexta,* amino acid isomerization of allatotropin peptides (MsAT, MsATL-I, MsATL-II, and MsATL-III) at different amino acid positions had no effect on the order of activation of MsATR2 and a previously identified receptor, MsATR1. Altogether, our results demonstrate that the function of amino acid isomerization as a modulator of receptor selectivity in allatotropins may be widespread among mollusks and less prevalent among organisms in other phyla.

MWRM 2026 MW430

Protecting long DNA molecules with an agarose-based inverted insert

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High-molecular-weight DNA is essential for long-read sequencing and accurate genome assembly, particularly for identifying large structural genomic variations. An agarose-based inverted insert was developed to protect long DNA molecules during cell lysis and sample preparation. In this design, cells or DNA are added to the center of the insert and surrounded by an agarose matrix that minimizes mechanical damage during cell lysis.
The inverted insert was evaluated using a 1 kb DNA ladder, λ DNA, *Saccharomyces cerevisiae* DNA, and *Escherichia coli* DNA. Results demonstrated that high-molecular-weight DNA remained intact within the inverted insert throughout the experimental period. However, DNA concentration gradually decreased over time due to diffusion from the insert. These findings demonstrate that the agarose-based inverted insert effectively preserves DNA integrity while highlighting the need to minimize diffusion-related DNA loss during extended processing.

MWRM 2026 MW143

Protein analyses using novel divergent field ion mobility focusing (DIFIMOF) separations with high-resolution tandem MS

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Macromolecular structure and heterogeneity are increasingly characterized by ion mobility spectrometry (IMS) in gases. Linear IMS using moderate electric fields captures the absolute mobility governed by ion geometry, but the orientational averaging limits structural specificity and 2-D IMS/MS peak capacity. Separations by field asymmetric waveform IMS (FAIMS) based on the high-field mobility increment are much more orthogonal to MS. The field gradient in curved FAIMS cells can focus ions depending on the waveform polarity and ion properties, improving sensitivity. We just demonstrated the DIFIMOF fractionation of protein oligomers and conformers (orthogonal to the underlying FAIMS dimension) by the super/sub linear scaling of compensation field (E_C) versus dispersion field for myoglobin (17 kDa), carbonic anhydrase (29 kDa), and alcohol dehydrogenase (ADH, 37 kDa).
Here we expand these analyses to a wider range of proteins (from 6 to 66 kDa) including BPTI, cytochrome *c*, lysozyme, and albumin. With the "−" waveform polarity, all exhibit rotary conformers at positive E_C values. Those increase at higher charge states (z) in the presence of disulfide bonds (BPTI and lysozyme) but drop at intermediate z otherwise. This reflects the unfolding induced by Coulomb repulsion,

which can be further examined by a new method comparing the actual $E_C(E_D)$ scaling with the ideal cubic for fixed ion geometries. Selected proteins above 12 kDa show the dipole-aligned species at negative E_C values. Scans in the "+" polarity reveal the aligned conformers at negative E_C while the rotary ones at positive E_C vanish at higher E_D levels. Smaller proteins exhibit well-delineated aligned conformers specific to each ***z***, showcasing the importance of dipole properties on the cusp of alignment. We now probe the DIFIMOF-fractionated species by collision-induced dissociation to detect and elucidate the distinct protomers yielding different backbone cleavages. These results demonstrate major novel capabilities for top-down proteomics and structural biology.

MWRM 2026 MW19

Pyruvate dehydrogenase complex inhibitors

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The pyruvate dehydrogenase complex (PDC) links glycolysis to the tricarboxylic acid (TCA) cycle and is negatively regulated by phosphorylation catalyzed by pyruvate dehydrogenase kinase (PDK). Overexpression of PDK decreases PDC activity and has been associated with numerous metabolic disorders, including several types of cancer, type 2 diabetes, and cardiovascular disease. We performed virtual screening of the ZINC and Enamine databases targeting the lipoamide-binding site of PDK to identify novel inhibitors. This approach identified a trifluoromethyl-benzothiophene scaffold that exhibited approximately 10-fold greater potency than our previous lead compound (IC_{50} ≈ 16 μM). Our ongoing efforts to optimize the activity of this lead scaffold will be presented.

MWRM 2026 MW346

Quantifying DNA loading density on biolayer interferometry probes using quantitative PCR

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Functional nucleic acid-based biosensors have significant potential for health monitoring and early disease detection. Aptamers are particularly promising recognition element as they have a wide target range, high stability, easy modification, and are cost-effective. However, aptamer surface density can strongly affect target binding, association and dissociation kinetics, response time, and sensor sensitivity. Despite the widespread use of biolayer interferometry (BLI) for aptamer characterization, the number and surface density of aptamer molecules on these probes remain poorly understood. In these experiments, we developed a quantitative PCR-based method to determine DNA

loading density on streptavidin-coated BLI probes. Desthiobiotin-modified DNA was immobilized on BLI probes and subsequently displaced using biotin wash. The recovered DNA was then quantified by real-time quantitative PCR. The threshold cycle from the BLI wash was then compared to a standard curve to determine the starting amount of aptamer on the probe. This was then used to calculate the density of aptamer on the probe at varying starting concentrations. Establishing the relationship between solution concentration, probe loading, and surface density will improve the interpretation of BLI binding measurements and support more controlled optimization of aptamer-based biosensors.

MWRM 2026 MW269

Quantitative analysis of pesticides in potatoes

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The purpose of this research was to determine a robust preparation method for the analysis of pesticides in russet potatoes and determine the concentration of pesticides in the sample using an Agilent 7890A gas chromatographer with an Agilent 5975 mass spectrophotometer. The extraction methods used were QuEChERs with a RESTEK kit and DLLME, which involve preparation, extraction, and drying that concentrates the analyte in a sample. The quantitation was done by creating calibration curves of pesticide standards – chlorpropham, chlorothalonil, and bifenthrin – using the peak areas and mass of pesticide in the GCMS injection and analyzing the potato samples using the NIST library. The GCMS retention time and the linear calibration equation for three pesticides were investigated; for chlorpropham they were found to be 9.435 minutes and y = 23,237,513.9448x − 921,498.4456; for chlorothalonil, 11.599 minutes and y = 99,834,892.6301x + 201,777.5105; and for bifenthrin, 17.156 minutes and y = 55,345,369.3561x + 8,589,949.5619. The internal standard used for the analyte concentration calculation had a retention time of 17.341 minutes and a linear equation of y = 1,645,100,686.0714x + 8,263,638.1364. One potato sample was determined to contain 0.048 microg of chlorpropham in a 1 microL injection. This preparation method, with the addition of extensive centrifuging, cooling, and a large sample size, was effective for preparing potato samples. The GCMS method was also effective for pesticide analysis. This information can be expanded to other produce to improve food safety research. While future testing is needed to finalize the method, extensive progress was achieved.

MWRM 2026 MW435

Quantitative assessment of the burden of per- and polyfluoroalkyl substances (PFAS) in South Dakota water systems via EPA Method 1633

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Per- and polyfluoroalkyl substances (PFAS) are a class of fluorinated chemicals used widely in consumer and industrial products, and posing a serious threat to global water systems. Increasing scientific evidence has associated certain PFAS compounds with adverse health effects, including elevated risks of cancers, thyroid disorders, liver toxicity, immune system disruption, neurodegeneration, and other health concerns. EPA method 1633 applies solid-phase extraction (SPE) followed by liquid chromatography-tandem mass spectrometry (LC-MS/MS) to measure PFAS concentrations in environmental water samples. Due to its high sensitivity, low detection limits, and reliable quantitative performance, this method is widely recognized as the gold standard for PFAS analysis. This study aims to adapt EPA method 1633 for the detection and quantification of PFAS in surface water samples collected from South Dakota. Method validation was performed via EPA method 1633 recommendations, by assessing calibration performance, method blanks, and recoveries of spiked quality control samples to ensure acceptable accuracy and precision. Several PFAS compounds, including perfluorooctanesulfonic acid (PFOS), perfluorobutanesulfonic acid (PFBS), and perfluorooctanoic acid (PFOA), were detected in South Dakota surface water systems.

MWRM 2026 MW86

Quantitative characterization of bromide- and bromate-dependent wave dynamics in the ferroin-catalyzed Belousov-Zhabotinsky reaction

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Oscillatory and propagating wave patterns are common in biological systems, including signaling processes involved in cardiac rhythms. The Belousov-Zhabotinsky (BZ) reaction system provides a nonlinear chemical model system for studying these behaviors. The BZ reaction is an autocatalytic oscillatory reaction involving bromate, bromide, an organic substrate, sulfuric acid, and a metal catalyst that participate in cyclic redox reactions. Although BZ reaction mechanisms have been studied extensively, quantitative relationships between initial reagent concentrations and wave dynamics remain incompletely characterized experimentally. Quantitative characterization of reaction-diffusion wave dynamics provides insight into the

mechanisms governing BZ wave behavior. BZ reaction-diffusion experiments were conducted in Petri dishes, with bromate and bromide concentrations systematically varied. Images were captured, and wave speed, wavelength, and period data were extracted with MATLAB-based time-lapse image analysis. Target, spiral, and chaotic wave patterns were observed, and wave dynamics were analyzed separately within each pattern. Concentration-dependent trends were observed within each pattern. Preliminary data suggest wave speed increases with initial bromate concentration; the effect of initial bromide concentration remains inconclusive. As concentrations of bromate increased, target wave patterns transitioned to spiral, then chaotic wave patterns. These results suggest that initial bromate concentrations influence BZ wave propagation speed and wave patterns and provide quantitative measurements for evaluating reaction-diffusion models of the BZ reaction.

MWRM 2026 MW137

Quantitative glycomics reveals brain carbohydrate signatures associated with dairy-derived sialic acid and cognitive health

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Dietary sialic acid, enriched in whey protein phospholipid concentrate (WPPC), has emerged as a promising bioactive component for supporting brain health and cognitive function. Building upon previous findings that WPPC supplementation alleviates high-fat diet-induced cognitive impairment, this project aims to elucidate the underlying glycomic mechanisms by quantifying sialic acid and other monosaccharide building blocks in rat brain tissues using targeted LC-QQQ-MS.
During the current funding period, a robust analytical workflow was established for brain tissue fractionation, acid hydrolysis, derivatization, and quantitative LC-MS analysis. Preliminary profiling of rat cerebellum demonstrated that galactose and N-acetylneuraminic acid (NeuAc) are the predominant carbohydrate building blocks, with protein- and lipid-enriched fractions reflecting abundant sialylated glycoproteins and glycolipids. While dominant monosaccharides were similar among dietary groups, several low-abundance sugars, including GlcNAc, GalNAc, xylose, fucose, and NeuGc, exhibited preliminary treatment-related trends, suggesting their potential as sensitive biomarkers of dietary intervention. Multivariate analysis further indicated that these minor carbohydrate species contribute more strongly to group discrimination than the abundant structural monosaccharides.
The next phase will extend this workflow to the cerebral cortex, a brain region more directly associated with learning and memory, and integrate glycomic profiles with behavioral outcomes to identify carbohydrate signatures associated with cognitive performance. Together, this work provides a quantitative glycomics framework for investigating the neuroprotective mechanisms of dairy-derived sialylated ingredients and supports the development of evidence-based dairy ingredients for brain health

MWRM 2026 MW164

Radical synthesis of α-hydroxy allenes utilizing triethylborane

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Allenes, or cumulenes, are functional groups consisting of cumulative π-bonds, and are useful intermediates in organic synthesis. This research project focuses on the development of a novel radical synthesis route to allenes. Traditionally, the most common method for the synthesis of allenes is S_N2' cuprate addition to alkynes. Organocuprates are commonly used due to their ability to participate in reproducible, clean transformations that result in high yield. With organocuprates being strong bases, they are highly susceptible to atmospheric moisture. This requires that cuprate addition to form allenes is done under anhydrous and inert atmospheric conditions.
The goal of this research is to develop a radical method using triethylborane/O_2 and various alkyl halides for the synthesis of α-hydroxy allenes. Ethynyl cyclohexene oxide (2) was used because the ring opening of the epoxide results in an alcohol that could be further functionalized. Preliminary studies suggest that a mixture of radical addition to the alkyne and the epoxide opening product are formed.



MWRM 2026 MW328

Rapid photoiniferter strategy for the synthesis of hyperbranched polymers

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Hyperbranched polymers represent an important class of branched polymer architectures with broad applications including drug delivery, coatings, catalysis and advanced functional materials. While RAFT has been widely employed to synthesize hyperbranched polymers, it is generally time-consuming (24-48 hours) and requires inert conditions. In this study, a rapid photoiniferter approach utilizing a xanthate photoiniferter in combination with a divinyl crosslinker was investigated. A series of hyperbranched N,N-dimethylacrylamide (DMA) polymers with varying degrees of branching was synthesized by altering the monomer-to-crosslinker ratio. The versatility of the method was further evaluated using additional monomers, including N-

isopropylacrylamide (NIPAM) and methyl acrylate (MA). The resulting polymers were characterized by gel permeation chromatography (GPC) to determine molecular weights and dispersities, while 1H NMR spectroscopy was used to determine monomer conversion and the degree of branching. Various solvents were evaluated with dioxane exhibiting the best overall performance, providing 90-95% monomer conversion within 25 min under UV irradiation (365 nm) for all three monomers. Furthermore, the polymerizations exhibited oxygen tolerance, although monomer conversions were slightly lower than those obtained under nitrogen. Overall, this photoiniferter strategy provides a rapid, versatile, and oxygen-tolerant route for the synthesis of hyperbranched polymers and is compatible with multiple monomers.

MWRM 2026 MW90

Recovery and reuse of imide fragments from hemiaminal-based aryldifluoromethyl-transfer reagents

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Aryldifluoromethyl groups are valuable motifs in medicinal chemistry because incorporation of the CF_2 unit can modulate lipophilicity, metabolic stability, and molecular recognition. However, many established methods for generating $ArCF_2$ nucleophiles rely on fluorocarbon feedstocks associated with ozone depletion or high global-warming potential. These limitations motivate the development of aryldifluoromethyl-transfer reagents that avoid problematic precursors while minimizing waste generated during reagent activation.
In this context, we have developed imide-derived aryldifluoromethyl-transfer reagents prepared without relying on fluorocarbon building blocks derived from ozone-depleting substances (ODS). Upon base-promoted activation, these reagents release an $ArCF_2$ anion equivalent while generating an imide-derived fragment. Our investigations revealed that phthalimide is formed following $ArCF_2$ release, prompting us to examine whether this fragment can be recovered and reincorporated into the synthesis of the $ArCF_2$-transfer reagent.
In this study, recovered phthalimide is evaluated for reuse in the synthesis of the aryldifluoromethyl-transfer reagent. In addition, the influence of N-substitution on reagent formation, stability, fragmentation efficiency, product distribution, and recovery of the corresponding imide-derived fragment is examined. Results from these recovery, reuse, and N-substitution studies will be presented.
Together, these studies establish the imide-derived fragment as a recoverable and reusable starting material for the preparation of this family of aryldifluoromethyl-transfer reagents, thereby improving material efficiency and supporting more sustainable strategies for installing difluoroalkyl groups in medicinally relevant molecules.

MWRM 2026 MW432

Recovery of high-molecular-weight DNA using a 3D-printed concentration device

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High-molecular-weight DNA is essential for genomic analyses, including long-read sequencing and genome assembly, but is difficult to recover because long DNA molecules are highly susceptible to mechanical fragmentation. To address this challenge, a 3D-printed device was developed to elute and concentrate high-molecular-weight DNA using a pulsed voltage. Large agarose inserts (2.7 × 6.6 × 7.2 mm) containing *Saccharomyces cerevisiae* chromosomes (200 kb–1.5 Mb) were placed in the device, and DNA was electrokinetically eluted into a recovery zone. A range of pulsed ON/OFF times, applied voltages (7.5 and 15 V), and run durations were evaluated to identify conditions that maximize DNA recovery. These results demonstrate the potential of the 3D-printed device to efficiently recover high-molecular-weight DNA for downstream genomic applications.

MWRM 2026 MW41

Reductive electrodeposition of uranium oxide materials from anhydrous uranyl triflate

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Potentiostatic deposition could be a viable method for reprocessing spent nuclear fuel, as the method employs reusable electrodes and is operationally straightforward. However, there are few studies of potentiostatic deposition of uranium conducted in non-aqueous media. In this presentation, a potentiostatic method for uranium electrodeposition from non-aqueous solutions will be discussed; our method involves formation of uranium oxide species by reduction of a “bare” uranyl ion precursor, uranyl triflate ($UO_2(OTf)_2$). With this method, we have established a relationship between electrochemical parameters and the efficiency of chemically reversible electrodeposition, aided by characterization of deposited materials with Raman and X-ray photoelectron (XP) spectroscopies. Studies with cost-friendly carbon electrodes and comparisons between a common electrolyte, tetrabutylammonium hexafluorophosphate ($TBAPF_6$), and a more chemically inert electrolyte, tetrabutylammonium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate ($TBA[BArF_{24}]$), have revealed distinct differences in chemical and electrochemical behaviors that will be discussed as well. Taken together,

our results suggest that uranyl triflate is an attractive precursor for fundamental studies of uranium electrochemistry and electrodeposition.

MWRM 2026 MW21

Reductive nitrogen metabolism by bryophyte non-symbiotic hemoglobins

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Bryophytes, an early divergent class of plants, including liverworts, mosses, and hornworts, have long been studied for the insight they provide into the evolutionary history of land plants. Studying bryophyte biochemical abilities allows for further understanding of how these abilities may have been retained or changed in more recently evolved land plants. All land plants express non-symbiotic hemoglobins (nsHbs); however, the physiological role of these nsHbs is still not well understood. Previous work by our group and others has shown that oxygen transport is not likely to be a primary function of nsHbs.
Numerous studies have found evidence that angiosperm nsHbs affect plant growth and stress responses through their ability to maintain NO homeostasis, including by participating in reductive nitrogen metabolism. Known oxygen transport hemoglobins, like human hemoglobin and myoglobin, have been demonstrated to reduce nitrite to nitric oxide and hydroxylamine to ammonium at slow rates. Higher green plants, on the other hand, express globins that have been shown to catalyze these same reactions at a much faster rate, likely because they must contend with higher nitrite concentrations, common during hypoxic conditions in waterlogged or flooded soils. We predict that by studying these same reactions in bryophyte globins, we can determine their importance in evolutionary history.
We report the kinetics of reductive nitrogen reactions by three representative bryophyte nsHbs. We found that the rates of these reactions for the bryophyte globins were as fast or faster than those of the same reactions catalyzed by other angiosperm nsHbs. These findings provide insight into the evolutionary strategies employed by early land plants as life transitioned from aquatic to terrestrial environments.

MWRM 2026 MW147

Regioselective pyridine synthesis via an iron-catalyzed [2+2+2] cycloaddition

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Multicomponent coupling is an attractive strategy in chemical synthesis. We have shown that a (β-dialdiminato)iron(I) system enables alkyne trimerization through isolable bimetallacycle intermediates. A variety of terminal alkynes cyclize via [2+2+2] cycloaddition through these complexes, leading to mixtures of two isomers resulting from bimetallacycle isomerism. Recent work has focused on incorporating multiple

components in these reactions. Particularly, when a nitrile substrate is included along with the terminal alkyne, a polysubstituted pyridine is produced in high yield as a single isomer. Optimization of the reaction conditions has led to an increase in the pyridine yield to 60-70%. Current work is focused on expanding the scope of substrates used and evaluating deactivation of the iron catalyst. For the latter, a potential byproduct has been identified using X-ray crystallography and is currently being investigated for reactivity.

MWRM 2026 MW263

Results of a regulatory assignment to determine opiate alkaloids on imported poppy seeds

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The poppy plant *Papaver somniferum* produces opiate alkaloids (OA), including morphine, codeine, and thebaine. Although poppy seeds do not contain significant amounts of OA, cross-contact can occur during harvest and post-harvest processing. The FDA is aware of consumers using poppy seeds to make a beverage known as poppy seed “tea,” in which the liquid used for steeping accumulates the OA residue from the surface of the poppy seeds. The agency has received reports of adverse events and deaths related to consumption of poppy seed “tea,” poppy seeds, and related products. To address this risk, two offices within FDA deployed an LC-MS/MS method for the quantification of morphine, codeine, and thebaine on poppy seeds, and this method was multi-laboratory validated. Subsequently, a regulatory assignment was issued, in which 11 import samples of poppy seeds from targeted high-risk firms were collected and analyzed. The most significant finding was that OA concentrations across the samples varied widely, within subsamples of a single collection, as well as across samples. Of the three OAs found in these samples, morphine is the most prevalent and typically present at the highest concentration. At least one sample showed high levels of morphine, codeine, and thebaine. While a small sample size limits broad market conclusions, this study demonstrates that OA concentrations on imported poppy seeds are highly variable. This significant variability indicates that a general assumption of safety for imported poppy seeds is not advisable, underscoring the need for additional sampling assignments and research. This work underscores the need to develop a draft guidance to establish an action level for opiate alkaloids on poppy seeds.

MWRM 2026 MW42

Reversible rare earth cation capture by Zn–Al layered double hydroxides synthesized via deep eutectic solvent route

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Rare earth elements (REEs) are indispensable for modern technologies, yet their selective and sustainable recovery from natural or secondary sources remains a significant challenge. Conventional extraction processes often require harsh chemical conditions and generate substantial waste. To address these issues, this work explores advanced functional materials capable of achieving efficient, environmentally friendly, and cost-effective REE separation and recovery. In this study, a choline chloride–urea deep eutectic solvent (DES) was employed to synthesize M–Al layered double hydroxides (LDHs; M = Mg, Co, Ni, Zn) under mild, non-hydrothermal conditions. The hydrolysis of urea in the presence of water facilitated the formation of highly crystalline, carbonate-intercalated LDHs. Among the resulting materials, Zn–Al LDH exhibited the most effective adsorption toward REEs in both single (Yb) and mixed (Yb–Nd) systems. Structural characterization using PXRD, SEM, and EDX confirmed that the Zn–Al LDH retained its crystallinity and morphology after adsorption. Importantly, the DES-derived Zn–Al LDH maintained reversible Yb adsorption–desorption performance over multiple cycles when regenerated with $Zn(NO_3)_2$ solution, demonstrating superior structural stability. Conversely, the traditional water-synthesized Zn–Al LDH showed irreversible Yb uptake despite higher initial adsorption capacity. Overall, these findings emphasize that DES-assisted synthesis effectively tailors the crystallinity, morphology, and recyclability of LDHs, providing a promising route toward reusable adsorbents for sustainable REE recovery.

MWRM 2026 MW369

Ring opening mechanism of epichlorohydrin in Sn-Beta: A DFT and microkinetic modelling study

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Epoxide ring opening (ERO) is a useful reaction in upgrading of chemicals and production of solvents and pharmaceuticals. However, its efficiency is limited by selectivity of ERO and reusability of catalytic materials. Zeolites, which are microporous silica, provide stability and ease of separation. Further, they have diverse pore environments and can be made catalytically active via various synthesis strategies. In

particular, zeolite Beta substituted with Sn (Sn-Beta) has high selectivity toward ERO due to the mild Lewis acid Sn. Sn-Beta has been found to contain distinctive sites, including closed (Sn fully coordinated within the zeolite framework), hydrolyzed-open (Sn with a hydrolyzed Sn–O bond exposing a silanol group), and open defect sites (Sn adjacent to a framework vacancy); however, the lack of knowledge regarding ERO mechanism affected by these distinctive sites limited the ability to control how synthesis and post-synthetic treatments translate into catalytic performance. Although previous studies have shown the dependence of rates and regioselectivity on solvents in Sn-Beta, how active sites in Sn-Beta affect the ERO mechanisms still lack in detail. Resolving this relationship is essential for the rational design of Sn-Beta catalysts with tailored activity and selectivity. In this study, we use ring opening of epichlorohydrin by methanol to elucidate the active site structure and mechanism underlying ERO by considering the collective effect of site type and co-catalyzation with solvent molecule methanol. DFT calculations show that open-defect sites and hydrolyzed-open sites give lower activation barrier of ring opening than closed sites. They also show that SN2 pathways are more favorable than SN1 pathways and that methanol stabilizes the transition states during ring opening. Microkinetic modelling reveals two reaction pathways: epichlorohydrin can directly open on site or mediated by a preadsorbed methanol. We found the ERO switches from directly ring opening pathway to methanol-mediated pathway with increasing methanol concentration on open-defect sites and closed site. For hydrolyzed-open site, the methanol-mediated pathway remains dominant at high/low methanol concentration. The knowledge provides detailed understanding of ERO mechanisms in Lewis acidic zeolite and will help contribute to the design of highly active and selective zeolite catalysts in the future.

MWRM 2026 MW105

RNAMotifDB: A hierarchical database of RNA secondary structure motifs for template-based tertiary structure prediction

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We introduce RNAMotifDB, a novel computational framework and database designed to support template-based prediction of RNA tertiary structures. Our pipeline begins with the systematic curation of high-resolution RNA structures from the Research Collaboratory for Structural Bioinformatics Protein Data Bank, followed by Dissecting the Spatial Structure of RNA-based segmentation to extract secondary structure motifs such as hairpins, internal loops, and bulges. The core innovation of RNAMotifDB lies in its three-tiered classification scheme: (1) geometric classification - grouping motifs by structural type and size, (2) sequence-based clustering - using configurable identity thresholds to define families, and (3) conformational grouping – leveraging RMSD - based hierarchical clustering (1.5 Å cutoff) to capture structural variants. To manage redundancy while preserving conformational diversity, we employ unweighted pair

group method with arithmetic mean clustering with International Union of Pure and Applied Chemistry (IUPAC)-coded sequence representations, selecting representative templates based on structural centrality metrics and annotate environmental features, including interactions with other nucleotides and proteins
The accompanying web platform (https://rnacossmos.com) will provide four primary functionalities: (1) sequence-based template retrieval, (2) motif identification from uploaded RNA structures via US-align structural comparison, (3) interactive 3D visualization using NGL Viewer, and (4) comprehensive downloads of curated motif templates and associated metadata. The classification pipeline has already processed a substantial number of motifs, and forthcoming validation will benchmark prediction performance against experimentally solved structures across diverse RNA families. RNAMotifDB has broad utility for the chemistry and structural biology communities: it enhances RNA 3D structure prediction by supplying curated, experimentally validated templates; supports evolutionary analyses of conserved structural elements; and serves as a teaching tool for visualizing RNA tertiary principles. Future developments include weekly updates with new PDB entries, machine learning integration for structural modeling and quality assessment, and expansion to RNA-protein interaction motifs. This resource bridges the gap between structural data and predictive modeling, offering a chemically informed and computationally robust tool for RNA structural biology.

MWRM 2026 MW32

RNA structure-based targeting of MALAT1 modulates triple-negative breast cancer cell behavior

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Triple-negative breast cancer (TNBC) is an aggressive breast cancer subtype characterized by the absence of hormone receptor and HER2 expression, leaving patients with limited targeted treatment options. Increasing evidence suggests that long noncoding RNAs (lncRNAs) play important regulatory roles in cancer progression and metastasis. One such lncRNA, MALAT1 (metastasis-associated lung adenocarcinoma transcript 1), has been implicated in tumor growth, migration, and metastatic potential in several cancers, including TNBC.
This project explores whether disrupting MALAT1 RNA stability can influence malignant behavior in TNBC cells. Small molecules predicted to interact with structural elements within the 3′ region of MALAT1 are being evaluated as potential RNA-targeting agents. Expression levels of MALAT1 will be quantified using quantitative RT-PCR in MDA-MB-468 TNBC cells and compared with nonmalignant breast epithelial cells (MCF-12A). Cytotoxicity assays will assess whether these compounds selectively affect cancer cell viability while sparing nonmalignant cells.
Beyond measuring transcript abundance, this work investigates whether destabilizing MALAT1 influences key cancer-associated phenotypes. Migration and invasion assays will be used to determine whether compound treatment alters the motility of TNBC cells. In addition, fluorescence in situ hybridization (FISH) may be used to visualize MALAT1

localization within intact cells and examine potential changes in RNA distribution following treatment.
By integrating RNA expression analysis with functional cellular assays, this study seeks to evaluate MALAT1 as a structurally targetable regulator of TNBC cell behavior. These findings may help establish RNA structure-based targeting as a promising strategy for the development of future therapeutics against aggressive breast cancers.

MWRM 2026 MW206

Room-temperature preparation of a luminescent crystalline gold chalcogenolate polymer

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Gold(I) organic chalcogenolates (Au(I)*X*) can form zero-, one-, or two-dimensional structures, with applications ranging from therapeutic activity in rheumatoid arthritis to thermochromism for temperature sensing. These Au(I)*X* hybrid molecules and materials can also serve as intermediates for the formation of gold molecular clusters and nanoparticles. We report the synthesis and characterization of a previously unreported Au(I)-methylbenzenethiol polymer and its structural solution, determined with small molecule serial femtosecond crystallography. In contrast to the synthesis of many Au(I)*X* polymers, our one-pot room-temperature synthesis results in a crystalline product without requiring elevated temperatures to induce long-range ordering. Aurophilic Au-Au interactions have been reported to drive the structural arrangements and photoluminescence of gold thiolate materials – we observe Au-Au distances as short as 3.097 A in our compound and note photoluminescence of the material under 365 nm light. Current investigations study the photoluminescent properties of this new phase and the impact of solvent choice on crystallinity.

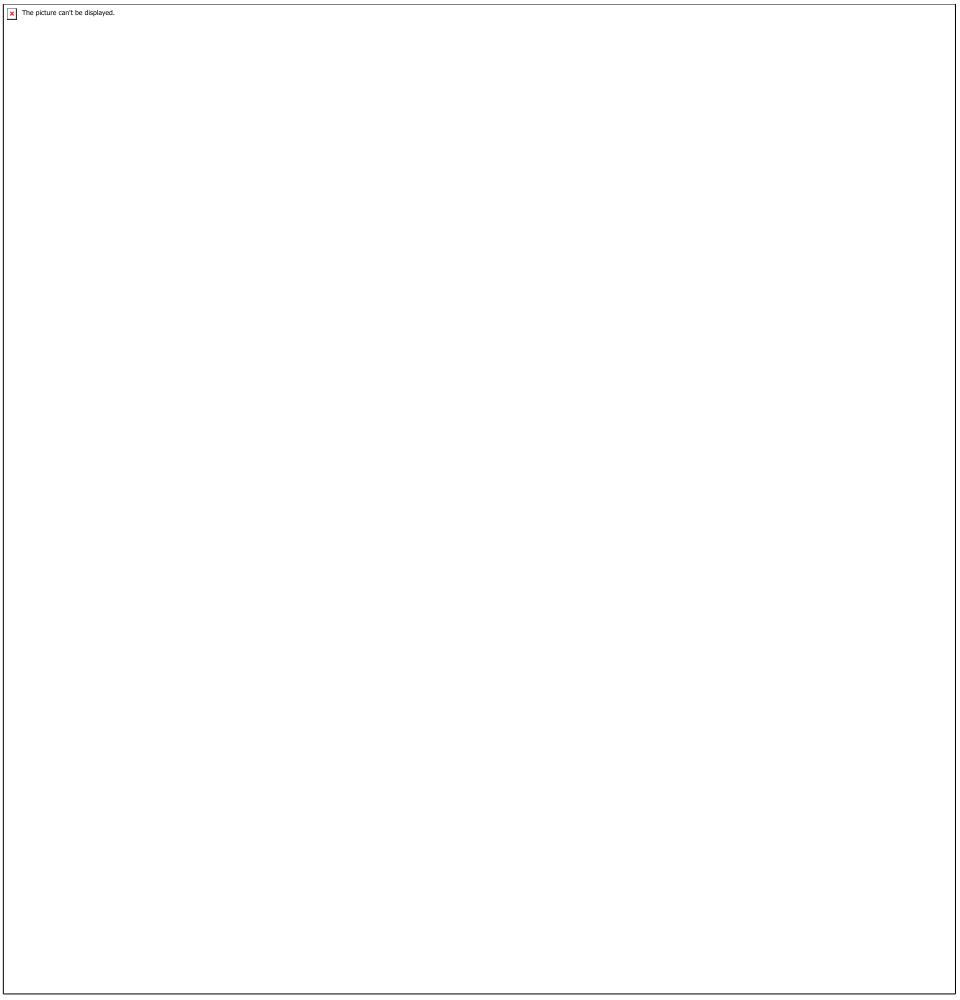
MWRM 2026 MW310

rPET at large: Smuggling sustainable Trojan units at scale

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The growing market for plastics and the mercurial market prices of fossil fuels create a great demand for a means to effectively recover these materials without leading them to deteriorate. Polyethylene terephthalate (PET), despite being the most widely produced and recycled polyester, degrades during thermomechanical recycling due to exposure to high temperatures, moisture, and oxygen-rich environments, limiting recycled material to low-end applications. In this work, we demonstrate that the incorporation of

trojan terephthalate units (i.e., dimethoxy terephthalates (DMTPA)) at low loadings (sub-5%) into PET permits Lewis acid-mediated deconstruction of the ester backbone into monomers with exposure to superheated water. These counits were synthesized through a scalable green chemistry route from dihydroxyterephthalate using dimethyl carbonate (DMC), eliminating the use of conventional toxic alkylating agents. The ortho dimethoxy moieties chelate with Lewis acids, rendering the carbonyl susceptible to electrophilic attack. Density Functional Theory (DFT) calculations further quantify the stability and reactivity criteria of the ester carbonyl by demonstrating that o-methoxy units twist the ester carbonyl out of the plane of the aromatic backbone, leaving the linkage similarly vulnerable. Upon incorporation in the polymeric backbone, these units lowered the overall crystallinity and suppressed the melting point. This ultimately led to a dampened diffusion barrier, enabling rapid depolymerization. We validated this strategy at pilot scale, producing ca. 100 kg of DMTPA-PET resin and demonstrating complete drop-in compatibility with existing manufacturing infrastructure through commercial-scale blow molding of bottles. Thus, this work establishes a molecular design strategy for engineering triggered recyclability directly into the PET backbone, offering a swift, scalable path towards closed-loop recycling.



MWRM 2026 MW12

Screening of bioactive algal lipids as natural antimicrobial agents

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The increasing prevalence of pathogens developing resistance to antibiotics has intensified the search for new antimicrobial agents that can provide a solution to this crisis of the future. Algae-derived lipids show promise as natural antimicrobial agents due to their ability to disrupt bacterial membrane integrity through both hydrophobic and amphiphilic interactions. Algae-derived bioactive lipids and glycolipids can alter membrane permeability and interfere with microbial growth, providing an alternative membrane-targeting strategy for the development of antimicrobial agents.
Our preliminary investigation with lipid extracted from wild algal strains occurring in the local surface basins of the Central Valley community showed inhibition for microbial assays conducted via Kirby-Bauer disk diffusion susceptibility test with Gram-positive and Gram-negative bacteria. Analyses of the bioactive constituents present in the algal oil and validation of its antimicrobial properties are currently ongoing. The results will implicate the capacity of these algae-derived bioactive lipids potency to compromise the integrity of bacterial membrane and thereby its potential to function as natural antimicrobial agents.

MWRM 2026 MW165

Screening small molecule benzannulated indole libraries against sinonasal undifferentiated carcinoma (SNUC)

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Sinonasal undifferentiated carcinoma (SNUC) is a rare and aggressive type of cancer originating in the epithelium layer of the nasal cavity or paranasal sinuses. First described and diagnosed in 1986 by Frierson as a distinct pathological entity, there are about only 200-400 known cases in the United States at present. The aggressive nature of the disease coupled with the stage of disease (clinically advanced and surgically unresectable) upon presentation lead to a poor survival rate. There is no standardized treatment. Several investigational drugs for SNUC include DNA repair inhibitors, poly ADP-ribose polymerase (PARP) inhibitors (olaparib/Lynparza), ataxia telangiecstasia mutated and Rad-3 Related (ATR) inhibitors (AZD6738), bromodomain and extra-terminal (BET) inhibitors (ODM-207). In this presentation we describe the screening of novel benzannulated indoles related to the trikentrins and herbindoles and their precursors against stable, human-derived SNUC cell lines as potential chemotherapeutic agents.

MWRM 2026 MW322

Selective degradation of the SARS-CoV-2 main protease (Mpro) through the application of proteolysis-targeting chimeras (PROTACs)

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Three COVID pandemics brought on by SARS-CoV have been documented in the last 20 years. Among the many coronaviruses, the main protease (M^{pro}) is highly conserved and essential for viral replication and pathogenicity, making it a desirable target for antiviral drug development. The recent development of first-in-class PROTAC degraders targeting M^{pro} marks a significant advancement in the field. Understanding the molecular mechanism underlying the PROTAC interaction with M^{pro} and CRBN could help optimize the design and efficacy of these degraders. We hypothesize that the PROTACs employed in this research will bind to specific regions of the M^{pro} and CRBN proteins and promote their binding. In the current work, we have developed a model of the M^{pro}-CRBN complex that enables us, for the first time, to perform molecular docking simulations to study the mechanism of M^{pro}-PROTAC-CRBN binding. The docking results were further validated by using machine learning and graph neural network methods to compare the M^{pro}-CRBN druggable site. We propose that M^{pro} and CRBN form a partially enclosed cavity where PROTAC binds during interactions. Finally, multiple PROTACs were rationally designed by introducing chemical mutations and docked onto the M^{pro}-CRBN protein complex. Based on our simulations, we have determined that PROTAC I and VII exhibit strong binding affinity to both target proteins. This work, with its potential to contribute to the fight against COVID-19, will aid targeted delivery of M^{pro} inhibitors and facilitate the development of potent, cost-effective, and low-side-effect PROTACs.

MWRM 2026 MW189

Selective diamondoid functionalization using direct photochemical methodologies

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Diamondoids are rigid caged hydrocarbons that can be superimposed upon the diamond lattice. The simplest member of the family, adamantane, and its derivatives have found widespread use in medicinal chemistry, materials science, and ligand design, while the more complex members of the family, starting with diamantane, have been largely unexplored and unutilized. Selective functionalization of these molecules is challenging as the number of very similar types of C–H bonds (secondary, 2°, and tertiary, 3°) increases rapidly. Using highly oxidizing pyrylium photocatalysts, we explored the prospect of direct oxidation of the diamondoids to capitalize on the

properties of the resultant radical cation to generate a neutral radical species after deprotonation and create C–C bonds from that. More recently our investigations have turned to the use of quinone species to facilitate catalytic formal hydride abstraction to generate C–N bonds selectively at the medial 1-position of diamantane with a variety of azole coupling partners such as pyrazoles, triazoles, and tetrazoles. Intermediate studies indicate a role for the HFIP solvent in trapping the less stable apical carbocation which remains inert in the reaction conditions unlike HFIP-trapped medial cations which can be converted much more readily. This transformation occurs under mild, air tolerant conditions in blue or near UV light and accomplishes the transformation directly from the hydrocarbon while most literature methods require additional prefunctionaliztion steps.

MWRM 2026 MW114

Selective formation of 1- and 1,8-substituted fluorenones and synthesis of fluorenylspirocyclopropene compounds

***John N. Brunn**, john.brunn@outlook.com, Ismael Nieto, Rami Batrice, Jaqueline L. Kiplinger. Los Alamos National Laboratory, Los Alamos, New Mexico, United States*

Fluorenes and fluorenones represent important classes of aromatic compounds noted for their fluorescent properties that find utility as optical materials, fluorescent tracers, and precursors to ligands for organometallic complexes, particularly Group III and IV transition metal catalysts. The syntheses of these classes of compounds often involve multi-step sequences that limit the functional group tolerance, yield, and selectivity of the desired products. Herein, we report improved reaction conditions to selectively furnish 1- and 1,8-substituted fluorenones in high yield. The success of this new synthetic route relies on a key bis-glyme ketal of fluorenone, which is formed in two steps from commercially available fluorenone. These fluorenone products enabled our foray into the synthesis of sterically congested fluorenylspirocyclopropenes, which are formed in a single step using diazofluorene derivatives and trimethylsilylacetylene.

MWRM 2026 MW114

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MWRM 2026 MW306

Selective nitrogen insertion functionalization of styrenic polymers

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Post-polymerization modification (PPM) provides a powerful means of introducing new functionality into pre-existing polymer frameworks without redesigning the underlying polymer synthesis. However, polymers containing inert hydrocarbon backbones often lack accessible reactive handles for such modification, limiting the structural diversity achievable through conventional methods. This work explores a new strategy for selectively incorporating nitrogen into polymers with inert backbones, offering an alternative route to nitrogen-functionalized materials with tunable properties. This poster highlights our progress in applying this strategy to styrenic polymers, demonstrating a viable route toward nitrogen-functionalized polymer scaffolds.

MWRM 2026 MW353

Self-assembly of gold-binding peptides on graphite

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Solid-binding peptides (SBPs) have emerged as versatile molecular building blocks because of their high affinity and selectivity toward specific inorganic surfaces. These short amino acid sequences can recognize and bind to target materials, making them promising candidates for applications such as enzyme immobilization, biosensing, nanofabrication, and biomaterial surface modification. In this study, the self-assembly behavior of two gold binding peptides, AuBP1 (WAGAKRLVLRRE) and AuBP2 (WALRRSIRRQSY), was investigated on graphite using atomic force microscopy (AFM). Graphite was selected as a hydrophobic surface to examine the nonspecific adsorption of these peptides in comparison to their well-known affinity for gold. The effects of peptide concentration, solution pH, adsorption time, and ionic strength on surface coverage and assembly morphology were studied. AFM imaging revealed variations in peptide organization under different experimental conditions, demonstrating that environmental parameters significantly influence peptide adsorption and self-assembly on graphite. These observations provide insight into the mechanisms governing peptide surface interactions beyond their target material. This work

establishes a foundation for understanding the behavior of these peptides on hydrophobic substrates and provides a basis for comparison with their interactions on gold. Future studies will extend this investigation to other different materials, including mica and self-assembled monolayers (SAMs), to develop a broader understanding of peptide adsorption across surfaces with different physicochemical properties. Such knowledge will contribute to the rational design of peptide-based surface functionalization strategies for further applications.

MWRM 2026 MW307

Sequential post-polymerization modification via amide activation and click chemistry

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Post-polymerization modification (PPM) offers a powerful route to functionalized polymers that are difficult to access through direct polymerization of functional monomers. This poster presents a sequential PPM strategy that first utilizes keteniminium-mediated functionalization to install reactive handles onto a polymer backbone, followed by click-chemistry conjugation. The reactivity and efficiency of this copolymer were demonstrated through a model copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC). In this work, this sequential strategy is utilized for the synthesis of multifunctional glycopolymers, opening a wide range of potential applications in targeted biotechnology.

MWRM 2026 MW339

Simplified TDDFT in CP2K: Efficient optical spectra of thiolate-protected gold nanoclusters

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The optical spectra of ligand-protected metal nanoclusters encode their electronic structure but simulating them with conventional time-dependent DFT becomes prohibitively expensive as cluster size grows, owing to the dense manifolds of low-lying excitations that accompany increasing core size. We present an implementation of simplified time-dependent density functional theory (sTD-DFT) [Bannwarth & Grimme, 2014] in the open-source CP2K package. The method replaces costly two-electron integrals with damped Coulomb interactions between Löwdin transition charges, accelerating spectral calculations by orders of magnitude while retaining the full response structure, including the de-excitation contributions that are absent from the sTDA kernel but are essential for reliable transition intensities. The implementation is validated against reference sTD-DFT codes on standard organic benchmark sets, and against conventional TDDFT results obtained with independent electronic-structure

packages at matched levels of theory. For the prototypical thiolate-protected cluster $[Au_{25}(SH)_{18}]^-$,sTD-DFT reproduces the experimental absorption profile and the underlying transitions with accuracy comparable to full TDDFT at a fraction of the computational cost, and its excitation energies and relative band intensities agree closely with published TDDFT results for this system. This work provides the nanocluster community with an efficient, freely available tool for simulating optical spectroscopy, opening a path to optical spectra of substantially larger gold and silver nanoclusters.

MWRM 2026 MW215

Simulations of ions diffusion with multilayer QM/MM adaptive partitioning methods

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Deciphering the mechanism of ion/molecule transport across transmembrane transport proteins, such as the NarK nitrate/nitrite antiporter, is a key step in understanding the protein's structure-function relations and how they are affected by mutations. Molecular dynamics simulations of these diffusion processes with static-boundary QM/MM methods are impractical due to the need of an exceedingly large QM zone to include the entire transmembrane pore and solvent molecules that may be involved in the ion solvation, which is computationally expensive. We hereby introduce adaptive-partitioning multilayer (APML) Q1/Q2/MM methods, where the protein residues and solvent molecules can be reclassified *on the fly* as Q1 (high level QM), Q2 (low level QM) or MM, depending on how important they are to the ion/molecule solvation through the transport process. Such importance is conveniently measured based on their evolving distances from the diffusing molecule or ion, although the use of other metrics is principally straightforward. Test computations demonstrate continuous energies and gradients for anion movements in a nitrate-water cluster model and in a model of NarK anion binding site. The new development opens the door to more efficient and accurate molecular dynamics simulations of the transport processes in complex environments.

MWRM 2026 MW142

Single molecule resolution dSTORM imaging with axially swept light-sheet microscopy

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Super-resolution microscopy has played a critical role in many advances in structural biology, allowing for the imaging of nanoscale structures using light-based microscopy techniques. Currently, widely used microscopy techniques used, such as confocal and

Total Internal Reflection Fluorescence (TIRF) microscopy, are lacking in their ability to image thick samples. Limiting sample selection to cultured cells or requiring extensive sample preparation techniques such optical clearing. An Axially Swept Light-Sheet Microscopy (ASLM) was built using an electronically tunable lens (ETL) to control the location of the waist, the thinnest portion of the light-sheet and allows for the waist to be scanned axially during imaging. Paired with Direct Stochastic Optical Reconstruction Microscopy (dSTORM), a technique that uses high powered lasers to induce blinking in fluorophores to generate super-resolution images by combining multiple frames, ASLM was used to produce super-resolution images of HELA cells. These images show the capability of ASLM as an optical sectioning technique and highlight the possibility of ASLM being used to image whole tissue samples at single molecule resolution.

MWRM 2026 MW289

Single-site bismuth alkoxide catalysts for the stereoselective ring-opening polymerization of *rac*-lactide

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Given the magnitude of the global plastic pollution problem, controlled methods for polymerizing bioderived monomers such as *rac*-lactide (*rac*-LA) are highly sought-after. While many metals, including, but not limited to tin, aluminum, and zinc have been investigated as Lewis acid catalysts for the ring-opening polymerization (ROP) of *rac*-LA, bismuth has gone largely unexplored, especially in the context of polymerization stereocontrol. In this work, three, single-site bismuth alkoxide catalysts bearing salen-type ligands with two-carbon, three-carbon, and binapthalene backbones were synthesized, characterized, and used for ROP of *rac*-LA. Notably, the Bi-based catalysts consistently yield highly heterotactic poly(lactide) in solvent (P_r > 0.99) and are extremely efficient and stereoselective as melt polymerization catalysts, achieving over 80% monomer conversion in minutes, while maintaining heterotactic enrichment in the polymer with P_r values of ~0.8–0.9. Moreover, both solvent and melt polymerization studies show good polymerization control, yielding polymers with narrow polydispersities and high molecular weights. The impact of ligand backbone flexibility on catalyst efficiency is examined and the role of monomer binding in the polymerization mechanism is probed. Finally, the relative air-stability of the catalysts is explored. Remarkably, comparable polymerization data is achieved when polymerizations are set up under normal, ambient conditions vs. those that are set up within an inert, N_2-filled glovebox.

MWRM 2026 MW287

Size-dependent effects of a hydrophobic solute on water structure and dynamics

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The interaction of water with hydrophobic solutes and interfaces is ubiquitous in chemistry and biology, yet key questions remain about the relative role of energetic and entropic driving forces. Here we use molecular dynamics simulations to investigate the effect of a spherical hydrophobic solute in water on the solution structure and dynamics. The emphasis is on the driving forces, *e.g.*, activation energies for dynamics and energetic and entropic contributions to the free energies determining structures. We particularly consider the effect of the solute size, which affects the hydrogen-bonding arrangements of the surrounding water molecules. Specifically, we use the fluctuation theory for dynamics to determine the water and hydrophobic solute dynamics, focusing on the diffusion coefficients and the associated activation energies. These are compared in the context of the solution structure, as represented in the pair radial distribution functions. The relative role of these effects in understanding the observed behavior as a function of solute size is examined and discussed. We see that the solution dynamics is both entropically and energetically driven. The solute diffusion has a significant entropic component, and water behavior is a bit more complex.

MWRM 2026 MW305

Skeletal editing of diene rubbers for controlled depolymerization

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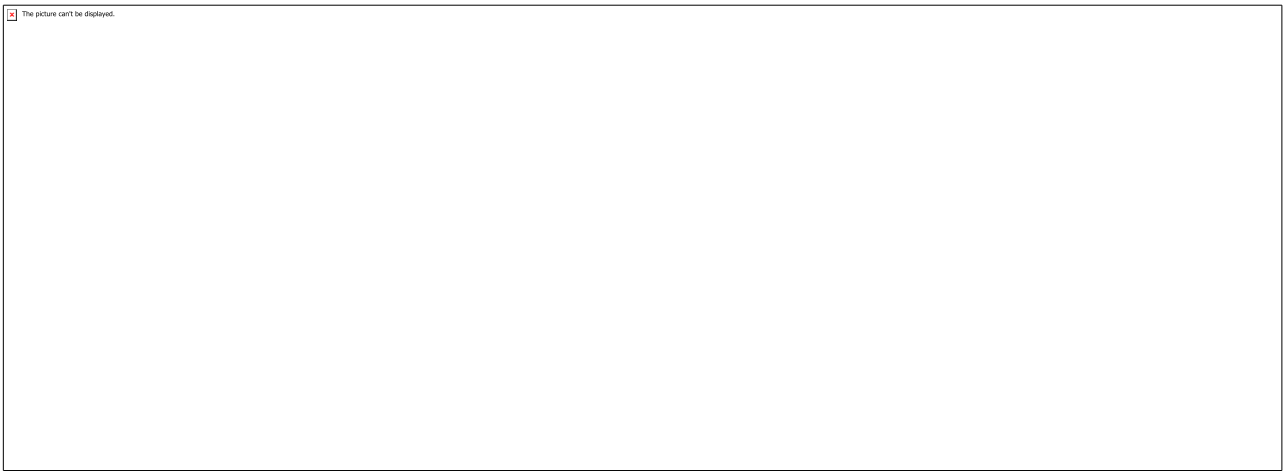
Diene rubbers like polybutadiene are made on a megaton scale and pile up as persistent waste, yet their carbon–carbon backbones offer limited option for controlled deconstruction. We show that a mild skeletal-editing reaction, redirected from small molecules to macromolecules, can serve as a general depolymerization strategy. Under mild, open-flask conditions, widespread backbone cleavage was observed in a tunable fashion. The resulting telechelic fragments can be re-functionalized, transforming commodity and post-consumer rubber into value-added building blocks for future use. To our knowledge, this is the first application of this chemistry for controlled polymer depolymerization.

MWRM 2026 MW361

Slower motions and dramatic conformational populations present in A:G mismatched DNA phosphates

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Mismatches such as A:G base pairs arise in DNA primarily due to improper nucleotide incorporation during replication as well as formation of a heteroduplex. Repair of these mismatches and prevention of deleterious mutations is vital to an organism's survival. Mismatch Repair (MMR) is the primary repair pathway for general DNA mismatches and follows replication to maintain genomic integrity; however, some details of mismatch recognition are unknown. Repair invariably requires precise and localized DNA-protein interactions and binding processes that depend on the specific properties, such as conformational structure and dynamics, of the repair protein and the damaged dsDNA substrate. Therefore, it is likely that the conformational properties of damaged, mismatched or modified DNAs will be different than canonical duplexed DNA. The work herein demonstrates a dramatic shift in timescale of motions and conformational populations for the phosphate flanking an A:G mismatched base pair. 31P NMR results show the motions are in the intermediate timescale (10^{-3} sec) which is orders of magnitude slower than prior results (10^{-5}–10^{-9} sec), and the population of the BII substate shifts to ~99%. These perturbations could be utilized in a phosphate tracking mechanism during indirect readout by repair enzymes such as MutS.



MWRM 2026 MW159

Small Science, Big Impact

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Addressing global crises in clean water, climate, and dwindling critical mineral resources demands a fundamental shift in how we understand chemical systems. This award lecture reflects on my career-long journey to uncover how “small science” — the molecular-level understanding and control of nanoscale interfacial processes and solid nucleation — can generate “big impact” across three pillars of sustainability: subsurface energy and carbon management, advanced nanomaterials for water purification, and resource recovery within a circular economy. Meeting these grand challenges requires decoding the atomic- and nanoscale mechanisms that govern them. At Washington University in St. Louis, the Environmental NanoChemistry Laboratory has advanced *in situ*, real-time, quantitative approaches that reveal complex chemical reactions at solid-water-gas interfaces.

Our research has helped shape the frontiers of the water-energy-resource nexus. In subsurface energy systems, we have uncovered the mechanisms of mineral nucleation in highly confined environments, informing safer and more effective strategies for geologic carbon dioxide sequestration and mineralization, underground hydrogen storage, and enhanced geothermal systems. In water purification, we have developed advanced nanomaterials, including bio-inspired photothermal materials and tailored nanostructures, to enable more sustainable and energy-efficient desalination. In resource recovery, we have leveraged nanoparticle nucleation and interfacial chemistry to engineer selective pathways for harvesting critical elements for energy technologies (*e.g.,* lithium, nickel, cobalt, and rare earth elements), as well as nutrients such as ammonia and phosphate, from unconventional resources. Ultimately, this lecture will illustrate how fundamental advances in solid nucleation and nanoscale interfacial chemistry can transform environmental liabilities into sustainable assets and help define a more resilient future.

MWRM 2026 MW253

Sodium versus lithium: How solvation improves battery behavior

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Increasing demand for lithium-ion (Li-ion) batteries necessitates diversification of battery materials to ease the strain on supply chains. Other alkali metals, such as sodium (Na),

are intriguing due to their global abundance. Owing to differences in atomic size and reactivity, research on lithium is not always directly transferable to sodium batteries. Herein, we compare LiTFSI and NaTFSI electrolytes in blends of diglyme and fluoroethylene carbonate. We initially observed with optical microscopy that Na systems electrodeposit more smoothly than Li in diglyme blends, motivating our subsequent measurements that show Na^+ interacting weakly with diglyme compared to Li^+. This causes profound effects on solution dynamics, manifesting in faster Na^+ transport. In support of this conclusion, we use fringe field NMR, viscosity-conductivity analysis, and molecular dynamics simulations to show that Na^+ moves more freely than Li^+, particularly in solvent blends dominated by diglyme. Ultrafast infrared techniques, including pump–probe anisotropy, show that Li^+ tends to structure the solvent more rigidly than Na^+, and this ordering effect can be sensed by distal molecules such as carbonate additives. In summary, our findings contribute to the emerging consensus that electrolytes engineered with weak solvation improve transport and charge transfer kinetics, highlighting the potential of Na-based systems as a more abundant alternate to Li-ion batteries.

MWRM 2026 MW275

Solute diffusion in nanoconfined partially miscible n-butanol/water mixtures

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Understanding molecular transport in nanoconfined liquid mixtures is essential for the rational development of high-performance membrane separation technologies. In this work, fluorescence correlation spectroscopy (FCS) and confocal Raman spectroscopy were employed to investigate the diffusion of Rhodamine B (RhB) in partially miscible *n*-butanol/water mixtures confined within anodic aluminum oxide (AAO) membranes containing 10 and 20 nm diameter nanopores. Mixtures spanning compositions from pure *n*-butanol to the bulk miscibility boundary were examined to determine how confinement influences solvent organization and solute transport. Raman measurements show that the confined liquid composition closely follows that of the bulk over most of the composition range, while a transition to a water-dominant environment occurs as the miscibility boundary is approached. The Raman spectra further indicate that the hydrogen-bonding network remains bulk-like in 20 nm pores but is partially disrupted in 10 nm pores, reflecting stronger interfacial effects under tighter confinement. FCS measurements reveal two distinct diffusion modes: a fast, bulk-like component associated with transport through the pore center and a slower, surface-mediated component governed by adsorption/desorption at the pore walls. The fast diffusion mode is only modestly slower than in bulk solution, whereas the slow mode strongly depends on RhB solubility and partitioning. Comparison of the two pore sizes demonstrates that pore surface chemistry, rather than geometric confinement alone, primarily controls the observed transport behavior. These findings establish a mechanistic framework linking solute partitioning, interfacial structure, and desorption-mediated diffusion in partially miscible nanoconfined liquids, providing new strategies for

tailoring chemical separations in nanoporous membranes through surface chemistry and confinement-induced phase behavior to improve separation performance.

MWRM 2026 MW234

Spectroscopic and mechanistic study of a manganese cerium adduct: Effect of electron-donating ligand on selectivity

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Cerium(IV) ammonium nitrate (CAN) is one of the most widely used cerium(IV) reagents in organic chemistry due to its high reduction potential (+1.61 V vs NHE), low toxicity, ease of handling, and good solubility in organic solvents. It generally acts as an efficient one-electron oxidant under mild conditions. Beyond organic reactions, CAN has also been shown to react with Fe(II) and Mn(II) complexes to form high-valent metal(IV)–oxo species, where the oxo ligand originates from water. Because the Ce(IV) centre can function both as a strong oxidant and as a Lewis acid, a variety of reaction pathways can occur, leading to structurally different intermediates. In some cases, mononuclear metal(IV)–oxo complexes are formed, while in others, oxo-bridged metal–cerium adducts are obtained. This variation raises an important question: which factors determine whether a metal–oxygen–cerium adduct, a terminal metal–oxo species, or other products form? In this context, a $[Mn^{IV}(O)(dpaq)]^{+}$–Ce^{4+} complex was previously reported by Nam and co-workers through the reaction of $[Mn^{III}(OH)(dpaq)]^{+}$ ($dpaq^{H}$ = 2-[bis(pyridin-2-ylmethyl)] amino-N-quinolin-8-yl-acetamido) with CAN. It has also been shown by Hitomi and co-workers that $dpaq^{5R}$ ligands with para-substituents on the amide nitrogen (R = OMe, H, Cl, NO_2) can significantly affect the Mn reduction potentials in $[Mn(dpaq^{5R})(NO)]ClO_4$ complexes. To better understand these effects, the reactivity of CAN with the Mn^{III} complex $[Mn^{III}(OH)(dpaq^{5OMe})]^{+}$ has been investigated, in which the electron-donating methoxy group stabilises higher oxidation states of manganese. In addition, the oxygen-atom transfer and hydrogen-atom transfer reactivity of the resulting manganese–cerium adduct intermediate has been examined and compared with previously reported Mn–Ce systems. Through these studies, clearer insight into the factors controlling reactivity and product formation in these systems is obtained.

MWRM 2026 MW224

Spectroscopic characterization and extraction optimization of catechins in green tea

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This research initiative immerses students in a multifaceted analytical chemistry investigation of catechins—polyphenolic antioxidants prevalent in green tea—through

the application of both classical and modern techniques. The project emphasizes hands-on experience with real-world sample analysis, method development, and critical data interpretation.
Catechins were extracted from various commercial green tea products, including loose leaves, powders, and dietary supplements, by trituration with ethyl acetate followed by solvent partitioning using a methanol and water solution. The resulting extracts were analyzed using UV-Visible spectroscopy to quantify catechin content. Selected samples were further characterized by liquid chromatography–mass spectrometry (LC-MS), confirming both the identity and purity of catechins and validating the effectiveness of the developed isolation protocol.
To enhance student understanding of electronic transitions and structure–property relationships, quantum chemical calculations were performed using Gaussian software. Theoretical UV-Vis spectra, generated via time-dependent density functional theory (TD-DFT), were compared with experimental data, allowing students to explore the relationship between molecular structure and spectroscopic behavior.
This integrated laboratory experience reinforces core analytical chemistry concepts—separations, spectroscopy, and computational modeling—while promoting scientific inquiry and interdisciplinary learning. Designed to be scalable and accessible in standard undergraduate teaching laboratories, the experiment also supports further exploration through pH-dependence studies, stability assessments, and statistical evaluation of extraction efficiency. This research-centered model will enhance student engagement and foster the development of practical analytical skills in the context of natural product analysis.

MWRM 2026 MW444

Spectroscopic investigation of the role of acid-base sites toward C-C bond formation on TiO2-based nanomaterials

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To determine the role of acid-base sites on $GaInTiO_2$, ammonia and acetaldehyde adsorption were examined at different temperatures using a specially designed ultra-high vacuum (UHV) infrared cell. The UHV cell is attached to a vacuum manifold which is continually pumped by a 60 L turbomolecular pump and a diaphragm roughing pump to obtain a routine pressure of $1x10^{-8}$Torr. It was found that at 233 K, acetaldehyde adsorbed through hydrogen bonding to surface hydroxyl groups as well as through Lewis acid sites over pretreated $GaInTiO_2$ surface. The formation of 2-butenal was observed as the product of aldol condensation reaction. This C-C bond formation is found to be due to the presence of Bronsted and Lewis acid sites. Upon controlling these sites with NH3 adsorption, the C-C bond formation can be totally suppressed, which in turn indicates that acid sites indeed are responsible for C-C bond formation.

MWRM 2026 MW237

Spectroscopic properties and reactivity of a Mn^{III}-hydroperoxo complex that is stable at room temperature

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The manganese lipoxygenase enzyme (MnLOX) which converts polyunsaturated fatty acids to alkyl hydroperoxides is found in fungi and plants to allow further metabolization of these substrates. It is proposed that the substrate oxidation is initiated by the transfer of a hydrogen atom from the C-H bond of the substrate to an active-site Mn^{III}-hydroxo center. Inspired by these enzymes, there are many examples of synthesized model manganese complexes to study the active site of enzymes. These synthesized models were able to activate H_2O_2 to conduct a series of reactions such as sulfoxidation, olefin epoxidation and C-H bond activation with high selectivity. It is generally proposed that in both enzyme and synthesized Mn catalysts a Mn^{V}-oxo is the key intermediate which is formed from the O-O bond cleavage of a Mn^{III}-hydroperoxo. This Mn^{III}-hydroperoxo intermediate possesses critical role in Mn catalytic cycle but there are a few reports on them. In this study, we formed a Mn^{III}-hydroperoxo supported by an amide-containing, pentadentate ligand ($dpaq^{6Me}$). The Mn^{III}-hydroxo complex $[Mn^{III}(OH)(^{6Me}dpaq)]^{+}$ reacted with H_2O_2 and $HClO_4$ to form a green intermediate, with a UV-vis band at 615 nm. On the basis of ^{1}H NMR, ESI-MS, EPR, FT-IR, and EPR data, we formulate this new intermediate as the Mn^{III}-hyrdroperoxo complex $[Mn^{III}(OOH)(^{6Me}dpaq)]^{+}$. This complex reacts with 10 equivalences of PPh_3 at 15 °C, and with 30 equivalences of TEMPOH at -35 °C. Based on kinetic studies, $[Mn^{III}(OOH)(^{6Me}dpaq)]^{+}$ reacts 600-fold faster with PPh_3 than its Mn^{III}-alkylperoxo analogue $[Mn^{III}(OO^{t}Bu)(^{6Me}dpaq)]^{+}$, and two-fold faster with TEMPOH than a similar Mn^{III}-hydroperoxo complex $[Mn^{III}(OOH)(dpaq^{2Me})]^{+}$. Time dependent computations (TD-DFT) were applied to compare electronic features of $[Mn^{III}(OOH)(^{6Me}dpaq)]^{+}$ with analogous Mn^{III}-hydroperoxo and Mn^{III}-alkylperoxo complexes.

MWRM 2026 MW341

Spin-phonon driven decoherence of molecular qubits in an open quantum system

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Molecular spin are promising candidates for quantum information science (QIS) due to their high tunability and potential to operate at ambient temperatures. A key feature for a successful qubit is its coherence, or its ability to maintain superposition. In the low temperature limit, coherence loss, or decoherence, is dominated by pure dephasing while, at moderate temperatures, the mechanism is more complex. An open quantum system framework is beneficial for modeling environmentally driven decoherence as it considers the interaction between the molecular system and its environment. Phonon

interactions are of particular interest as they contribute to population relaxation, which limits coherence lifetimes. We rely on *ab initio* electronic structure methods to parameterize open quantum system methods and then obtain environmentally driven dynamics. The leading approach in computing papulation relaxation times involves finite differences methods, which include a large number of electronic structure calculations. Alternatively, linear vibronic coupling (LVC) has been proposed as a cheaper alternative. This work aims to adapt a LVC model, previously used for single molecule magnets, and compare it to the finite differences method for decoherence in molecular spin qubits. Investigating how spin-phonon driven population relaxation contributes to decoherence can help inform molecular design principles.

MWRM 2026 MW05

Stabilization of aryl diazonium groups for intracellular affinity-driven labeling of proteins

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Cellular signaling is mediated by small molecules, proteins, or peptide ligands that activate surface receptors to initiate biochemical pathways. Affinity-driven labeling techniques have been developed to probe these interactions by converting the receptor-ligand interaction into a covalent linkage between the two molecules. Current intracellular labeling systems use photoreactive species that remain inert until released by light, but these techniques lack protein selectivity, resulting in off target reactivity and reduced labeling efficiency. The off-target reactivity of these techniques led us to explore aryl diazonium chemistry as a strategy for intracellular affinity-driven labeling because of its selectivity for tyrosine and histidine residues in proteins. Aryl diazonium chemistry successfully labels extracellular targets but has shortcomings for intracellular labeling of protein-protein interactions due to the aryl diazonium's instability at physiological conditions. While some modified aryl diazonium species have been developed to enhance the stability of the aryl diazonium, these species may not be stable enough to pass through the cell membrane and label an intracellular target. To address these shortcomings, we envisioned adding a photocleavable protecting group onto the aryl diazonium ion, which couples the controlled release of photoreactive groups with the protein selective properties of the aryl diazonium. The triazene group has been shown to provide stability to the aryl diazonium at biological conditions with reversible photocleavable and acid labile properties. We have shown that a triazene

protecting group can be added to an aryl diazonium-containing peptide, released by pH or light, and recaptured by phenol. Further studies will determine whether the triazene group can efficiently undergo photocleavage for affinity-driven labeling of intracellular proteins. This work looks to establish the first photocleavable, affinity-driven labeling system providing a method for the identification of novel intracellular receptor-ligand interactions.

MWRM 2026 MW139

Stereochemical evaluation of cell-cell signaling peptides in *Platynereis dumerilii*

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Platynereis dumerilii, a marine annelid, produces proneuropeptides throughout its lifetime. These inactive precursors are cleaved into neuropeptides, which are modified to perform various functions. As the annelid grows, proneuropeptide transcript expression decreases, suggesting neuropeptides are crucial in early development. One understudied neuropeptide modification is the conversion of an L-amino acid to its corresponding D-amino acid, forming a D-amino acid-containing peptide (DAACP). Only two receptor classes are known to recognize DAACPs for endogenous cell signaling: the achatin receptor in both *P. dumerilii* and *Aplysia californica* and the allatotropin-related peptide (ATRP) receptor in *A. californica.* Because L-ATRP and D2-achatin contributes to cell-cell signaling in both organisms, we hypothesize that juvenile *P. dumerilii* endogenously produces L- and D2-isomers of achatin and ATRP.
We synthesized isotopically labeled peptide standards $^{13}C_2$-L-achatin and $^{13}C_2$-D2-achatin for the identification of endogenous L- and D2-achatin within the animal. For the identification of L- and D2-ATRP, *P. dumerilii* neuropeptide extracts were digested with Asp-N for identification of the shorter, truncated analogues. Therefore, isotopically labeled $^{13}C_6{}^{15}N_4$-L-ATRP (1-7), $^{13}C_6{}^{15}N_4$-D2-ATRP (1-7), and $^{13}C_6{}^{15}N_4$-L-ATRP (8-14) were synthesized. The use of isotopically labeled synthetic peptides ensured that the synthetic standards would not be mistaken for endogenous peptides when performing multiple reaction monitoring (MRM). The co-elution of the synthetic and endogenous peptide provided strong evidence that the correct diastereomer was identified. Further verification of the endogenous peptides was determined through MS/MS fragmentation and *de novo* sequencing.
These experiments revealed that *P. dumerilii* endogenously produces both L- and D2-achatin, as well as endogenous L-ATRP, but not D2-ATRP within the detection limits of these experiments. Endogenous neuropeptides were identified and confirmed by the co-elution of isotopically labeled peptide standards and the verification of fragment ions: b_2 and y_2 for L- and D2-achatin, b_3, b_5, b_6, and y_5 for L-ATRP (1-7), and b_4, b_5, and b_6 for L-ATRP (8-14). These novel findings indicate that DAACP-producing organisms do not produce the same DAACPs, suggesting these peptides serve specific biological functions.

MWRM 2026 MW64

Stereoselective α-sialylation through electrophilic peroxide–enabled etherification

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Sialylated glycans participate in numerous biological recognition processes, including pathways associated with cancer immune evasion, multidrug resistance, and metastasis. However, the chemical synthesis of α-linked sialosides remains challenging because formation of the sterically hindered, equatorial anomeric linkage is complicated by the adjacent electron-withdrawing carboxylate, the absence of effective neighboring-group participation, and competing elimination pathways. This work investigates electrophilic peroxide–enabled etherification as a mechanistically distinct approach to constructing the α-alkoxy carboxylate acetal motif characteristic of sialic acid. Our strategy employs protected glucose- and galactose-derived tetrahydropyranyl monoperoxyacetals as electrophilic alkoxyl-transfer reagents. These substrates are coupled with an α-alkoxy ester nucleophile generated from methyl tetrahydropyran-2-carboxylate, providing a simplified model for formation of the sialic acid anomeric C–O bond. Protected carbohydrate monoperoxyacetal electrophiles have been synthesized and characterized, and ongoing studies are evaluating the effects of base identity, counterion, solvent, temperature, and reaction stoichiometry on productive coupling and peroxide decomposition. Product formation and stereochemical outcomes are being assessed using chromatographic, mass-spectrometric, and multidimensional NMR techniques. These studies will establish the feasibility and controlling factors of peroxide-mediated glycosyl ether formation and provide a foundation for extending this chemistry to stereodefined α-sialylated glycans for use as cancer-associated glycan probes.

MWRM 2026 MW211 - Withdrawn

MWRM 2026 MW68

Stripping-induced acidification accelerates zinc anode corrosion

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Aqueous zinc metal batteries rely on reversible Zn plating and stripping, yet mechanistic understanding of the anode has focused predominantly on plating. This gap is particularly consequential in full cells with Zn-free cathodes, where discharge begins with Zn stripping and anode losses directly consume the finite Zn inventory. Here, we

reveal a fundamental asymmetry between these processes: plating depletes Zn2+ and promotes interfacial basification, whereas stripping accumulates Zn2+ and creates an acidic, corrosive interfacial environment. Transport simulations and electroanalysis establish opposing concentration polarization and identify Zn2+ saturation as a limiting condition for stripping, analogous to depletion at Sand's time during plating. Operando fluorescence microscopy directly visualizes the resulting opposing pH gradients, while electrochemical mass spectrometry demonstrates that stripping-induced acidification enhances hydrogen evolution despite anodic polarization. High-rate stripping further leaves electrochemically accessible residual Zn and destabilizes the passivation layer, coupling electrolyte and electrode instabilities during Zn removal. Together, these findings establish stripping as a distinct source of Zn anode instability and provide a framework for understanding Zn reversibility across plating, stripping, and rest.

MWRM 2026 MW35

Structural characterization of the *Homo sapiens* ornithine decarboxylase antizyme (OAZ) RNA regulatory element

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Riboswitches are segments of non-coding RNA located in the 5' untranslated region of messenger RNA that regulate downstream gene expression upon binding to specific cellular metabolites. Metabolite binding yields conformational changes in the riboswitch, which directly regulate gene expression by affecting transcription, translation, or RNA processing. Polyamines are organic compounds essential for cellular growth, survival, and differentiation. They also function as ligands, interacting with DNA, RNA, and proteins to influence essential cellular binding and function of these molecules. Although most riboswitch regulatory elements have been characterized in bacteria, the role of eukaryotic riboswitches in polyamine biosynthesis remains largely unexplored. A notable example of a conserved eukaryotic riboswitch candidate is the Ornithine Decarboxylase Antizyme RNA (OAZ RNA), which is present in multiple organisms. Recent studies from Dr. Soukup's laboratory provide substantial evidence for a riboswitch function in human OAZ RNA, based on studies of riboswitch-ligand interactions and conformational dynamics. My project aims to investigate further the interactions between Homo sapiens OAZ RNA and varying concentrations of polyamines, focusing on conformational changes and subsequent effects on gene expression. In-line probing (ILP) will serve as the primary assay to analyze these structural interactions. This approach will determine whether OAZ RNA demonstrates one of the defining features of riboswitches: ligand-induced conformational changes, assessed using different concentrations and types of polyamines. Therefore, additional

research into riboswitches as regulatory elements and their ligand specificity is critical for advancing their application as potential targets for cancer treatment.

MWRM 2026 MW403

Structural responses of pea protein to low urea concentrations: Molecular dynamics study

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Pea protein functionality depends strongly on molecular conformation and intermolecular interactions and can be affected by modifiers, such as urea. This study investigated how low urea concentrations alter pea protein structure at the molecular level. All-atom molecular dynamics simulations were performed using the pea protein structure 7U1I containing all three chains in aqueous control, 1 M urea, and 2 M urea systems with the CHARMM36 force field and TIP3P water. After energy minimization and NVT/NPT equilibration, each system was simulated for 200 ns at 300 K and 1 bar. Structural responses were evaluated using backbone root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), radius of gyration (Rg), hydrogen bonding, and secondary structure analysis.
During 100-200 ns, mean RMSD values were 0.3268, 0.5265, and 0.4226 nm for the control, 1 M, and 2 M systems, respectively, showing that both urea systems deviated more from the initial structure than the control, with the greatest deviation at 1 M. Mean RMSF increased from 0.1262 nm for the control to 0.1514 and 0.1646 nm at 1 and 2 M with pronounced flexibility observed in residues 205-220 and 330-345, indicating enhanced local flexibility. Protein-urea hydrogen bonds increased from 184.7 at 1 M to 358.8 at 2 M, confirming stronger direct protein-solvent interactions at the higher concentration. In contrast, Rg remained within 3.4536-3.4735 nm, intramolecular protein hydrogen bonds remained near 954-959, and helical and β-structure contents were maintained within 14.35-15.50% and 36.88-37.38%, respectively.
These results indicate that low urea concentrations induce distinct concentration-specific conformational responses in pea protein. Urea increased global deviation, local flexibility, and direct protein-urea interactions without causing substantial expansion, disruption of the internal hydrogen-bond network, or loss of ordered secondary structure within 200 ns.

MWRM 2026 MW136

Structure-activity relationship optimization of a bismuth-cyclized cell-penetrating peptide enables minimally charged, high-efficiency intracellular delivery

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Cell-penetrating peptides (CPPs) are powerful tools for delivering membrane-impermeable biological cargos in vitro and in vivo, enabling applications ranging from therapeutic delivery and biomolecular imaging to agricultural biopesticides. However, most conventional linear CPPs rely on a high density of cationic residues (usually ≥6 Arg/Lys) to facilitate cellular uptake, which often leads to dose-limiting cytotoxicity and nonspecific interactions with intracellular protein-nucleic acid complexes. Reducing this charge requirement without compromising delivery remains a significant challenge. Herein, we conducted a structure-activity relationship (SAR) analysis and medicinal chemistry optimization of the bismuth-mediated bicyclic CPP, BCP16, a conformationally constrained scaffold formed through Bi(III)-mediated complexation of thiol-rich precursors. Using flow cytometry, confocal microscopy, and an EDTA competition assay to evaluate cellular uptake, bismuth-coordination strength, proteolytic stability, and cytotoxicity across a series of analogs, we identified BCP16e as the lead optimized candidate. BCP16e carries a net charge of only +2 at physiological pH yet exhibits 2.2-fold greater cytosolic entry efficiency than parent BCP16, along with 2.3-fold tighter bismuth coordination, comparable proteolytic stability (t1/2 ~24 h), and a favorable cytotoxicity profile (IC50 ≥ 35 μM). In vivo dose-escalation studies further established an LD50 of >15 mg/kg with no observed mortality, indicating a substantially improved therapeutic index relative to conventional high-charge CPPs. To demonstrate functional cargo delivery, we conjugated BCP16 and BCP16e to a peptidyl cargo targeting the Keap1-Nrf2 interaction; the BCP16e conjugate showed approximately 2-fold greater potency than the BCP16 conjugate in an ARE luciferase reporter assay, confirming that reduced cationic charge translates into improved functional delivery, not just enhanced cytosolic entry. These findings demonstrate that efficient cellular translocation can be achieved without high cationic charge density, establishing a design framework for minimally charged, high-efficiency intracellular delivery vehicles for therapeutic applications.



MWRM 2026 MW65

Structure and selectivity differences in the ring hydrogenation of furan 2,5-dicarboxylic acid by supported Pt catalysts

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The biomass-derived platform chemical furan 2,5-dicarboxylic acid (FDCA) may be converted to the valuable monomer adipic acid (AA) and tetrahydrofuran 2,5-dicarboxylic acid (THFDCA), as well as the specialty chemical 2-hydroxyadipic acid (2-HAA) via catalytic hydrogenation. However, these transformations require preserving the carboxyl group, which in the presence of metals undergo reduction to alcohols and alkanes or decarboxylation/decarbonylation in high or low H_2 concentrations, respectively. The variables controlling selectivity in the reduction have not been systematically investigated for FDCA hydrogenation, motivating the present work. Reactivity experiments combined with DFT calculations were used to elucidate reaction pathways, selectivity dependence, and the nature of the observed disparity in the hydrogenation of FDCA in the supported Pt catalysts studied. We have demonstrated that Pt catalysts favor ring opening to the valuable specialty chemical, 2-hydroxyadipic acid and the turnover frequency is dependent upon the Pt particle size in these catalysts. The observation suggests that terrace sites are more selective to ring opening than edge sites but the latter contribute significantly to observed reaction rate. DFT calculations demonstrated that FDCA adsorbs asymmetrically on Pt (111) crystal facets, which could promote ring-opening on Pt. This study uncovers the potential of traditional catalysts within this emerging bio-based economy.

MWRM 2026 MW406

Structure-guided computational modeling of molecular tweezers targeting histone proteins in pediatric high-grade glioma

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Pediatric High-Grade Glioma (pHGG) is an aggressive and often fatal pediatric brain tumor characterized by limited treatment options and poor prognosis. One of the most common genetic alterations associated with pHGG is the H3 G34R histone mutation, which disrupts chromatin organization and contributes to tumor progression. Molecular tweezers are synthetic supramolecular compounds capable of selectively binding positively charged amino acid residues and have shown therapeutic potential in several protein misfolding disorders. In this study, we performed a structure-guided computational analysis to evaluate molecular tweezers as potential binders of the H3 G34R mutant histone protein. The amino acid sequence of the histone protein was

obtained from UniProt, and three-dimensional structural modeling was performed using AlphaFold 3. Four molecular tweezer variants (MT1–MT4) were evaluated through molecular docking simulations, and the stability of the top-performing complex was further assessed using molecular dynamics (MD) simulations. Docking results demonstrated favorable binding interactions between all molecular tweezers and the mutant histone protein, with MT4 exhibiting the strongest binding affinity, achieving docking scores as low as −143.18 kcal/mol. MD simulations indicated stable protein–ligand interactions, supported by Root Mean Square Deviation (RMSD) and Root Mean Square Fluctuation (RMSF) analyses. Structural analysis suggested that the positively charged arginine residue introduced by the G34R mutation interacts favorably with the electron-rich cavity of the molecular tweezer. These findings suggest that molecular tweezers may serve as promising candidates for selectively targeting mutant histone proteins in pediatric high-grade glioma and provide a computational framework for the future design of histone-directed therapeutics.

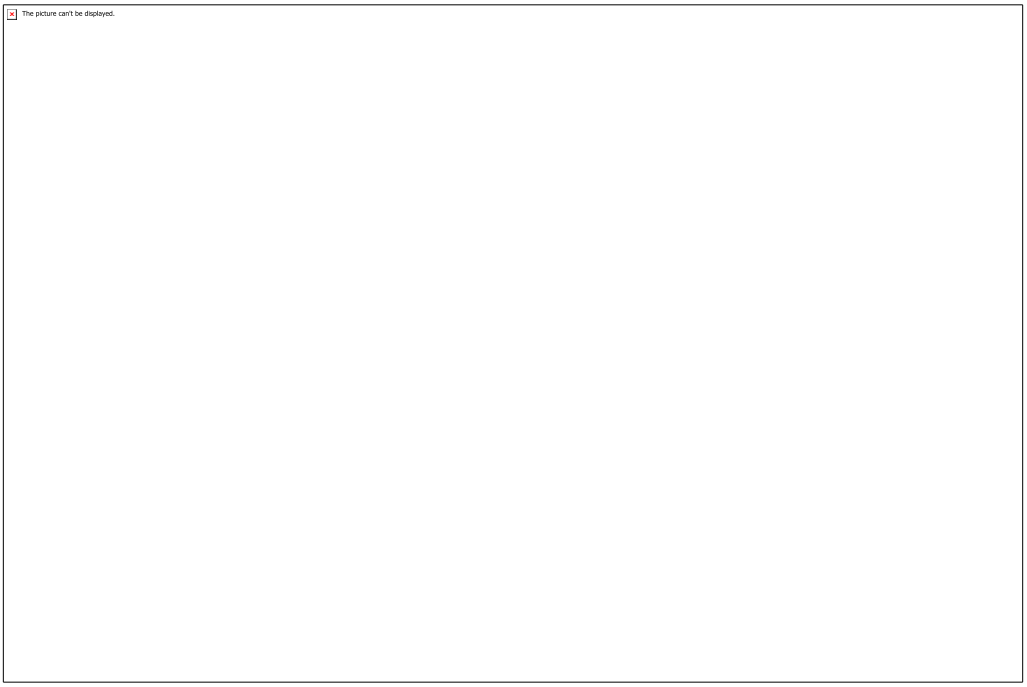
MWRM 2026 MW115

Structure-guided design of broad-spectrum coronavirus protease inhibitors bearing a 1,3,2-oxazaphospholidin-3-one scaffold as a versatile design element

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The continued emergence of SARS-CoV-2 variants and the risk of future zoonotic coronavirus spillover highlight the need for broad-spectrum antivirals targeting conserved viral proteins. Coronavirus 3C-like protease (3CLpro) is an attractive therapeutic target because it is essential for viral replication and highly conserved across coronaviruses. Guided by structural insights, we designed and synthesized a new class of 3CLpro inhibitors incorporating a 1,3,2-oxazaphospholidin-3-one scaffold as a versatile design element. The scaffold combines favorable drug-like properties, including multiple hydrogen-bond acceptors, three-dimensional architecture, limited conformational flexibility, stereochemical diversity, and high synthetic tractability, while providing a platform for exploring new chemical space and optimizing protease active-

site interactions. The resulting compounds potently inhibited both SARS-CoV-2 and MERS-CoV 3CLpro, with lead compounds 1 and 2 exhibiting IC_{50} values of 0.34 and 0.23 μM against SARS-CoV-2 3CLpro and 0.12 and 0.09 μM against MERS-CoV 3CLpro, respectively. Both compounds also demonstrated potent antiviral activity against SARS-CoV-2 in cell culture (EC_{50} = 60 and 50 nM) with low cytotoxicity. Representative inhibitors also exhibited low- to sub-nanomolar inhibition of human cathepsin L, supporting a dual mechanism that suppresses both viral entry and replication. High-resolution cocrystal structures confirmed covalent binding of the inhibitors to the catalytic cysteine residues of SARS-CoV-2 and MERS-CoV 3CLpro and revealed conserved interactions that guide further optimization. Collectively, these findings establish the 1,3,2-oxazaphospholidin-3-one scaffold as a promising platform for developing broad-spectrum coronavirus therapeutics with dual-target antiviral activity.



MWRM 2026 MW291

Structure-property relationships in glycerol-crosslinked and HMDS-modified soybean oil-based polyurethane coatings

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The development of sustainable coating materials is essential to reduce reliance on petroleum-derived systems while maintaining high performance. In this study, a bio-based polyol derived from soybean oil was synthesized through sequential epoxidation and ring-opening reactions and used as a replacement for conventional petroleum-based polyols in polyurethane (PU) coatings. To enhance the mechanical properties, glycerol (GLY) was incorporated as a multifunctional crosslinking agent in combination with methylene diphenyl diisocyanate (MDI). The effect of GLY content (0–20 wt% relative to soybean oil polyol) on mechanical performance was systematically investigated, with the highest tensile strength (47 MPa) observed at 10 wt% GLY, indicating an optimal crosslinking density. Following this optimization, hexamethyldisilane (HMDS) was introduced as a silicon-based modifier (10–50 wt%) to improve surface-related properties such as hydrophobicity, durability, and resistance to environmental contaminants. The incorporation of 10 wt% HMDS resulted in the best balance of mechanical performance, achieving a tensile strength of 37 MPa. Higher HMDS loadings led to reduced crosslinking efficiency and phase inhomogeneity, ultimately decreasing mechanical strength. The optimized formulation was further evaluated for thermal stability, chemical resistance, ink repellency, and dirt resistance. The results demonstrate that the strategic combination of glycerol crosslinking and controlled silicon incorporation enables the development of high-performance, bio-based PU coatings with improved mechanical and surface properties, offering a viable and sustainable alternative to conventional coating materials.

MWRM 2026 MW24

Strucural analysis of *Crassostreas gigas* OAZ RNA

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Riboswitches are segments of non-coding RNA found within messenger RNA that influence the expression of the downstream coding RNA. When interacting with its specific ligand, riboswitches undergo a conformational change that ultimately influences downstream expression. This change in gene expression is a feedback mechanism, affecting the same metabolic pathway its ligand functions in. While there are many studies on bacterial riboswitches, the Soukup lab studies potential eukaryotic riboswitches, mainly Ornithine Decarboxylase Antizyme (OAZ) RNAs. One such potential riboswitch is found in the OAZ RNA of a species of oyster, *Crassostrea gigas*, and is believed to interact with polyamines to control a specific feedback mechanism involving Ornithine Decarboxylase (ODC) and the synthesis of polyamines. In-Line Probing (ILP) experiments can be utilized to analyze structural changes of this RNA segment upon binding to varying concentrations of various polyamines. Early data from ILP experiments with *Crassostrea gigas* OAK RNA shows that spermine binding results in a structural change to the RNA segment, whereas other polyamines do not induce any changes. Current experiments aim to examine whether the binding of spermine analogs, spermidine and pentamine, result in a structural change of the RNA segment.

The study of riboswitches in bacteria have demonstrated significant impacts on regulating metabolic pathways which could then be used as novel antibiotic treatments. The identification of similar riboswitches in eukaryotic species, provides an opportunity for the development of novel antibiological agents.

MWRM 2026 MW268

Super-resolved single molecule detection and tracking studies of Rhodamine B adsorption on fresh and aged polyethylene terephthalate and polystyrene microplastic models

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The millions of tons of microplastics distributed around the world are of significant environmental concern. One source of concern is their ability to accumulate and transport organic micropollutants (OMs) in aquatic systems. Understanding how OMs interact with microplastics is critical for predicting their environmental transport and impact. Indeed, numerous bulk studies of OM accumulation on microplastics have appeared in the literature, although many of these studies employ unrealistically high OM concentrations. These earlier studies have also largely ignored the importance of the spatial heterogeneity of microplastic surfaces. In this work, super-resolved single-molecule tracking (SMT) is used to study the accumulation of Rhodamine B (RhB) dye, serving as a proxy for OMs, on fresh and artificially photo-aged polyethylene terephthalate (PET) and polystyrene (PS) microplastic models. Artificial aging of thin-film polymer models is accomplished via UV-ozone exposure. The model microplastics are initially characterized by classical water contact angle measurements, spectroscopic ellipsometry, and IR spectroscopy to track age-dependent changes in hydrophobicity, thickness, chemical composition. Macroscopic batch adsorption data demonstrate distinct equilibrium behaviors and binding capacities for PET and PS as a function of aging. Wide-field fluorescence SMT videos acquired at the water/polymer interfaces under picomolar RhB concentrations reveal the significant nanoscale heterogeneity of the microplastic surface and its evolution as the plastics age. Ultimately, comparing the SMT datasets for PET and PS reveals how polymer-specific chemical structures and morphological variations guide the nanoscopic pathways of OM accumulation on aged microplastics.

MWRM 2026 MW196

Super-resolved single-molecule studies of Rhodamine B accumulation on fresh and aged polyethylene terephthalate

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Microplastics (MPs) are an important environmental concern because of their ability to adsorb and transport organic micropollutants in aquatic environments. In this study, super-resolved single-molecule tracking (SMT) was used to investigate the accumulation and transport of Rhodamine B (RhB), a model organic micropollutant, on fresh and artificially aged polyethylene terephthalate (PET) surfaces. PET thin films were used as model microplastics, and aging was induced by UV-ozone exposure. Surface characterization using water contact angle measurements, spectroscopic ellipsometry, and FTIR showed progressive decreases in hydrophobicity, film thickness, and carbonyl index as aging progressed. SMT imaging at the water/PET interface enabled direct observation of both mobile and immobile RhB molecules, representing weakly and strongly bound populations, respectively. Step-size analysis showed that RhB surface transport occurs through desorption-mediated diffusion, in which molecules briefly escape into solution before readsorbing at new surface sites. As PET aged, the overall density of adsorbed RhB decreased, while the fraction of strongly bound molecules increased, indicating age-dependent changes in surface chemistry. Super-resolution imaging also revealed repeated adsorption at specific nanoscale locations, demonstrating spatially heterogeneous binding environments on the PET surface. Recent preliminary surface-modification studies will also be presented, in which aged PET films were exposed to hexamethyldisilazane (HMDS) vapor to passivate accessible oxygen-containing surface groups. HMDS treatment increased the water contact angle, consistent with greater hydrophobicity of the aged PET surface. Ongoing SMT measurements are being used to determine how this chemical passivation affects RhB adsorption density, immobilization, and surface diffusion. These results provide molecular-level insight into how weathering and surface chemistry control organic pollutant accumulation on PET microplastic surfaces, and demonstrate how SMT resolves heterogeneous adsorption behavior beyond conventional ensemble measurements, with relevance to understanding and predicting microplastic-associated pollutant risks in natural environments.

MWRM 2026 MW36

Surface organometallic chemistry as a synthetic tool for reactive ruthenium cations

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Molecular ($RPN^{H}P$)Ru(CO)(H)(X) pincer complexes are highly selective and active catalysts for the hydrogenation of unsaturated polar bonds, aldehyde coupling, and other reactions. However, accessing and exploiting the corresponding low-coordinate, highly reactive [($RPN^{H}P$)Ru(CO)(H)]$^{+}$ cations remains a distinct challenge in solution. Molecular attempts to isolate these coordinatively unsaturated species typically fail; complexes with sterically small R groups rapidly undergo dimerization and precipitation into inactive species, whereas larger aryl groups suffer from ortho-methyl activation. To circumvent these solution-phase deactivation pathways, we utilized surface

organometallic chemistry (SOMC) to stabilize these elusive intermediates via chemisorption to an oxide. This work highlights the utility of weakly-coordinating sulfated zirconium oxide (SZO) to generate and isolate well-defined, monomeric $[(RPN^{H}P)Ru(CO)(H)]^{+}$ surface species. By pairing molecular pincer precision with surface site-isolation, the solid support successfully suppresses bimolecular dimerization and unwanted ligand activation, even when utilizing sterically unencumbered R groups.
Spectroscopic characterization and mass balance data confirm that the resulting SZO-supported complexes are highly electrophilic, well-defined, and isolated monomers. When evaluated for catalysis, these surface-stabilized species display exceptional activity, outperforming or competing effectively with traditional molecular precursors in hydrogenation and C-H functionalization reactions. Ultimately, this work demonstrates that the surface is not merely a passive anchor for heterogenization, but a powerful synthetic tool to access unique, highly active, low-coordinate catalytic architectures that are otherwise impossible to isolate in the fluid phase.

MWRM 2026 MW421

Surrogate reference standards for RP-HPLC quantification of paracetamol: Influence of structural variability on assay values

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The study explores the use of surrogate reference standards for RP-HPLC quantification of paracetamol in tablets, and the effect of the relative structural variations of the surrogate candidates on assay values. A cost-effective isocratic HPLC method was developed, utilizing a mobile phase of methanol and water (65:35 v/v) at pH 3.10, with a C-18 Copsil column and UV detection at 235 nm. A mixture comprising the target analyte (paracetamol) and surrogate reference standards (p-aminophenol, caffeine, acetanilide, and aspirin) was analyzed at a flow rate of 1.5 mL/min. The study established surrogate constant (S_{∞}) for all the surrogate reference standards and employed in a derived equation to evaluate paracetamol content. The results showed that these compounds could successfully quantify paracetamol in the absence of a paracetamol reference standard, with all measurements falling within compendial monograph limits, although structural analogs of the surrogate reference standards to the target analyte provided least mean difference of assay values and greater accuracy. These findings highlight the flexibility of reference standard selection in HPLC quantitation and offer a practical approach for researchers, small-scale pharmaceutical industries, and laboratories in resource-constrained settings.

MWRM 2026 MW187

Synthesis, characterization and evaluation of self-decontaminating cotton fabric for organophosphate detoxification

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Nerve agents are highly toxic organophosphorus compounds that disrupt the central nervous system and pose significant risks to both military personnel and civilian populations. Since the early twentieth century, organophosphorus compounds have been developed for use as pesticides and chemical warfare agents. Exposure can cause severe cholinergic symptoms, potentially resulting in incapacitation or death. To mitigate these hazards, considerable research has focused on the development of antidotes and chemical detoxification strategies. Detoxification commonly involves cleavage of the stable P–O bond in phosphate esters to produce less toxic products. Because phosphorus has a strong affinity for oxygen, nucleophilic functional groups such as oximes can attack the phosphorus center and promote bond cleavage. Imidazole groups, which are frequently present in enzyme active sites, can also participate in catalytic reactions while maintaining relatively low toxicity.
In this study, new bifunctional small-molecule organophosphate scavengers containing both oxime and imidazole functionalities were synthesized. These compounds can degrade organophosphate agents under non-aqueous conditions at ambient temperature and near-neutral pH (8.5). An important feature of this work is that the scavengers can also be grafted onto cotton fabrics. The resulting functionalized textiles may provide protective materials capable of degrading nerve agents upon contact, offering potential applications in military uniforms and other chemical-protective clothing.

MWRM 2026 MW236

Synthesis, isolation, and redox chemistry of heterobimetallic uranium/europium complexes

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Despite the importance of mixtures containing lanthanides and actinides in the nuclear fuel cycle and separations of critical minerals/materials, there are few examples of well-defined coordination complexes that contain both 4f and 5f ions, and even fewer for which systematic studies of redox properties have been reported. And, although heterobimetallic complexes featuring secondary redox-inactive cations have received significant attention in the literature in recent years, studies of species containing secondary redox-active cations remain quite rare. In this presentation, the synthesis, isolation, and chemical and electrochemical properties of mixed U/Eu heterobimetallic complexes will be described. The complexes are supported by a non-macrocyclic

organic ligand which enables the binding of both the uranyl ion and a europium cation in close proximity. Spectroscopic studies of the various species that are accessible on this platform will be discussed, including the results of experiments aimed at assigning formal metal oxidation states. Our latest results will be discussed, including studies of oxidation-state-dependent reactivity.

MWRM 2026 MW45

Synthesis, preliminary characterization, and toxicity studies of three amino acid Schiff-base ligands and their potential binding sites to Ni (II) ion: Comparison with computational density functional theory (DFT) studies

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Three Schiff-base ligands derived from amino serine, leucine and phenylalanine and salicylaldehyde, benzaldehyde and N-4-dimethylaminobenzaldehyde respectively were successfully synthesized and partially characterized. In addition, three Ni(II) complexes were synthesized *in situ* and characterized with the above Schiff-bases. The structures of these complexes were investigated experimentally and computationally using density functional theory (DFT) technique to determine the potential binding environment with the Ni(II) center. Simulation of different models of the complexes were fully optimized using computational DFT B3LYP technique and the results revealed that models 4a, 5a, and 6a correspond to complexes-I, II, & III respectively. All the three complexes adopt a stable square planar geometry around the Ni(II) center. The complexes were partially characterized using melting point/decomposition temperatures, solubility test, FT-IR and UV-visible spectroscopy and the results compared with calculated results. The melting points/decomposition temperatures of all the complexes were different from the melting points of the starting amino acids used in their syntheses and the complexes were found to be soluble in water and other polar solvents. Experimental FT-IR and UV-Visible results agree with calculated results within accepted levels (5-10 %). The experimental imine v(C=N) stretching frequencies of all the three complexes agrees well with the calculated results while the rest of the stretching frequencies show some discrepancies. Furthermore, the UV-Visible spectra the three electronic transitions HOMO-6àLUMO, HOMO-2àLUMO+1, and HOMOàLUMO+1 for complex-I, two transitions HOMO-2àLUMO+1 and HOMO-1àLUMO for complex-II, and two transitions HOMO-7àLUMO and HOMOàLUMO+1 for complex-III. The complexes were non-toxic towards prokaryotic gram positive (*Staphylococcus aureus, Staphylococcus epidermis, Streptococcus mutants*) and gram negative (*Aquaspirillum serpens Escherichia coli*) bacterial and eukaryotic (*Saccharomyces cerevisiae*) bacterial.

MWRM 2026 MW151

Synthesis, spectroscopy, and redox studies of Fe, Mn, and Co thiolate complexes supported by a triaryl tetradentate ligand

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Square pyramidal transition metal complexes that contain a planar tetradentate N_4 ligand and a single axial thiolate represent an important class of bioinorganic model complexes. The N_4S coordination environment and structure are reminiscent of those found in heme systems, most notably the cytochrome P450 enzymes, which rely on a Fe porphyrin core with an axial thiolate ligand to mediate key oxidative transformations in human metabolism. Due to their biological significance, substantial effort has been devoted to developing synthetic analogues that reproduce the reactivity of P450 and related metalloenzymes. These biomimetic complexes frequently incorporate Fe, Mn, or Co centers supported by nitrogen-rich macrocycles or chelating ligands that enable systematic exploration of structure function relationships, redox behavior, and catalytic pathways relevant to enzymatic transformation using dioxygen.
Recent studies from our group have demonstrated that weak field tetradentate ligands derived from *o* phenylenediamide and incorporating flanking NMe_2 substituents promote dinuclear assembly with divalent Fe, Mn, and Co. Subsequent reactivity studies have revealed that treatment of these dinuclear complexes with S_2Ph_2 oxidizes the metal and breaks apart the dinuclear structure to yield mononuclear N_4S complexes. The resulting M(III) thiolate complexes mimics the defining geometric features of cytochrome P450 heme thiolate active sites. Notably, these complexes display distinctive variations in the displacement of the metal from the plane defined by the equatorial nitrogen donors. This structural parameter changes systematically with both metal identity and redox state, thereby providing a sensitive metric for comparison to ligand field strength, covalency, and redox tuning within this series.
The structural and electronic features of the new M(III) thiolate complexes will be described, as elucidated using a combination of single-crystal X-ray diffraction (XRD), UV-visible (UV-vis) spectroscopy, and X-ray absorption spectroscopy (XAS). Additionally, chemical reduction of the M(III) thiolate complexes using cobaltocene will also be discussed. Collectively, these studies provide further insight into the redox flexibility of the ligand framework and the stability of the thiolate coordination environment, offering a more complete picture of the electronic and structural factors governing this biomimetic series.

MWRM 2026 MW128

Synthesis and characterization of four zingerone derivatives

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S. maltophilia is an emerging global pathogen that is detrimental to immunocompromised individuals. This gram negative bacteria displays multiple-drug-

resistance and readily contaminates hospital devices and contacts lenses. Zingerone has been shown to inhibit biofilm formation of *S. maltophilia*. Zingerone is a naturally occurring phenolic compound derived from the decomposition of gingerol during the drying of ginger root. In previous studies, zingerone has been observed to have antioxidant, anti-aging, anti-cancer, anti-inflammatory, and antimicrobial properties both alone and as an antibiotic promoter. Four zingerone derivatives were synthesized and characterized. Derivatives include: reduction of the ketone to an alcohol, acetylation, a Williamson ether synthesis, and a novel ketal formation. Compounds were purified and characterized by ATR-IR, GCMS, ^{1}H NMR, and ^{13}C NMR. Future work includes testing of inhibition of biofilms.

MWRM 2026 MW181

Synthesis and characterization of hemiaminals and hemiaminolates as modular aryldifluoromethyl-transfer reagents

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Fluorinated groups are widely used in drug discovery, yet many established methods for installing difluoroalkyl fragments rely on ozone-depleting substances or fluorocarbon feedstocks with high global-warming potential. The continuing phaseout of these materials motivates the development of alternative fluorine-transfer reagents derived from more sustainable building blocks.

Herein, we report a modular family of fluorinated hemiaminal and hemiaminolate reagents prepared without relying on ODS-derived fluorocarbon precursors. Fluorinated hemiaminals are accessed through nucleophilic addition of organomagnesium reagents to phthalimide, followed by acid-promoted electrophilic fluorination. The corresponding hemiaminolates provide an additional means of tuning reagent activation through variation of the countercation. Together, these compounds function as precursors to aryldifluoromethyl anion equivalents.

Representative reagents were characterized by multinuclear NMR spectroscopy, including ^{1}H, ^{13}C, and ^{19}F NMR, supporting the assigned structures and their difluoroalkyl connectivity. The modular architecture permits variation of the aryl group, imide scaffold, N-substituent, and countercation, providing opportunities to examine how these features influence stability and reactivity.

Preliminary studies demonstrate that the fluorinated hemiaminals undergo fragmentation under mild basic conditions. Formation of $ArCF_2H$ following protonation,

together with diagnostic ^{19}F NMR observations, is consistent with generation of an aryldifluoromethyl anion equivalent. These results establish a foundation for directing fragmentation toward productive carbon-carbon bond formation.
Current efforts focus on extending this reactivity beyond protonation through trapping of the generated $ArCF_2$ nucleophile with synthetically useful electrophiles. Progress toward reactions with aryl and alkyl carbonyl compounds and Pd-catalyzed cross-coupling with aryl electrophiles will be presented. In parallel, sodium and potassium hemiaminolates are being investigated as internally activated precursors that may generate $ArCF_2$ nucleophiles without requiring an external base, thereby suppressing competing protonation and favoring productive electrophile capture.
Overall, this reagent family provides a tunable platform for generating aryldifluoromethyl nucleophiles from non-ODS-derived building blocks and supports the development of more sustainable approaches to nucleophilic difluoroalkylation

MWRM 2026 MW83

Synthesis and characterization of novel aryl-cyanoximes

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A series of novel monosubstituted and disubstituted aryl-cyanoximes containing $-CF_3$, chloro, sulphonyl and NO_2- groups were designed and subsequently synthesized from respective acetonitriles using a nitrosation reaction with gaseous methyl-nitrite under inert gas protection. Preparation and isolation of new cyanoximes was optimized by changing time of the reaction and by solvent of recovery. Obtained compounds were characterized by means of NMR spectroscopy and X-ray analysis.

MWRM 2026 MW23

Synthesis and characterization of N-quaternized ammonium pectin derivatives for tunable antimicrobial activity

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Pectin, a plant-derived polysaccharide structurally similar to hyaluronic acid, was chemically modified to produce N-quaternized ammonium derivatives with tunable antimicrobial properties. Pectin quaternization reactions were carried out in water, DMF,

and water/DMF mixtures under basic conditions to minimize hydrolysis of the quaternizing agents Quat-188 and glycidyltrimethylammonium chloride (GTMAC). Modification of pectin with Quat-188 resulted in a degree of substitution of approximately 24%, as determined by 1H NMR spectroscopy. Both the native and modified polymers were further characterized by FTIR to confirm structural changes associated with quaternization. The degree of quaternization of the GTMAC-modified pectin derivatives will be determined. Antimicrobial assays shows antimicrobial activity against *S. aureus* and *E. coli* This study aims to expand the application of plant-based polysaccharides in biomedical materials with controlled biological activities.

MWRM 2026 MW225

Synthesis and characterization of sodium trioxodinitrate ($Na_2N_2O_3$; Angeli's salt). introduction to nitroxyl (HNO) chemistry in upper-division undergraduate laboratory

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Angeli's salt ($Na_2N_2O_3$) undergoes spontaneous self- decomposition in physiological buffer (pH 6.8- 7.4), to nitroxyl (HNO) and nitrite. The current interest in Angeli's salt is due its potential clinical application (as a HNO/NO donor) in cardiovascular diseases such as heart failure. In the upper-division synthesis and characterization laboratory, students prepared Angeli's salt by the reaction of hydroxylamine with n-butylnitrate in methanol/NaOH. The percent purity of the compound was determined from the measured absorbance at 250 nm in 1M NaOH (molar absorptivity = 8100 M^{-1} cm^{-1}). Students followed the first-order decomposition at 237 nm ($t_{1/2}$, ≈ 7 minutes in the presence of O_2 at 25°C). The measured nitrile levels (Griess method using sulfanilic acid/ α-naphthylamine azo-dye (red-violet; 550 nm) are consistent with the established stoichiometry of the reaction: $2HN_2O_3^- = N_2O + H_2O + 2NO_2^-$. In independent undergraduate research projects, students examined the substitution of cyanide at tetracyano-Ni(II)center. In addition, we probed the electron -demand in the reaction of nitroxyl with a series of substituted thiophenols.

MWRM 2026 MW239

Synthesis and crystal structures of heavy metal thiosalicylate complexes

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2-Mercaptobenzoic acid, commonly called thiosalicylic acid, ($C_7H_6O_2S$) is a useful organic compound that contains both a carboxylic acid and a mercaptan functional group. With its low cost and close proximity of functional groups, it a useful precursor in many organic reactions and can also be used as a stabilizing agent in the synthesis of metal nanoparticles. Additionally, when complexed with ethyl mercury it forms Thiomersal (which has antiseptic and antifungal properties). These latter two applications frame a continued interest in how this ligand can interact with metal cations. When deprotonated, the thiosalicylate anion has both a soft donor in thiolate and a hard donor in carboxylate, which provides a compact ligand to react with a variety of hard and soft metal cations; however, care must be taken when performing reactions so as not to simply form the 2,2′-dithiodibenzoate species. The single crystal investigation explored here provides unique insights into how this flexible ligand is able to interact with different heavy metals. Herein we will discuss the synthetic strategies and single-crystal structural characterizations of new metal thiosalicylate complexes.

MWRM 2026 MW299

Synthesis of aliphatic poly(ester carbonate) copolymers using novel chloroformates and their hydrolytic and enzymatic degradation

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Aliphatic polyesters and polycarbonates have been widely investigated due to their biodegradability, which is important for both biomaterials and sustainable plastics. In this work, we explore the synthesis and copolymerization of a new aliphatic monomer, 2-(chlorocarbonyl)ethyl chloroformate (CFEO), with aliphatic diols. In addition to developing copolymerization reactions, this presentation will compare the degradation behavior of alternating and statistical copolymers of the poly(ester carbonate)s (PEC) synthesized with 1,10-*n*-decanediol and the analogous polyester, poly(decelyene succinate) (PDS), and polycarbonate, poly(decylene carbonate) (PDC). The degradation behavior of these copolymers were studied by exposing them in the form of pellets to basic conditions with $NaOH_{aq}$ and enzymatic conditions using Novozyme 435. PDC is the most stable and resistant to degradation under both conditions, while PDS and the PECs undergo significant degradation after 3 days of exposure to $NaOH_{aq}$ and Novozyme 435.

MWRM 2026 MW383

Synthesis of a quaternized polyampholytic pectin derivative and Tanfloc-based multilayer coatings for antimicrobial biomedical interfaces

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Polysaccharide-based polyelectrolytes have attracted significant attention for biomedical applications due to their biocompatibility and ability to form functional surface coatings. However, conventional anionic polysaccharides often lack intrinsic antimicrobial activity and require additional functionalization. In this study, we developed quaternized pectin-derived polymers (polyampholytes) containing permanent cationic ammonium groups to investigate their potential as functional polyanions for bioactive coatings.
Pectin was chemically modified with glycidyl trimethylammonium chloride (GTMAC). The optimized synthesis conditions were achieved in aqueous media, enabling controlled variation of the degree of quaternization by adjusting GTMAC concentration. Proton nuclear magnetic resonance spectroscopy confirmed the successful incorporation of quaternary ammonium groups, and the degree of quaternization was quantified by proton NMR.
Compared with native pectin, the quaternized derivatives exhibited significantly lower hydrodynamic diameters while maintaining a negative overall surface charge in ultrapure water. The quaternized pectin derivative with approximately 45% quaternization was selected for surface engineering studies. Titanium substrates were functionalized using layer-by-layer (LbL) assembly. The pectin derivative and pectin were paired with Tanfloc, a cationic polyphenolic polymer derived from condensed tannins containing flavan-3-ol repeat units. Multilayer coatings comprising 6 or 12 layers were fabricated, with the outermost layer composed of the quaternized pectin derivative. Surface characterization by contact angle measurements revealed changes in wettability after multilayer deposition, with water contact angles increasing from approximately 40° for untreated titanium to approximately 50-55° after polymer coating. Energy-dispersive X-ray spectroscopy (EDS) spectra and elemental mapping confirmed successful deposition and homogeneous distribution of the multilayer coatings on titanium substrates.
These findings demonstrate a versatile strategy for designing functional polysaccharide-based polyelectrolytes and Tanfloc-containing multilayer interfaces. We are investigating coating morphology, thickness, antimicrobial activity, and hemocompatibility to establish structure–property relationships and evaluate the potential of quaternized pectin/Tanfloc coatings for cardiovascular biomaterial applications.

MWRM 2026 MW88

Synthesis of aspirin using $FeCl_3$ in a variety of solvents

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It is well known that iron trichloride, $FeCl_3$, is used to test for the presence of residual salicylic acid in classic aspirin synthesis experiments done in undergraduate chemistry labs. More recently it has been found that this Lewis acid can be used, in place of a Bronsted acid, to catalyze the synthesis of aspirin from salicylic acid and acetic anhydride under neat conditions. In all cases to date, aqueous forms of this catalyst have been used and it is seen that as such the catalyst can be very active; in fact the reaction can be completed within ten minutes and at room temperature with only small amounts of the catalyst used. Given the solubility of $FeCl_3$ in organic solvents, anhydrous conditions for aspirin synthesis using salicylic acid and acetic anhydride were considered. This was done to both examine the breadth of conditions that can be used for iron trichloride catalyzed aspirin synthesis, and to also ensure that the lewis acid itself, and not hydrous byproducts, were able to catalyze this reaction. Through this work it was found that new solvents including diethyl ether, acetone, cyclohexane and ethyl acetate, along with catalytic amounts of anhydrous $FeCl_3$, are effective for the synthesis of aspirin. The results of these various conditions are reported. The most effective of the organic solvents was found to be ethyl acetate. Even with only a mole to mole ratio (acetic anhydride to salicylic acid) of 1.35 to 1 the reaction run near room temperature was complete within 20 to 30 minutes resulting in aspirin at 70 to 80 percent yield.

MWRM 2026 MW178

Synthesis of Balgacyclamide C analogs in pursuit of discovering the biological pharmacophore: Retention of the lower peptide fragment

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The balgacyclamide family consists of three heterocyclic and macrocyclic peptides, balgacyclamide A-C. These natural products were isolated from *Microcystis aeruginosa*, a phototropic cyanobacteria, which is found in eutrophic water bodies worldwide. Balgacyclamide A and B have been reported to have anti-parasitic activity toward *P. falciparum*; however, there has been no biological activity reported for balgacyclamide C (Balg C). The aims of this project are to determine the biological pharmacophore of each family member and reveal how that is related to its overall biological activity. Current literature hypothesizes that the degree of unsaturation of the heterocyclic rings is correlated with biological activity. Based upon this, our lab hypothesizes that the upper fragment in the Balg family that contains the oxazoline and thiazole is the active pharmacophore of the molecule. To test this hypothesis, analogs of the Balg family have been synthesized that have replaced the upper heterocyclic rings with a carbon chain and retained the lower peptide component. There are two main differences in the lower peptide fragment of these three members: the peptide sequence and whether it is linear or cyclized. Balg A and B both contain valine, threonine and alanine; however, the threonine in Balg A is cyclized to give an oxazoline ring, whereas Balg B is an open chain. The lower peptide chain of Balg C is linear and contain phenylalanine, threonine

and glycine. Based upon our computation docking studies, the difference between an aliphatic (valine) and an aromatic side chain (phenylalanine) could play a large role in the overall biological activity, in addition to the difference in having the lower fragment cyclized versus linear. The biological activity of these analogs will be assessed and gain, or loss of activity will be observed to help determine the biological pharmacophore of the molecule.

MWRM 2026 MW173

Synthesis of Balgacyclamide C analogs in pursuit of discovering the biological pharmacophore: Retention of the upper heterocyclic ring system

***Ryan Bachman**, ryan101@ksu.edu, Meghan Rice, Ibrahim Ciftci, Arnaldo Torres Hernandez, Ryan J. Rafferty. Chemistry, Kansas State University, Manhattan, Kansas, United States*

The balgacyclamide family consists of three heterocyclic and macrocyclic peptides, balgacyclamide A-C, which were isolated from Microcystis aeruginosa, a phototropic cyanobacteria, found in eutrophic water bodies worldwide. Balgacyclamide A and B have been reported to have anti-parasitic activity toward P. falciparum; however, the biological activity for balgacyclamide C (Balg C) has not been reported. The aims of this project are to determine the biological pharmacophore of each family member and see how that is related to its overall biological activity. Current literature hypothesizes that the degree of unsaturation of the heterocyclic rings is correlated with biological activity. Based upon this, our lab hypothesizes that the upper fragment in the Balg family that contains the oxazoline and thiazole is the active pharmacophore of the molecule. To test this hypothesis, analogs of the Balg family have been synthesized by retaining the heterocyclic upper fragment and replacing the lower fragment with carbon chains. There is one amino acid difference between balg A, B and C in the upper heterocyclic ring fragment. Balg A and B have valine, whereas Balg C has phenylalanine. Based upon our computation docking studies, this difference between an aliphatic and an aromatic side chain could play a large role in the overall biological activity. The biological activity of these analogs will be assessed and gain or loss of activity will be observed to help determine the biological pharmacophore of the molecule.

MWRM 2026 MW312

Synthesis of PLB-g-PMMA by grafting MMA from PLB

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Poly(lactic acid) (PLA) is one of the most widely available compostable polymers produced from renewable feedstocks. However, post-polymerization functionalization of PLA remains difficult because its backbone does not contain reactive pendant groups suitable for subsequent chemical modification. Incorporation of a bromine atom at the α-

position of an ester carbonyl introduces a versatile reactive site that can be used for further functionalization. In this study, 2-bromo-3-hydroxypropionic acid (BrH), a brominated constitutional isomer of lactic acid, was synthesized and copolymerized with lactic acid to produce poly(2-bromo-3-hydroxypropionic acid-co-lactic acid) (PLB). The pendant α-bromoester groups incorporated into the PLB backbone are intended to serve as initiating sites for the atom transfer radical polymerization (ATRP) of methyl methacrylate (MMA) through a grafting-from approach, yielding poly(2-bromo-3-hydroxypropionic acid-*co*-lactic acid)-*graft*-poly(methyl methacrylate) (PLB-g-PMMA). Before conducting graft polymerization from the PLB backbone, the reactivity of the α-bromoester functionality was evaluated using a small-molecule model initiator. For this purpose, BrH was converted to methyl 3-acetoxy-2-bromopropionate (acetoxy-BrH). ATRP of MMA was then performed using acetoxy-BrH as the initiator, CuBr as the catalyst, and methylated polyethyleneimine (MePEI) as the ligand. The reactions were then investigated at different temperatures and reaction times to assess the initiation efficiency of the α-bromoester group and identify suitable polymerization conditions for the subsequent synthesis of PLB-g-PMMA, without cleavage of the PLB backbone.

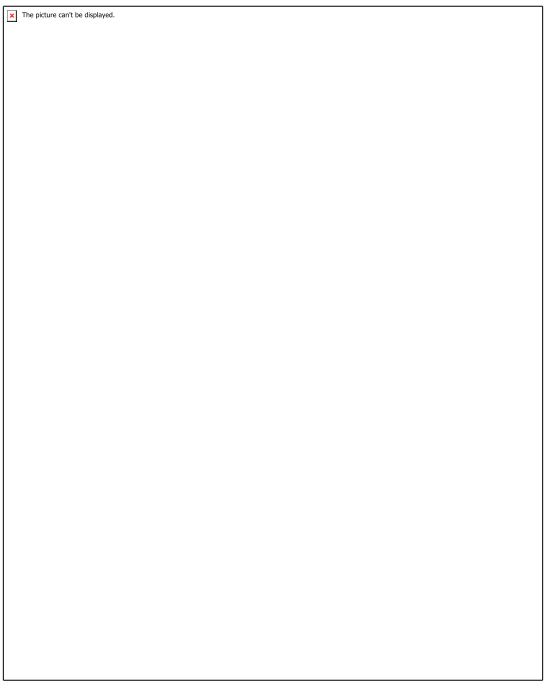
MWRM 2026 MW146

Synthesis of rigid quaternary ammonium compounds (QACs) for use as capping agents to create fluorescent lanthanide metal-organic framework (MOF) antimicrobial materials

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Antimicrobial resistance (AMR) is a problem that is estimated to have caused 1.27 million global deaths in 2019 by the World Health Organization. Our group is interested in making quaternary ammonium compound (QACs) surfactants, which are broad-spectrum bactericides and important materials in combating AMR.
Molecular QACs are effective at killing bacteria, but they can be harmful to eukaryotic (*i.e.* human) cells when delivered as small molecules. To reduce environmental exposure to QACs, we propose putting QACs on the surfaces of larger particles. Our group has synthesized *rigid* antimicrobial surfactants that are more effective at killing bacteria, by recent MIC data, than *flexible* commercial surfactants. Lanthanide metal-organic frameworks (MOFs) are highly fluorescent materials that can incorporate antimicrobial compounds at their edges using capping agents, such as carboxylates, to bind to open coordination sites on the MOFs. We are investigating antimicrobial potency by altering the length between the carboxylate that binds to the MOFs and the QAC that kills bacteria. The fluorescent MOF/QACs can then be probed spectroscopically to

determine binding and antimicrobial effectiveness. The synthesis of these asymmetric, rigid QACs (Fig. 1) and the capped MOFs will be discussed.



MWRM 2026 MW152

Synthesis of stable multinary MOFs

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Metal-organic frameworks (MOFs) have emerged as a versatile class of crystalline, porous materials with significant promise for gas storage, separation, and catalysis. A particularly powerful subset multinary MOFs feature organic linkers arranged in well-defined, ordered distributions within each unit cell, enabling precise control over pore chemistry and the study of cooperative interactions between distinct functional groups. However, realizing stable, permanently porous multinary frameworks remains a central synthetic challenge. Our lab is currently addressing this challenge through two parallel synthetic efforts: (1) replacing long dipyridyl glycol pillar linkers in our KSU-1 and KSU-100 frameworks with shorter, functionalized bipyridine alternatives to reduce pore size and improve framework robustness, and (2) synthesizing multinary Zr-based MOFs via sequential linker installation (SLI), exploiting the superior chemical and mechanical stability of Zr secondary building units. Together, these efforts are advancing our ability to rationally design porous materials in which the spatial arrangement of functional groups can be systematically tuned to enhance separation performance.

MWRM 2026 MW175

Synthetic efforts towards a histidine analog of Reniochalistatin E for cancer drug delivery

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In 2014, Lin and co-workers discovered five cyclic macrocyclic peptide natural products from the marine sponge Reniochalina stalagmitis during their search for proline-rich bioactive compounds. Among them, Reniochalistatin E (RenE) was the only macrocycle shown to exhibit biological activity, displaying cytotoxicity against HeLa and RPMI-8226 cell lines with IC50 values of 17.3 and 4.9 μM, respectively. Inspired by this, our lab initiated the first total synthesis of RenE in 2017 and later completed a phenylalanine analog in 2025. Our synthetic route delivered RenE in 15 steps with an overall yield of 5%, and the compound demonstrated moderate activity against the MM.1R multiple myeloma cell line. Looking to understand the chemical structure and how it relates to anti-cancer activity, a phenylalanine variant was developed and evaluated. This analog, and the original RenE, was shown to more effectivity shut down cancer cells when combined with known anti-cancer agents in a synergistic manner. It is hypothesized that the aromatic rings present are responsible for this enhanced cancer fighting ability and by fine-tuning the chemical structure, we could make further improvements. To test this, we propose a histidine analogue that has a superior ability to interact with other aromatic rings in a process known as π-stacking. If correct, this RenE-histidine analogue will lay the foundation for future analogue development and inform further modifications to build a more powerful and targeted anti-cancer strategy.

MWRM 2026 MW61

Synthetic efforts towards Cahuitamycin

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The cahuitamycin family comprises peptide-based natural products first isolated by the Sherman group in 2016 from *Streptomyces gandocaensis* and characterized for their ability to inhibit biofilm formation. Among them, Cahuitamycin C (Cah C) displayed the most potent activity (IC50 = 14.5 μM). While structural assignments were initially proposed for Cah A–C, subsequent synthetic efforts have raised questions about their accuracy. In 2023, the Wuest lab reported a total synthesis of the originally proposed structure of Cah A and demonstrated it to be incorrect. Concurrently, our group initiated a synthetic campaign toward Cah C and reached a similar conclusion. Our ongoing efforts have led to a new structural hypothesis, which, along with the preceding synthetic investigations, will be presented to address the evolving structural reassignment of the cahuitamycin family.

MWRM 2026 MW108

Systematically improving the quality of atomically accurate RNA 3D structures

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Advances in cryo-electron microscopy and X-ray crystallography have greatly increased the number, size, and complexity of experimentally determined RNA structures, including ribosomes and other ribonucleoprotein assemblies. As RNA models grow to thousands of nucleotides and tens of thousands of base-pairing interactions, manual inspection of local structural quality becomes impractical. Existing RNA annotation and validation tools provide interaction annotations and global quality metrics but offer limited guidance for identifying incorrectly modeled base pairs or diagnosing the geometric defects responsible for reduced structural quality. To address this challenge, we developed an automated computational framework that identifies RNA base pairs directly from atomic coordinates and evaluates RNA quality at the base-pair, and backbone level. Individual base pairs are evaluated using empirical geometric and hydrogen-bond reference distributions, while backbone conformation is assessed through backbone geometry and sugar-pucker analysis. The framework reports quantitative scores together with residue-level diagnoses of the geometric and conformational features responsible for reduced quality. Benchmarking against DSSR across nonredundant PDB RNA structures showed near-complete agreement for canonical base-pair identification while maintaining high performance across noncanonical interaction classes. Quality scores correlate with experimental resolution and established global validation metrics while providing complementary residue-level information beyond existing approaches. Lower-quality RNA models contain more low-scoring interactions enriched in hydrogen-bond, shear, stretch, and opening defects. PDB-REDO validation showed that low-scoring interactions improve substantially following automated re-refinement, whereas high-scoring interactions remain largely unchanged, demonstrating that the framework identifies refinement-correctable modeling errors. Ribosome-sized RNA structures are analyzed in less than one second, enabling residue-level quality assessment during iterative refinement and large-scale RNA analysis. Together, this work provides a scalable framework for systematic identification of local modeling errors, supporting the generation of more accurate RNA structural models for downstream structural and functional studies.

MWRM 2026 MW265

Textural property evaluation of mesoporous silica induced by acid, solvent, thermal treatment and methylene blue uptake

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The synthesis of a hydrothermally stable form of mesoporous silica was optimized to yield a large surface area sorbent from organic matter in wastewater. Optimization of

the surface area and pore-size distribution was performed by examining the effects of the acid catalyst, the ethanol: isopropanol volume ratio and calcination temperature. Each optimization affected the surface area and pore size distribution of the sorbent, and thus its performance for removing organics from water. Improved performance is associated with increased hysteresis loop between adsorption and desorption isotherms, which is normally associated with a mesoporous adsorbent. The final material was sieved (-40+60) to obtain a high-surface-area sorbent with known particle size distribution. The sorption of organics from water was demonstrated using methylene blue, which allows sub-ppm concentrations to be easily determined by UV-VIS. The mesoporous silica material was characterized using BET, FT-IR, and TGA. Surface areas up to 924 m^2/g were obtained. The absorption isotherms and maximum capacity were determined for the -40+60 sieved sorbent and the resulting sorbent powder. After considering several adsorption models, the Langmuir isotherm was chosen to model the data. From fitting the Linearized Langmuir Isotherm, the resulting adsorption capacity was determined to be 189 mg/g for the sieved material and 79 mg/g for the powder, which is less porous. These results indicate that the mesoporous silica could be an effective way to remove cationic dyes and potentially other organic species at the ppm level from wastewater.

MWRM 2026 MW208

Theoretical and computational treatments of molecular binding in the context of lipid membranes

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The equilibrium dissociation constant and the binding free energy of two molecular moieties in bulk solution are two classic and extremely familiar concepts. The binding free energy of two molecular moieties in solution can be characterized experimentally and can also be computed using molecular dynamics simulations by relying on rigorously formulated free-energy simulation methodologies. In contrast, formulating these same concepts in the context of membranes requires some caution. For instance, standard computational free-energy methodologies are not applicable to integral transmembrane (TM) proteins because the association process is completely restricted to the two-dimensional space of the membrane. Another situation is that of peripheral membrane-binding proteins, where the binding process brings an unbound protein in three-dimensional bulk solution to a bound state in which it is restricted to the two-dimensional surface of the membrane. How to rigorously formulate the proper statistical mechanical description of these different situations, and design effective computational methods to treat these problems, remains a challenge. Here, rigorous statistical

mechanical theoretical frameworks will be formulated for the treatment of integral transmembrane (TM) proteins and peripheral membrane-binding proteins. These new methods will be illustrated by considering the association of the glycophorin A homodimer and the binding of Bacillus thuringiensis phosphatidylinositol-specific phospholipase C (BtPI-PLC) to the membrane surface.

MWRM 2026 MW97

Thermodynamic characterization of naturally occurring RNA octaloops

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RNA plays essential roles in gene regulation, catalysis, and therapeutic targeting, with its biological function tightly linked to its three-dimensional structure. Accurate RNA structure prediction typically begins by determining the secondary structure through free energy minimization using nearest-neighbour parameters. However, predictive accuracy remains limited because many structural motifs, particularly hairpins, are not well characterized thermodynamically. Although hairpins are the most common RNA secondary structure motif, octaloops, which contain eight nucleotides in the loop, have been examine in only a few thermodynamic studies. This work aims to determine the thermodynamic parameters (Gibbs Free Energy, Enthalpy, and Entropy) for 20 abundant, naturally occurring octaloop sequences to develop an octaloop-specific thermodynamic model. Frequent octaloop sequences were identified from secondary structure databases and designed to preferentially form unimolecular hairpins rather than bimolecular duplexes under high salt conditions (1 M NaCl) required for optical melting experiments. Equilibrium calculations were used to ensure that each construct maintains a hairpin population exceeding 90%. RNA oligonucleotides were synthesized by Integrated DNA Technologies and subsequently purified using Sep-Pak and thin layer chromatography. The purified oligonucleotides were optically melted across a 50-fold concentration range. Thermodynamic parameters were extracted using MeltWin 3.5 and will be incorporated into a linear regression analysis to produce a predictive model describing octaloop stability. By expanding the thermodynamic database for RNA hairpin loops, this project will improve the accuracy of RNA secondary structure prediction algorithms and support deeper insights into RNA function.

MWRM 2026 MW282

Thermodynamic kinetics of gold ion retrieval by linear and branched cross-linked polyethyleneimine networks

***Merina Sah**[1], msmn5@umsystem.edu, Peng Tao[2], Zhonghua Peng[1], Xiaobo Chen[1]. (1) Chemistry, University of Missouri-Kansas City, Kansas City, Missouri, United States(2) Chemistry, Southern Methodist University, Dallas, Texas, United States*

Gold is a precious metal due to its intrinsic value and scarcity and has been extensively used in catalysis, jewelry, medicine, and electronics. The demand for gold has been increasing with the growing need for device manufacturing because of its unique physical and chemical properties. Gold is a very efficient conductor of electricity, and resistant to corrosion, used in gold-based electronic devices such as connectors, switches, hybrid circuits, soldered joints, connecting wires and connection strips. Electronic waste (e-waste) contains gold about 200-350 g/t, much higher than those found in natural ores (5-30 g/t).
Adsorption-based gold recovery technology is regarded as a highly effective, simple, economic and environmentally friendly method. However, this method has been observed with some longstanding challenges such as the low adsorption capacity, slow adsorption kinetics and low ion selectivity. In this project, we propose systematic experimental and theoretical studies to gain fundamental insights on interactions between gold ions and novel adsorbents based on intrinsically porous triazine-crosslinked polymer networks (TCPEIs) exhibit unprecedentedly high adsorption capacity and selectivity towards $[AuCl_4]^-$ ion in a wide pH range with ultrafast adsorption and desorption kinetics.
This project includes the effect of temperatures on adsorption kinetics and rates by performing adsorption of gold metal ions by linear and branched TCPEIs. For quantification, Atomic Absorption Spectroscopy (AAS) and UV-Vis Spectroscopy were used and the data obtained from AAS are used to determine amount of Au (III) adsorbed on adsorbent at different contact time (Cs in mg/g), Adsorption efficiency in percentage (η %), Equilibrium Capacity (q_e), Adsorption equilibrium constant (Keq), the change in Gibbs free energy (ΔG°), change in enthalpy (ΔH°), change in entropy (ΔS°) from Van't Hoff equation and plot and activation energy (E_a) by using Arrhenius equation and plot. Also, the kinetic models mainly Pseudo-First order and Pseudo-Second order are fitted to determine which model best describes the mechanism of gold adsorption on adsorbents.

MWRM 2026 MW207

Three-dimensional electrospun Zn/PCL and core–shell Zn/PCL@PCL scaffolds with tunable zinc release

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Developing three-dimensional (3D) scaffolds remains a major challenge in tissue engineering. In this study, highly porous 3D zinc nanoparticle/polycaprolactone (Zn/PCL) scaffolds were fabricated using electrospinning and a thermal-induced self-agglomeration (TISA) process. Scaffold morphology and structure were characterized by SEM. Zinc release in physiological saline was quantified by ICP-MS and analyzed using kinetic models. Zn/PCL scaffolds exhibited concentration-dependent biphasic release profiles dominated by Fickian diffusion, with release rates tunable through zinc nanoparticle loading. To further regulate zinc release, core–shell Zn/PCL@PCL fibers

were fabricated by coaxial electrospinning. The resulting 3D scaffolds showed significantly slower zinc-release kinetics than blend Zn/PCL scaffolds with similar zinc contents while maintaining a porous nanofibrous architecture. These results demonstrate that combining electrospinning, TISA processing, and core–shell fiber design provides a versatile strategy for developing 3D scaffolds with controllable zinc delivery.

MWRM 2026 MW170

Total synthesis of Reniochalistatin E analogs to enable drug delivery & potentiation

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Reniochalistatin E (Ren. E) is a macrocyclic, octapeptide marine natural product derived from *Reniochalina stalagmitis* and has been shown to possess cytotoxicity against myeloma (IC50 = 4.9 μM, RPMI-8226) and gastric cancer cells (IC50 = 9.7 μM, MGC-803). Additionally, its first total synthesis by our lab (2017) and subsequent total syntheses of analogs (2025-present) have shown that the highly aromatic drugs 6-thiopurine and Doxorubicin exhibit synergism with our synthetic compounds. Our hypothesis is that aromatic residues in Ren. E undergo pi-pi stacking with these drugs to enhance their cytotoxicity. Our lab's current interest to understand Ren E's structure-activity relationship (SAR) has led to our ongoing evaluation for its potential use as a drug conjugation platform. This work accomplished the gram scale synthesis of a heptapeptide intermediate used to access these analogs along with the synthesis and conception of various amino acid-based drug handles to continue SAR and drug platform evaluations.

MWRM 2026 MW166

Total synthesis of the trikentrins and the trikentramides using one-pot tandem Bartoli syntheis/indole aryne Diels-Alder cycloaddition methodologies

An Nguyen*, annwdb@umkc.edu, William McAtee, Christopher Brown, Mark Rayhart, Katie Smith, Gesung Rissler, Sarah Powell, Maura Grijalva, Cassidy Hill, Elise Kraenow, Blake Harmon, Carolyn Lower, Xaviera Muhammad, Jacob Rodriguez, Joey Long, Keith R. Buszek. Department of Chemistry, University of Missouri-Kansas City, Kansas City, Missouri, United States*

The trikentrins and the trikentramides are members of the uncommon benzannulated group of indole natural products. These and the structurally similar herbindoles exhibit significant biological activities across a broad spectrum of therapeutic areas, including antitumor, antimicrobial, antiparasitic, and analgesic. Other members of this

architecturally complex, biologically active compound class include the penitrems, nodulosporic acids, and teleocidins. Our laboratories have focused on the trikentrins as platforms for the development of new reaction methodology and as drug discovery templates. In this presentation we describe an efficient and novel approach to the trikentrin core that builds on our previous work using the Bartoli indole synthesis from 1,2,5-tribromo-3-nitrobenzene followed by an unprecedented one-pot cascade of reactions: regioselective Grignard exchange, elimination, and subsequent 6,7-indole aryne cycloaddition. Elaboration of this core without the need for transition metal-catalyzed cross-coupling reactions affords *cis*-trikentrin A in only four additional steps. With this target in hand, trikentramide A and B were readily synthesized in one additional step. This practical and scalable approach is amenable to other members of the trikentrins, trikentramides, and herboindoles as well as for diverse library synthesis.

MWRM 2026 MW166

Total synthesis of the trikentrins and the trikentramides using one-pot tandem Bartoli syntheis/indole aryne Diels-Alder cycloaddition methodologies

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MWRM 2026 MW06

Toward high-throughput quantitative measurements of RNA-protein binding

***Prathapa D. Perera**, pperera3@huskers.unl.edu, Joseph D. Yesselman, Catherine D. Eichhorn. Chemistry, University of Nebraska-Lincoln, Lincoln, Nebraska, United States*

Ribonucleoproteins (RNPs) are RNA-protein complexes that are critical to cellular function. Disruption of RNA-protein interactions contributes to a range of neurodevelopmental and neurodegenerative disorders. Quantitative characterization of RNA-protein interactions is necessary to determine binding affinities and assess how structural changes influence protein binding. Traditionally, techniques such as ITC, NMR spectroscopy, fluorescence polarization (FP), and filter binding assays have been used for this purpose, as they provide detailed thermodynamic and structural information. These techniques are, however, inherently low throughput. In recent years, the growing need to characterize RNA-protein interactions across large RNA libraries has led to the development of high-throughput approaches. However, many existing high-throughput techniques offer limited experimental flexibility and provide global binding measurements, lacking nucleotide-resolution information on protein-induced changes in RNA structure, limiting our ability to identify specific nucleotides involved in RNA-protein binding and to characterize the structural changes that occur upon protein binding. To address these challenges, we developed a DMS-MaPseq-based approach for quantitative characterization of RNA-protein interactions at nucleotide resolution. Combining chemical probing with high-throughput sequencing, DMS-MaPseq measures DMS modification of solvent-accessible adenine and cytosine residues. Protein binding protects interacting nucleotides from DMS modification, reporting nucleotide-resolution chemical footprints of RNA-protein interactions. To validate this approach, we utilized the well-characterized MS2 RNA–MS2 coat protein model system. We first benchmarked DMS-MaPseq using ITC and measured a binding affinity (K_d) of 19.8 ± 4.50 nM. DMS-MaPseq revealed ten- to twenty-fold reductions in DMS reactivity at established MS2 binding residues upon protein binding. Building on this validation, we then generated a library of MS2 aptamer variants to evaluate the impact of sequence on MS2 protein recognition. These results demonstrate that DMS-MaPseq can identify RNA-protein interactions at nucleotide resolution and serve as a scalable high-throughput approach for quantitative measurements of RNA-protein binding across large RNA libraries.

MWRM 2026 MW06

Toward high-throughput quantitative measurements of RNA-protein binding

***Prathapa D. Perera**, pperera3@huskers.unl.edu, Joseph D. Yesselman, Catherine D. Eichhorn. Chemistry, University of Nebraska-Lincoln, Lincoln, Nebraska, United States*

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MWRM 2026 MW75

Toward predictive design of functional polymeric materials: A three-phase interaction framework

***Ji Qi**, qiji0811@126.com, Jikai Zhao. Kansas State University, Manhattan, Kansas, United States*

Functional polymeric materials are increasingly expected to combine mechanical robustness, sustainability, and multifunctionality. However, material development often remains empirical because the interactions among polymers, fillers, and solvents are rarely considered as an integrated system. Here, we present a three-phase interaction framework for understanding and designing functional polymeric materials. The framework describes key interactions among polymer, filler, and solvent phases and illustrates how these interactions collectively influence material structure, properties, and performance. Representative biomacromolecules are discussed as versatile components that can serve as network formers, reinforcing fillers, or interfacial mediators. This perspective highlights opportunities for transitioning from empirical formulation toward predictive material design and provides a general framework for developing next-generation functional polymeric materials.

MWRM 2026 MW317

Towards a consistent framework for efficient simulation of phase transitions of proteins, nucleic acids and metabolites

***Jianhan Chen**, jianhanc@umass.edu. Chemistry, University of Massachusetts Amherst, Amherst, Massachusetts, United States*

Biomolecular condensates form and dissolve through spontaneous phase separation, driven primarily by dynamic, multivalent biomolecules such as intrinsically disordered proteins (IDPs), single stranded RNAs and DNAs.These condensates play crucial roles in a myriad of cellular processes, including RNA storage and processing, stress response, metabolism, and cellular signaling. Efficient coarse-grained (CG) models are required to reach the length and time scales of biomolecular phase transitions. Existing CG models of dynamic nucleic acids and proteins, however, are largely limited to one or two beads per residue, and lack the detail necessary to capture diverse interactions of nucleic acids and proteins, particularly peptide backbone-mediated interactions and nucleic acid base stacking, base pairing, and Mg2+ coordination. In this talk, I will discuss our recent progresses towards developing intermediate resolution CG models of proteins and nucleic acids, namely, HyRes and iConRNA/iConDNA. Our results show that these models provides a powerful framework for direct simulation of both homotypic and heterotypic nucleic and protein phase transitions, enabling molecular studies of how conformational dynamics and its response to complex condensate environments control the phase behavior and condensate material properties.

MWRM 2026 MW73

Training-free data-driven prognosis of lithium-ion battery anomalies and thermal runaway

***Lin Liu**, linliu@ku.edu. Mechanical Engineering, University of Kansas, Lawrence, Kansas, United States*

Lithium-ion battery safety is governed by coupled electrochemical, thermal, and mechanical degradation processes that may evolve from subtle performance anomalies into rapid thermal runaway. Physics-based prognostic models generally require detailed constitutive relationships and boundary conditions, whereas conventional machine-learning approaches often depend on extensive labeled training datasets. This work presents data-driven prognosis (DDP), a deterministic framework for detecting battery instabilities using measured or simulated operating data without offline model training. DDP assumes the local existence of a conservation principle but does not require prior knowledge of its global mathematical form or the underlying failure mechanisms. At each analysis step, data from two consecutive time instances are used to calculate a dimensionless local length scale and the corresponding composite curvature of the system’s state-space manifold. Battery stability is then assessed through complementary indicators describing path dependency, critical chain formation, residual curvature, and energy exchange amplitude. Application of the framework to lithium-ion battery cycling data demonstrates that DDP can identify deviations from normal

degradation behavior and predict failure before conventional end-of-life criteria are reached. Integration of DDP with an electrochemical-thermal cell model further enables the analysis of temperature escalation and the progression of local anomalies toward thermal runaway. These results demonstrate the potential of DDP to provide interpretable and computationally efficient early warnings using heterogeneous electrochemical and thermal data. The framework offers a promising foundation for real-time battery health monitoring, safer battery-management systems, and prognosis of anomalies in other multiscale and multiphysics energy systems.

MWRM 2026 MW53

Transferable and accurate machine-learned potential for exploring the potential energy surfaces of gold chloride nanoclusters

***Jonathan T. Bvunzawabaya**, jtbvunza@ksu.edu, Christine M. Aikens. Chemistry, Kansas State University, Manhattan, Kansas, United States*

Ligand-protected gold nanoclusters are promising materials for catalysis, sensing, and biomedicine, with gold chloride complexes serving as key precursors in their synthesis. In the absence of X-ray crystal structures, density functional theory (DFT) is widely used to reliably predict cluster geometries. However, its high computational cost limits its application to long-timescale molecular dynamics (MD) simulations, warranting the development of accurate machine-learned force fields (ML-FFs) to explore the potential energy surfaces (PES) of complex gold chloride nanoclusters. Herein, we develop an ML potential trained on a reference dataset comprising four theoretical gold chloride motifs: $Au_{18}Cl_{24}$, $Au_{24}Cl_{20}$, $Au_{28}Cl_{20}$ and $Au_{38}Cl_{24}$ sampled across temperatures from 300 K to 500 K. Transferability was assessed in LAMMPS by comparing ML-FF energy predictions against single-point VASP calculations for 10 structurally diverse clusters entirely excluded from training. The model achieves high predictive accuracy, yielding mean absolute deviations (MADs) ranging between 0.5 and 6 meV/atom across the test suite. Following literature reports characterizing the presence of Au_{32} species in synthesis seed solutions, we utilized our potential to examine the PES of the pseudo-icosahedral $Au_{32}Cl_{20}^{-12}$ cluster. Simulated annealing MD simulations revealed a novel, lower-energy conformational space (minimizing to -9.224 eV) that directly challenges previous structural baselines. While literature models describe the cluster as a highly rigid, symmetric $Au_{12}@Au_{20}$ double-shell framework protected by static, uniformly distributed terminal Au-Cl bonds, our ML-FF trajectories identify a dynamic structural relaxation stabilized by a cooperative network of Au-Cl-Au bridging bonds. These findings underscore the capacity of trained ML-FFs to not only replicate expensive ab-initio metrics with remarkable efficiency but to effectively map uncharted potential energy surfaces and correct static structural assumptions in complex cluster synthesis.

MWRM 2026 MW169

Transforming Reniochalistatin E into a modular drug delivery platform

***Noah J. Burgoon**, noahburgoon22@gmail.com, Matthew Barnett, Ryan J. Rafferty. Chemistry, Kansas State University, Manhattan, Kansas, United States*

Reniochalistatin E (RenE) is a marine-derived macrocyclic peptide natural product first isolated by Lin and co-workers in 2014 from the sponge Reniochalina stalagmitis. Among the five proline-rich cyclic peptides identified in this study, RenE was the only compound reported to possess cytotoxic activity, exhibiting IC50 values of 17.3 μM against HeLa cells and 4.9 μM against RPMI-8226 multiple myeloma cells. Motivated by these findings, our laboratory completed the first total synthesis of RenE in 2017 and subsequently developed a phenylalanine analog in 2025. The optimized synthetic route afforded RenE in 15 steps and 5% overall yield, enabling biological evaluation against the MM.1R multiple myeloma cell line. To investigate the relationship between structure and biological activity, the phenylalanine analog was synthesized and evaluated alongside the parent natural product. Both compounds exhibited enhanced cytotoxicity when used in combination with established anticancer agents, suggesting a synergistic effect. Current structure activity relationship studies are focused on understanding the contribution of the aromatic residues to this enhanced activity and leveraging these insights to guide the design of more potent analogs. The incorporation of an alkene functional handle is currently underway which will provide a versatile platform for late-stage conjugation of an interchangeable therapeutic payloads. If successful, this would expand the utility of RenE as a targeted drug delivery scaffold.

MWRM 2026 MW120

Tröger's base as a multifunctional platform for metallodrug and supramolecular design

***Asanga K. Mannapperuma**, mmannapp@ksu.edu, Boris B. Averkiev, Christer B. Aakeroy. Department of Chemistry, Kansas State University, Manhattan, Kansas, United States*

The design and synthesis of new organic ligands and metal complexes with potential therapeutic applications remain an active area of interdisciplinary research. Tröger's base (TB) is a rigid, V-shaped, chiral supramolecular scaffold that enables precise three-dimensional positioning of functional groups, making it an attractive platform for the development of metal-based therapeutic and supramolecular systems. Functionalized TB derivatives bearing pyridyl and benzaldehyde substituents provide versatile platform for metal coordination and further molecular modification. These ligands can form well-defined complexes with biologically relevant metal ions including Cu(II), Zn(II), Ru(II), and Ag(I), several of which have attracted considerable interest in the development of anticancer agents. The inherent cleft geometry and chirality of the TB framework also offer opportunities for directing supramolecular organization through predictable non-covalent interactions. This study further explores the incorporation of hydrogen- and halogen-bonding functionalities and their influence on the structural organization and stability of TB-derived systems. By combining metal coordination, modular functionalization, and supramolecular recognition within a single rigid scaffold,

TB derivatives offer a versatile platform for the rational design of structurally defined systems with potential biomedical applications. The synthesized ligands and metal complexes were characterized using Fourier-transform infrared spectroscopy (FT-IR), ^{1}HNMR and 13CNMR spectroscopy, powder X-ray diffraction (PXRD), single-crystal X-ray diffraction (SCXRD), and differential scanning calorimetry (DSC).

MWRM 2026 MW120

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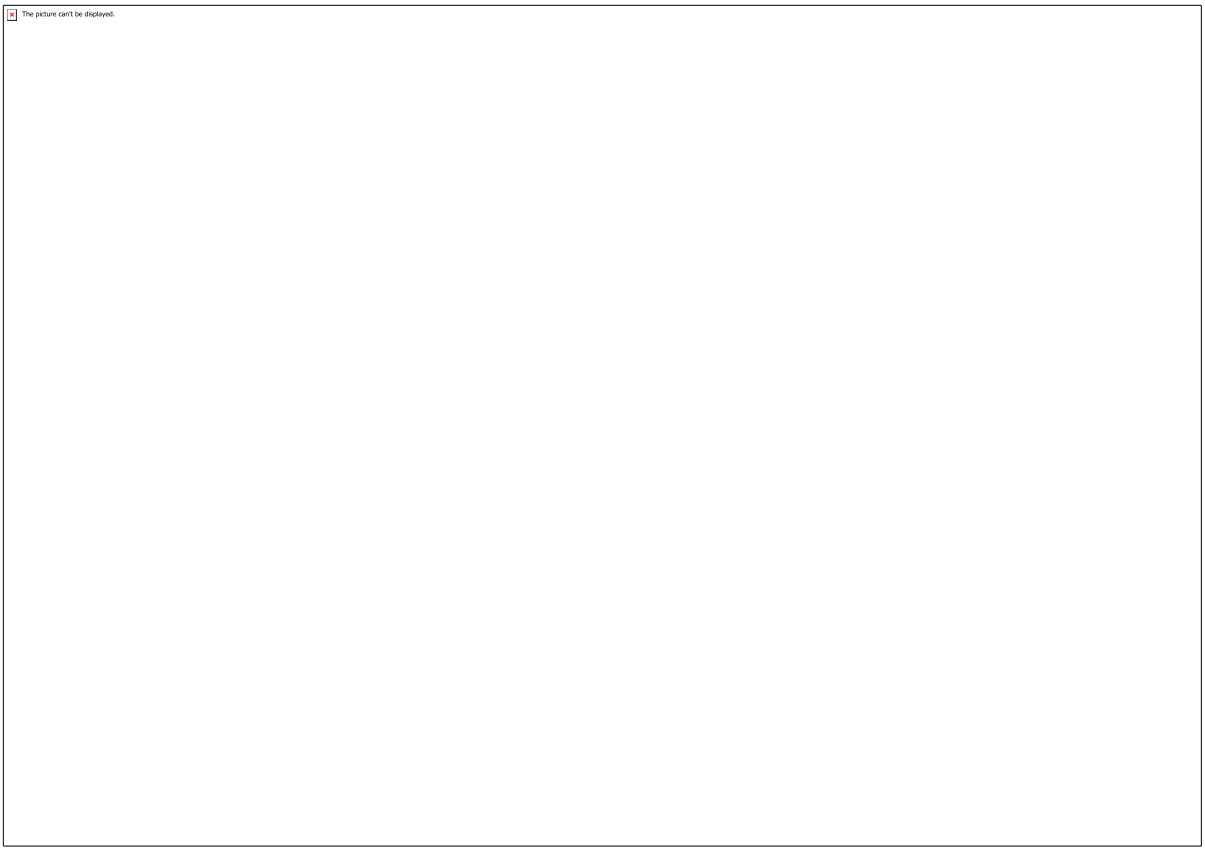
MWRM 2026 MW294

Trojan terephthalates for scalable depolymerization

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The escalating reliance on plastics and the price volatility of fossil fuels demand recycling strategies that recover monomers without degrading material quality. Polyethylene terephthalate (PET), despite being the most widely produced and recycled polyester, degrades during thermomechanical recycling, limiting recycled material to low-end applications. Herein, we demonstrate that incorporating dimethoxy functionalized Trojan terephthalates (DMTPA) at 2.5-5 mol% enables depolymerization to monomers in pressurized subcritical water at 180 °C. We developed a scalable O-methylation route to synthesize DMTPA using DMC (dimethyl carbonate) and DMS (dimethyl sulfide) under conditions that result in DMC decomposition (250 °C, 1100-1500 psi), generating supercritical CO_2 and methanol in situ, eliminating the need for toxic alkylating agents such as methyl iodide, dimethyl sulfate, and other cosolvents. Density functional theory (DFT) reveals that ortho-methoxy groups twist the ester carbonyl out of plane by 23.7 °, disrupting resonance and increasing susceptibility to nucleophilic attack. DMTPA facilitates Lewis acid coordination and reduces crystallinity, leading to rapid bulk hydrolysis; calculations show that $ZnCl_2$ is more effective than $Zn(OAc)_2$ for depolymerization. Pilot-scale production (>70 kg), solid-state polymerization to bottle-grade intrinsic viscosity, and injection stretch blow molding of commercial spirit bottles confirm full drop-in compatibility with existing manufacturing. The limited incorporation of Trojan terephthalates maintains the performance properties of conventional PET while adding inherent chemical recyclability, thus creating a synthetic approach to circular plastics.



MWRM 2026 MW368

Tuning ion association via surface interactions: When bulk-centric pictures may disappoint

***Ryan Jorn**, ryan.jorn@wichita.edu. Chemistry and Biochemistry, Wichita State University, Wichita, Kansas, United States*

Rationalizing changes in the reactivity of high concentration electrolytes often focuses on correlations between bulk solvation structures and the electrochemistry of the electrode/electrolyte interface. However, this approach neglects the role of the interface itself in modifying the solvation environment near the electrode surface. Our work seeks to investigate changes in electrolyte structure and dynamics at interfaces relevant to metal-ion electrolytes for rechargeable batteries using a range of simulation strategies from ab initio to coarse-grained molecular dynamics. In this talk, we will contrast two classes of electrolytes that represent two opposite extremes: carbonate solvents, which evidence significant changes in ion association at aged interfaces, and ether solvents, which maintain bulk solvation structures as a result of strong ion chelation. The role of changing concentration and applied bias voltages will be considered for both lithium-ion and sodium-ion mixtures. It will be shown that with increasing electric fields, reliance on bulk solvation structures even at clean graphite surfaces becomes tenuous and we

present a new hypothesis that increased concentration is necessary to overcome anion electrostatic repulsion. We will conclude with discussion of the impact of polarization on general trends and the development of enhanced sampling methods to study the free energy barriers for ion transport.

MWRM 2026 MW198

Two-photon absorption spectroscopy in service of microscopy imaging and dynamics

***Christopher G. Elles**, elles@ku.edu, Joohyun Lee, Crest Koemel, Joseph Sommers, Weston Henning. The University of Kansas Department of Chemistry, Lawrence, Kansas, United States*

Two-photon fluorescence imaging, 3D printing, photodynamic therapy, and many other applications achieve localized excitation of target molecules with very high spatial resolution by taking advantage of the requirement for high-intensity radiation to induce the simultaneous absorption of two photons. Unlike one-photon excitation, two-photon absorption (2PA) occurs only at the focus of a laser beam or at the point where two laser beams cross, providing very high spatial selectivity. Traditional two-photon techniques typically use monochromatic lasers and therefore are limited to a single excitation energy. However, we are developing an approach using ultrafast pump-probe techniques to enable broadband 2PA spectroscopy measurements that simultaneously cover a wide range of excitation energies. This talk will discuss the development of new methods for rapid and reproducible broadband 2PA measurements, the quantitative measurement of accurate 2PA cross sections using stimulated Raman scattering of the solvent as an internal standard, and the potential for making information-rich 2PA measurements with microscopic spatial resolution. The dynamics of molecules following two-photon excitation will also be discussed. Ultrafast spectroscopy measurements comparing the dynamics following one- and two-photon excitation provide additional insights into the excited-state relaxation of target molecules. Differences on the ultrafast time scale have the potential to reveal unique information about the native environment of a chromophore.

MWRM 2026 MW199

Two-photon excited fluorescence measurement of coumarin 153 using broadband two-photon absorption spectroscopy combined with sensitive fluorescence detection

***Joohyun Lee**[1], hanamitch@gmail.com, Chase Courbot[2], Crest Koemel[1], Joseph Sommers[1], Christopher G. Elles[1]. (1) Chemistry, University of Kansas, Lawrence, Kansas, United States(2) Chemistry, NC State University, Raleigh, North Carolina, United States*

Broadband two-photon absorption (BB-2PA) spectroscopy, using a non-degenerate pumping scheme with a single-wavelength pump and broadband probe pulses, has been shown to provide a complementary 2PA cross-section profile compared to conventional degenerate 2PA measurements. Due to its simultaneous broadband detection, BB-2PA also demonstrated significantly more efficient data acquisition, whereas conventional methods require cumbersome single-wavelength scanning across the entire 2PA energy range. However, both techniques require considerably high concentrations of sample solution because both measurements rely on small differential transmission upon the 2PA transition. While the two-photon excited fluorescence (2PEF) technique using a degenerate pump beam still has to undergo single-wavelength scanning to indirectly measure the 2PA cross-section profile, it can provide accurate values without demanding such high concentrations because the measurement relies on sensitive fluorescence detection where background signals do not exist. In this work, to leverage the advantages of each technique, we added on fluorescence detection to our BB-2PA setup, in which 2PA transitions still occur in a non-degenerate manner, and the subsequent fluorescence is sensitively detected to provide a 2PA profile. Due to the independent detection setup but still sharing the identical pump-probe geometry, we could simultaneously measure signals from BB-2PA and 2PEF. Using this method, we measured BB-2PA and 2PEF of coumarin 153 in methanol, a well-established 2PA standard with a well-defined fluorescence quantum yield, and directly compared the resulting spectra. We also performed a concentration-dependent study to determine whether any aggregated species distort the inherent 2PA profile of the sample solution. Lastly, we also examined how combined BB-2PA and 2PEF spectroscopy of 2PA chromophores in different solvents can sensitively report their local environment via spectral shifts and changes in fluorescence quantum yields.

MWRM 2026 MW447

Ultrafast study of a pH-sensitive azobenzene photoswitch in basic conditions

Jaden Riddle*, jadenriddle28@gmail.com, Weston Henning, Christopher G. Elles. The University of Kansas, Lawrence, Kansas, United States*

Azobenzene derivatives boast unique isomerization dynamics that vary based on solvent and substituent effects. This inherent versatility of azobenzene makes it an appealing parent compound for fields requiring kinetic and energetic specificity, such as pharmacology and solar energy harvesting. Although many substituent and solvent effects on azobenzene isomerization are well documented, little literature is available on the effect of high pH on isomerization for azobenzenes with ionizable, electron-donating substituents, including hydroxyl moieties (-OH). In pursuit of quantifying and describing the effects of electron-rich ionized azobenzenes, an initial experiment was conducted using transient absorption (TA) spectroscopy to examine the trans to cis isomerization of a pH-sensitive azobenzene derivative, 4,4’-dihydroxyazobenzene (DHAB), in basic conditions. A pump-probe TA setup utilized femtosecond laser pulses at two distinct wavelengths to excite DHAB to the first and second excited states, followed by a white-light probe to record absorption data of the transient species. The resulting data indicate

the presence of a long-lived, unstable intermediate species formed during molecular relaxation. Quantum calculations were performed to estimate the molecular orbitals and transition energies of basic DHAB and may support the presence of an atypical isomerization pathway induced by the electron-donating effects of the deprotonated para-hydroxyl moieties. This result could suggest the possibility of manipulating azobenzenes to achieve longer-lived, more reactive excited states when excited by high-energy photons, expanding the possibilities of azobenzene applications.

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MWRM 2026 MW325

Understanding polymer-metal interactions through amino acid-functionalized polymers

***Graham Moran**, gcmoran2@ksu.edu, Patricia R. Calvo. Chemistry, Kansas State University, Manhattan, Kansas, United States*

Metal-chelating polymers offer a versatile platform for applications such as water purification, metal recovery, and drug delivery. Despite recent progress in this area,

many fundamental aspects are poorly understood including the importance of ligand design, polymer molecular weights, and polymer architecture. This study focuses on the synthesis of a linear polymer library with different amino acid functionalized polymers and their interactions with various metals. Reversible addition-fragmentation chain transfer (RAFT) polymerization of pentafluorophenyl acrylate (PFPA) was employed to create well-defined linear polymers of controlled molecular weight, followed by post-polymerization functionalization with various amino acids to introduce different chelating ligands. The polymers were characterized by ^{1}H NMR and size-exclusion chromatography (SEC), confirming narrow molecular weight distribution and functionalization was quantified using ^{19}F NMR as well as IR spectroscopy. Dynamic light scattering (DLS) of the functionalized metal chelating polymers was conducted to determine the size and zeta potential both with and without the metals present to see how the polymer conforms in water. Isothermal titration calorimetry (ITC) was used to determine the metal-binding thermodynamics with different metals of various hardness and size. Future work will investigate the selectivity of metal binding with the polymers by ICP-OES. The findings of this study aim to enhance the understanding of polymer-metal binding interactions, an area that is less understood compared to small-molecule chelators.

MWRM 2026 MW44

Understanding the tunable properties of aza-crown complexes of the uranyl ion

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Crown ethers represent a diverse family of ligands that can be tuned to bind most metals. However, stable chelation/coordination of the uranyl ion (UO2n+) by crown ether derivatives has not received the attention it deserves. Recently, our group has demonstrated that uranyl crown ether complexes can be prepared in a heterobimetallic system templated with an accessory Pt(II) center (J. Am. Chem. Soc., 2024, 46, 9597-9604), suggesting new opportunities in design of tunable uranyl complexes through use of all-organic crown-type ligands. In this presentation, the chemistry of recently prepared aza-crown complexes will be described, including both their solution properties as well as solid-state structure from X-ray diffraction analysis. Electrochemical and spectroscopic measurements have been carried out and shown that aza-crown ligands strongly influence the properties of the uranyl core motif, particularly in comparison to the prior heterobimetallic system that our group is continuing to study as well. Taken together, the findings available so far suggest that important consequences result from incorporation of derivatized nitrogen atoms into the crown ligands supporting uranyl complexes.

MWRM 2026 MW446

Uniformity from disorder in electrochemical reaction networks

***Olivia Underwood**, olivia.underwood@slu.edu, Istvan Z. Kiss. Chemistry, Saint Louis University, St. Louis, Missouri, United States*

Uniform chemical reactivity is generally expected in systems operating under nearly identical conditions. However, in networks of interacting chemical reactions far from thermodynamic equilibrium, symmetry breaking can lead to heterogeneous behavior despite nominally uniform environments. Electrochemical reactions provide a prime example of such coupled systems, where interactions and heterogeneities strongly influence collective dynamics. In particular, negative feedback, often arising from external constraints, can induce symmetry breaking and generate spatiotemporal patterns.
In this study, we investigate how a specific form of heterogeneity; variations in individual electrode resistance that modify double-layer charging times, affects spatial uniformity in coupled electrochemical systems. The nickel electrodissolution reaction is studied using two-electrode arrays. Under negative coupling, the system exhibits antiphase oscillations in dissolution rates when the coupling strength exceeds a critical threshold. We then introduce heterogeneity and examine its effect on electrode uniformity by varying the resistance of individual electrodes while keeping the mean total resistance constant. Uniformity is quantified by the mean difference in electrode potentials relative to the homogeneous case. We find that negative coupling is essential for heterogeneity to enhance uniformity and that stronger negative coupling amplifies this effect. As the degree of heterogeneity increases, the mean potential difference initially decreases, indicating improved uniformity, reaches a minimum at an optimal level of heterogeneity, and then increases approximately linearly with further increases in heterogeneity. These experimental observations are reproduced by numerical simulations based on a kinetic model of nickel electrodissolution.
Our results demonstrate the counterintuitive phenomenon that introducing heterogeneity can improve uniformity in coupled electrochemical systems. These findings provide new insights into the interplay between coupling and disorder in nonlinear electrochemical systems and may inform the design of electrochemical technologies, including sensors, reactors, and batteries, where uniform operation is often desirable.

MWRM 2026 MW446

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MWRM 2026 MW424

University of Kansas nanofabrication facility: Equipment and capabilities

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The University of Kansas Nanofabrication Facility (KUNF) is a core lab operated through the KU Office of Research and the Center for Molecular Analysis of Disease Pathways. KUNF primarily serves researchers developing micro- and nanofluidic devices for biomedical applications, while also supporting a broad range of research projects requiring micro- and nanofabrication capabilities. The facility includes approximately 1,300 sq ft of ISO class 5, 1,700 sq ft of ISO class 6, and 1,250 sq ft of ISO class 7 cleanroom space. Available capabilities include photolithography, nanoimprint lithography, plasma etching by ICP-RIE, wet etching, thin-film deposition,

scanning electron microscopy, atomic force microscopy, contact angle goniometry, ellipsometry, profilometry, wafer dicing, wire bonding, laser ablation and engraving, 3D printing, hot embossing, and COMSOL-based device modeling. The facility also provides microscopes for general inspection, ovens and furnaces, ultrapure water access, and dedicated process fume hoods.
KUNF is led by Dr. Susan M. Lunte and directed by Ryan Grigsby. Facility services and access are available to researchers from Kansas universities, as well as non-Kansas academic institutions and private industry users through contracted consultation, training, facility access, and staff-supported services. Training is provided to new investigators and graduate students in micro- and nanofabrication procedures, cleanroom practices, and equipment operation. Hourly and per-use rates apply for facility access, equipment usage, and staff labor, while initial consultation is provided at no cost.

MWRM 2026 MW179

Unlocking Lagunamide C: Structure-activity-relationship studies of the polyketide and penetration investigations of the polypeptide backbone

***Benjamin C. Rudeen**, bcrudeen@ksu.edu. Chemistry, Kansas State University, Manhattan, Kansas, United States*

In 2011 Tan and co-workers isolated lagunamide C (LagC), a depsipeptide from the cyanobacterium Lyngbya Majsucle in Singapore. It was shown to possess potent cytotoxicity against a panel of cancer cell lines: lymphoma (P388, IC50 24.4 nM), lung (A549, IC50 2.4 nM), prostate (PC3, IC50 2.6 nM), colon (HCT8, IC50 2.1 nM), and ovarian (SK-OV3, IC50 4.5 nM). LagC can be broken down into two structure motifs; the polyketide and polypeptide backbone. Through our total synthesis efforts and the work by Kigoshi the structure was revised and found to be an analog of odoamide. However, in our work we were able to show that the polyketide is the active cytotoxic unit and speculated that the polypeptide backbone is responsible for cellular penetration. To be presented will be our total synthesis efforts of LagC, the structural-activity-relationship studies performed upon the polyketide, and our investigations into cellular uptake and penetration by the polypeptide.

MWRM 2026 MW279

Unravelling the driving forces behind confined water dynamics in nanoscale silica slit pores

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The behavior of confined aqueous solutions can differ dramatically from the bulk. The study of these confined systems has garnered interest over the years. However, the root cause for this deviation from bulk-like behavior is still not well known. They are often thought to arise from either confinement effects or interfacial effects. At its core, the question is whether the water dynamics are influenced by only short-ranged surface effects or longer-ranged confinement effects. Molecular dynamics simulations of water in neutral β-cristobalite silica slit pores of varying pore widths are used to probe the water dynamics to elucidate how these effects shape the dynamics of water. We show that the impact of confinement interfacial effects is multifaceted and depends on the property being considered. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

MWRM 2026 MW250

Unravelling the impact of interfacial pH swings on nitrate electroreduction selectivity

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Nitrate is a widespread pollutant with significant environmental and human health impacts. Electrochemical nitrate reduction is a promising strategy to convert nitrate into value-added ammonia, but ammonia selectivity remains limited by poorly controlled interfacial reaction environments. Interfacial pH is a key parameter governing selectivity because it directly influences proton availability for the multi-electron, multi-proton conversion of nitrate to ammonia. Previous studies have shown that the temporal evolution of interfacial pH can strongly affect the product distribution during nitrate reduction.

Pulsed electrochemical operation has emerged as a strategy to control the near-surface pH by periodically replenishing reactant species at the electrode surface. Although pulsed operation is expected to influence the interfacial environment, it remains unclear which pulse conditions effectively stabilize local pH and how these dynamics impact nitrate reduction selectivity.

In this work, attenuated total reflection–surface-enhanced infrared absorption spectroscopy (ATR–SEIRAS) is used to quantify local pH within 10 nm of the catalyst surface. Rapid spectral collection at 180 spectra per minute enables direct, time-resolved measurement of interfacial pH dynamics during pulsed electrochemical operation, capturing transient microenvironmental changes that have remained largely inaccessible experimentally. Complementary bulk electrolysis experiments are performed to accumulate products for quantification. Gas chromatography is used to analyze hydrogen and nitrogen, while ultraviolet-visible spectroscopy is employed to quantify nitrate, nitrite, and ammonia concentrations in the electrolyte.

By systematically varying the pulse duty cycle and current density, we investigate how pulsed operation influences local pH dynamics and identify operating regimes in which the near-surface pH remains stable. Correlating product distribution with transient interfacial pH behavior reveals how local reaction conditions govern nitrate reduction selectivity. These insights will establish quantitative design criteria for pulsed electrolysis and identify operating protocols that promote ammonia formation through control of the interfacial environment

MWRM 2026 MW248

Unusual reactivity of 2D transition metal carbides (MXenes)

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A large family of two-dimensional transition metal carbides and nitrides (MXenes) raises interest for many applications due to their high electrical conductivity, mechanical properties [1], potentially tunable electronic structure [2], nonlinear optical properties [3], and the ability to be manufactured in the thin film state [4]. However, their chemistry that is key to development of these applications, still remains poorly understood [5,6]. In this presentation we will discuss recent progress in understanding fundamental MXene chemistry and harnessing it for suppressing unwanted reactions and prolonging stability of these materials.
For example, suppressing oxidation and hydrolysis at high pH was demonstrated as an effective way to prolong shelf-life and stability of MXene aqueous colloids [7]. Use of polyphosphate also has been shown to improve chemical stability of MXene aqueous colloids [8].
Other selected examples illustrating connections between understanding MXene chemistry and development of their applications will also be considered.

MWRM 2026 MW244

Uranium redox at very positive potentials with oxygen-donor crown ethers

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The redox properties of the uranyl dication underlie virtually all processes used for preparing nuclear fuels and reprocessing of spent fuels, making development of strategies for controlling the reduction potential of uranium species an attractive target for future developments. In this presentation, the synthesis and electrochemical

characterization of uranyl species supported by a crown-ether ligand featuring six oxygen donors will be discussed. These efforts are motivated by the observation that few uranium species have been prepared which are supported by charge-neutral chelating ligands. The U^{VI} complex supported by the ligand studied here undergoes chemically reversible reduction to a corresponding U^{V} species at a more positive reduction potential than the others reported to date for cycling of non-oxo-functionalized uranyl moieties. Voltammetry and bulk electrolysis have been used to study the preparation of the U^{V} species from U^{VI} by electrochemical reduction, and optical spectroscopy has been used to identify key electronic features of the new compounds. Our most recent results will be presented as well, including spectroscopic titration studies of the water reactivity of this system and insights into potential hydrolysis products.

MWRM 2026 MW412

Using activation energies to elucidate the effects of osmolytes on water dynamics

***Abigail Kerr**, abbeykerr932@gmail.com, Anjali Radhakrishnan, Ward H. Thompson. Chemistry, The University of Kansas, Lawrence, Kansas, United States*

Osmolytes have been extensively studied for their stabilizing and destabilizing effects on protein structures. The mechanism underlying this behavior is still debated and has been attributed to either direct osmolyte-protein interactions or an indirect effect through which the osmolyte modifies the solvating water network. Previously, our group studied the osmolytes urea and TMAO for their ability to disrupt water diffusion and hydrogen-bond exchange times, with a focus on the energetic and entropic driving forces that were calculated by the fluctuation theory for dynamics approach and measured by NMR. These results showed that adding TMAO increased the water diffusion activation energy while adding urea had nearly no effect. In this work, we investigate the role of the osmolyte steric bulk and symmetry in modifying the water structure and dynamics by examination of a series of methylated urea solutes. We consider both the water self-diffusion coefficient and hydrogen-bond exchange time along with the corresponding activation energies. We discuss the influence of increased steric bulk on water dynamics with increased concentration of methylated urea solutes, and we provide insight into the structural contributions to this behavior through the disruption of the hydrogen bond network as well as diffusion within osmolyte solvation shells for water. The similarities and differences amongst bulk and symmetry of methylated urea systems are particularly discussed.

MWRM 2026 MW219

Utilization of chemical demonstrations as an experiential and collaborative learning strategy for general chemistry students

***George P. Nora**, George.Nora@northern.edu. Northern State University, Aberdeen, South Dakota, United States*

This poster presents the results of a group-based learning project in the general chemistry lab sequence at Northern State University (NSU). Students worked in varied teams and were asked to plan and carry out a chemistry demonstration show. Each group focused on key concepts covered throughout the two-semester course. This project served as the final assessment for General Chemistry II lab, asking students to apply their knowledge in a creative and practical way.

Teams designed and performed demonstrations covering topics like acid-base titrations, identifying ions, how temperature affects reaction speed, and precipitation reactions. Working together gave students a chance to share feedback with each other in real time and discuss ideas together. By splitting up tasks and working through problems as a group, students strengthened their understanding of chemistry. This approach also gave them practice in explaining scientific ideas, following lab safety rules, and working cooperatively.

Many studies show that group-based learning helps students remember material longer and improve their reasoning abilities, compared to working alone. Instead of just listening to lectures, students play a direct role in solving real problems and building knowledge with their peers. This makes the experience more engaging and gives students a clearer sense of how chemistry applies outside the classroom.

In addition to the academic benefits, students in this setting often develop stronger communication, teamwork, and problem-solving skills. The experience can help them feel more connected to their classmates and more confident in their abilities. These skills are highly regarded in both academic and professional environments. Because of these advantages, group-based learning has become common in many courses, and it continues to be refined through research into how group size, teaching methods, and assessment styles affect student outcomes.

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MWRM 2026 MW218

Utilization of eye tracking to add to the validity of data obtained using the resonance concept inventory

***Mary Simon**, marysimon@unomaha.edu, Sachin Nedungadi. University of Nebraska Omaha, Omaha, Nebraska, United States*

Resonance is a fundamental organic chemistry concept that is commonly misunderstood by undergraduate students. This misunderstanding leads to alternate conceptions that prevent students from understanding more advanced organic chemistry concepts. A 14-item Resonance Concept Inventory (RCI) was developed to help organic chemistry instructors detect student alternate conceptions. Think-aloud interviews were conducted during the development of the RCI to establish evidence based on response process validity. To gain further insight into the process that students employ, an exploratory study utilizing eye tracking was conducted. The eye movements and fixations of 26 first-semester undergraduate organic chemistry students were recorded while they answered the 14 RCI items. Heat maps, gaze plots, and areas of interest were used to compare correct and incorrect responders. The results suggest that correct responders focus on more relevant features of the items, and they exhibit a reasonable process to arrive at the correct answer.

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MWRM 2026 MW194

Vertically-stood anodic alumina membranes as unique platforms to study nanoconfined molecular diffusion and surface adsorption using single-molecule localization microscopy

***Takashi Ito**, ito@ksu.edu, Akash Nathani, Daniel A. Higgins. Chemistry, Kansas State University, Manhattan, Kansas, United States*

In-depth understanding of mass transport mechanisms within nanoscale pores is essential for future development of advanced chemical separation and energy storage materials. Our groups systematically investigate molecular-level diffusion dynamics in cylindrical nanopores such as those of anodic aluminum oxide (AAO) membrane using fluorescence correlation spectroscopy (FCS) and single-molecule localization microscopy (SMLM). Our FCS studies with laid-down AAO membranes, which comprise nanopores oriented vertically to an underlying coverslip, have revealed a two-component mechanism involving faster, hindered bulk-like diffusion and slower, desorption-mediated diffusion. However, the vertically-oriented nanopores are less suitable than horizontally-oriented nanopores for detailed measurements of single-molecule diffusion dynamics using SMLM. Herein, we will present a novel imaging platform based on vertically-stood AAO membranes, which comprise AAO nanopores oriented parallel to coverslip surface, for SMLM measurements of nanoconfined diffusion and adsorption dynamics. A piece of an AAO membrane (≈ 5 × 5 mm^2) was mounted on a notched opening (≈ 1 × 1 mm^2) fabricated in the wall of a cylindrical glass

cell. The bottom edge of the membrane was polished on lapping films to obtain a smooth surface, and then the glass cell was adhered to a glass coverslip with a clearance of ≈ 10 μm between the smoothed membrane edge and the coverslip. The resulting membrane was illuminated by excitation light emerging from the objective at an oblique angle to obtain SMLM data with reduced background fluorescence, as with highly inclined laminated optical light sheet microscopy. Importantly, this platform is applicable for direct observations of detailed adsorption and diffusion dynamics at the single-molecule level by simply adjusting the illumination positions, on the edge and side face of the membrane, respectively. In addition, this platform permits the easy replacement of solutions within the AAO nanopores to investigate the effects of solution composition on the adsorption and diffusion dynamics as well as the assessment of single-molecule orientational dynamics.

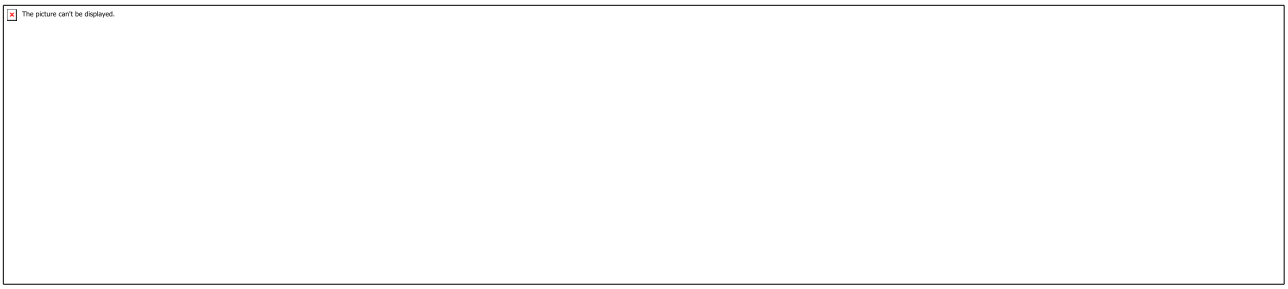
MWRM 2026 MW366

Virtual screening for modulators of the J-domain of DNAJA1

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The Computational Chemical Biology and Molecular Modeling (CCBMM) Core is a service lab dedicated to providing the computational resources and expertise to enhance the productivity of researchers of chemical biology and translational science in biomedical research. The CCBMM is introduced followed by an introduction of Pocket Optimization and Exemplar Screening, which enable the screening of tens of millions of drug-like compounds against an ensemble of protein structures.

DNAJA1 is an HSP40 protein that is responsible for the stabilization of conformational mutant p53, preventing its degradation. There is therapeutid potential for targeting DNAJA1, which would deplete mutant p53. Exemplar Screening was used to screen ten million compounds against an ensemble of DNAJA1 J-domain structures. 32 compounds were purchased and tested for the degradation of mutant p53, and a SAR-by-catalog approach was used to identify more potent modulators of DNAJA1, resulting in the identification of compound A11 which leads to the degradation of both DNAJA1 and mutant p53. A11 suppressed migration and filopodia formation in a manner dependent on DNAJA1 and conformational mutp53. A11 shows promise as a treatment against cancers expressing conformational mutant p53.



MWRM 2026 MW126

Visible-light-driven defluorination of perfluoroalkyl carboxylic acids through an inner-sphere transition-metal photocatalytic pathway

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The activation of carbon–fluorine (C–F) bonds remains challenging because of their exceptionally high bond dissociation free energies compared with other carbon–halogen bonds. Consequently, per- and polyfluoroalkyl substances (PFAS) are highly persistent, leading to widespread environmental contamination and growing concerns about their effects on human health.
In this study, we investigate the visible-light-driven defluorination of perfluoroalkyl carboxylic acids (PFCAs) using a readily accessible transition-metal photocatalyst under blue-light irradiation. The method is effective for C2–C9 PFCAs, including widely detected compounds such as perfluorooctanoic acid and perfluorononanoic acid. Several fluorinated monocarboxylic acids, perfluorinated dicarboxylates, and related carboxylate derivatives also undergo defluorination in good yields, demonstrating the generality of the transformation.
Mechanistic studies reveal that visible light and the reaction solvent play crucial roles in catalyst activation. UV–vis studies indicate that the photocatalyst undergoes ligand dissociation to form a bis-ligated complex, which subsequently participates in an inner-sphere mechanism. Upon visible-light irradiation, the activated catalyst promotes substrate decarboxylation followed by defluorination. Further mechanistic studies suggest perfluoroalkyl radical and metal-perfluoroalkyl species as potential intermediates.
These findings provide valuable mechanistic insights into transition-metal-photocatalyzed PFAS defluorination. Future work will focus on developing photocatalytic systems based on earth-abundant transition metals and achieving PFCA hydrodefluorination with transition metal photocatalysts.

MWRM 2026 MW11

Volatile organic compound enrichment from exhaled breath using cryogenic condensation for electrochemical sensing

***Lida Khalafi**, lida.khalafi@avila.edu. Chemistry, Avila University, Kansas City, Missouri, United States*

Noninvasive analysis of exhaled breath provides a promising approach for monitoring biomarkers associated with human metabolism, disease progression, and exposure to environmental and occupational hazards. However, the extremely low concentrations of volatile organic compounds (VOCs) in breath remain a major challenge for direct detection using portable analytical platforms. Here, we report a simple and effective breath condensation strategy based on a modified syringe equipped with a freezer-cold jacket to enhance the collection and detection of breath VOCs.

The cryogenic condensation approach enables efficient trapping and enrichment of volatile species from exhaled breath, generating a condensed breath sample suitable for downstream electrochemical analysis. As a proof of concept, we focus on the detection of ethanol and acetaldehyde, two important volatile metabolites with applications in alcohol monitoring, metabolic studies, and biomedical diagnostics. Under normal physiological conditions, ethanol and acetaldehyde concentrations in exhaled breath are significantly lower than those in blood, with reported breath-to-blood concentration ratios of approximately 1:2000 and 1:900, respectively. The developed condensation method overcomes this limitation by concentrating these volatile compounds into a small liquid phase, resulting in analyte concentrations that can exceed those present in blood samples.

The condensed breath samples obtained using this platform provide sufficient volume and analyte concentration for analysis with commercially available screen-printed electrodes, enabling the development of compact and potentially field-deployable electrochemical sensing systems. The combination of cryogenic enrichment and electrochemical detection offers a low-cost alternative to conventional breath analysis methods that often require complex instrumentation, such as gas chromatography and mass spectrometry.

This work demonstrates the potential of a simple sample preparation strategy to bridge the gap between trace-level breath biomarkers and accessible electrochemical sensing technologies. The proposed approach may enable improved sensitivity for portable breath diagnostics and provide a versatile platform for monitoring VOC biomarkers in clinical and point of care applications.

MWRM 2026 MW188

Wavelength-selective photochemistry via distinct reactive intermediates

***Logan Evans**, logan71999@gmail.com, Alexander S. Ramos, Stephan Zeng, David Martin. Chemistry, University of Iowa, Iowa City, Iowa, United States*

Iron(III) halide species have been shown to undergo Ligand-to-Metal Charge Transfer (LMCT) at near-UV wavelengths. Our group expanded on these systems by pushing the LMCT window further into the visible region through the addition of bromide to the iron center. This allowed for C-H alkylation reactions catalyzed by visible light using the iron salt TBA[$FeCl_3Br$]. Through substrate exploration and mechanistic studies, we showed that this iron salt can perform alkylations at 390 nm through the release of a chlorine radical, and at 456 nm through the release of bromine radical. This mild wavelength-selective behavior was intriguing to us, and we envisioned a reaction pathway that would allow for differing product classes based entirely on the wavelength of irradiation. Typically, the selectivity of organic reactions can be impacted through the tuning of a multitude of variables, including reagent choice, catalyst choice, and conditions such as temperature or solvent. In photochemical transformations, wavelength becomes a new parameter that can influence reactivity and selectivity. Through rigorous optimization, we detail a wavelength-selective reaction that enables access to [2+2] cycloaddition products at near-UV irradiation and C-H alkylations at 456 nm irradiation using electronically differentiated alkenes. Control experiments provide evidence that the simple iron(III) catalyst is necessary to promote a photocatalytic alkylation reaction under blue light irradiation but plays no role in the [2+2] reaction. Our substrate scope unveils that more electron poor Giese acceptors have attenuated [2+2] reactivity and enhanced alkylation reactivity, while the inverse is true for electron rich Giese acceptors. This work unveils a new method for wavelength-selective photochemistry, allowing for substrate exploration of differing product classes at the flip of a switch. Further mechanistic studies are underway to probe the nature of TBA[$FeCl_3Br$] and provide insight on competing mechanistic proposals.

MWRM 2026 MW27

WDR45: A beta-propeller protein associated neurodegeneration (BPAN) protein packaged in exosomes

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Autophagy is the process of intracellular degradation in which cellular contents are enclosed in autophagosomes and fused with the lysosome. Recent research shows extracellular vesicles, including exosomes, are secreted during autophagy to regulate cellular homeostasis, store energy and nutrients, and remove damaged cellular material. This process involves the ATG18 protein family, whose mammalian orthologs are WIPI proteins. WDR45 encodes WIPI4, a β-propeller scaffold protein essential for early autophagosome formation through phosphatidylinositol-3-phosphate-dependent

membrane recruitment. Mutations in WDR45 cause the lethal disorder BPAN by disrupting autophagic flux, promoting abnormal protein accumulation, iron dysregulation in the substantia nigra, and progressive neurodegeneration. Our BioID data suggested a correlation among exosomal markers and WDR45. To investigate this relationship, N2a cells were cultured under starvation conditions without FBS and treated with Rapamycin or Torin-1 to induce autophagy. Exosomes were isolated and analyzed by Western blot, confirming the presence of CD81 and WDR45 within exosomes. We also confirmed isolation of exosomes from wild-type mouse brains. Dynamic light scattering analysis showed an exosome diameter of 45 nm, consistent with exosome size and supporting the integrity of our isolation protocol. These findings support the association of WDR45 with exosomes.

MWRM 2026 MW54

What does a foundation model for atoms know? Running and reading Universal interatomic potentials, from nanocrystal precursors to oxide defects

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Pretrained universal machine-learned interatomic potentials can be used in two ways: run as simulators or read as representations. We show one example of each. First, frozen per-site embeddings from a pretrained MACE model, passed to a two-layer neural network, predict DFT oxygen-vacancy formation energies for about 250 oxides with no supercell construction or relaxation. In element-wise cross-validation, which holds out all compounds of a given cation, the error is 0.38 eV versus 0.72 eV for a model trained from scratch. Re-scoring a thermochemical water-splitting screen changes 45 percent of classifications, and new DFT calculations support the revisions. Second, molecular dynamics with the UMA potential, validated against DFT to about 1 meV per atom, resolves the speciation of Mn(II) halide complexes in oleylamine; Mn K-edge EXAFS reproduces the coordination trend and matches Mn–halide distances within 0.02 Å. Both studies follow one arc: validate against theory, extrapolate beyond it, verify independently.