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Breakfast and Registration (ISA 7th Floor)	08:00am - 09:00am
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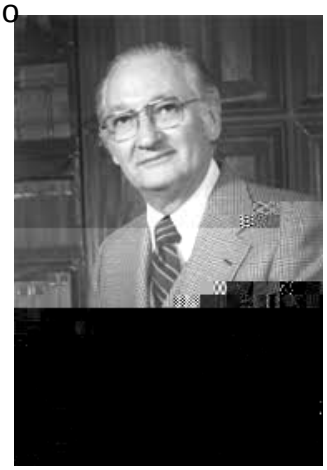
Oral Session C (ISA 2023)	09:10am - 11:20am
Lunch (ISA 7th Floor, Chipotle)	11:30am - 01:30pm
Poster Session (ISA 7th Floor)	12:15pm - 01:45pm
Oral Session D (ISA 1051)	02:00pm - 04:10pm
Oral Session E (ISA 1061)	02:00pm - 04:10pm
Castle Introduction (ISA 1061, Edward Turos, Ph.D.)	04:20pm - 04:40pm
Plenary Presentation (ISA 1061, Hans Renata, Ph.D.)	04:40pm - 05:40pm
Award Ceremony (ISA 1061)	05:45pm - 06:00pm

Remembering Raymond N. Castle

Raymond N. Castle was born on June 24, 1916 in Boise, Idaho



Oral Session Breakdowns

Oral Session A (ISA 3048)

Barbara Chiu	09:10am - 09:30am
Jessica Young	09:35am - 09:55am
Ashton Taylor	10:00am - 10:20am
Intermission	10:20am - 10:35am
Nathan Grimes	10:35am - 10:55am
Steven Soini	11:00am - 11:20am

Oral Session B (ISA 3050)

Cole Gibson	09:10am - 09:30am
Alexander Mariscal	09:35am - 09:55am
Gina Pantano	10:00am - 10:20am
Intermission	10:20am - 10:35am
Ankai Wang	10:35am - 10:55am
Herrmann Antoine	11:00am - 11:20am

Oral Session C (ISA 2023)

Intermission	09:10am - 09:35am
Harriet Thompson	09:35am - 09:55am
Yafeng Wang	10:00am - 10:20am
Intermission	10:20am - 10:55am
Benjamin Smith	11:00am - 11:20am

Oral Session D (ISA 1051)

Sean Bradley	02:00pm - 02:20pm
Krishna Yadavalli	02:25pm - 02:45pm
Ruixuan Gao	02:50pm - 03:10pm
Intermission	03:10pm - 03:25pm
Mohammad Nazmus Sakib	03:25pm - 03:45pm
Joshua Welsch	03:50pm - 04:10pm

Oral Session E (ISA 1061)

Rose Pittman	02:00pm - 02:20pm
Matthew Saunders	02:25pm - 02:45pm
Julian Melendez	02:50pm - 03:10pm
Intermission	03:10pm - 03:25pm
Paul Orndor	03:25pm - 03:45pm
Nicole A. Miller	03:50pm - 04:10pm

Oral Presentation Abstracts (Morning Session A)

Utilizing the MAtCH Model to Analyze Student Problem-Solving

Within the eld of chemistry education, problem-solving has been recognized as an important skill lacking in many undergraduate students. Due to the overuse of algorithmic questions in exams, students have di culty approaching conceptual problems that require them to apply previous

commercially sourced from Deurion and were also used as the nebulization source. Various higher frequency SAW chips were fabricated in-house at frequencies ranging from 16-98 MHz.

Presented by: Ashton Taylor (Graduate, Analytical Chemistry)

Vapor Modi er Control to Enhance FAIMS Analysis with Mass Spectrometry

Innovated B/N Frustrated Lewis Pairs for CO reduction: a DFT study

Challenges in global energy shortage have promoted studies in nding alternative and sustainable energy resources, for example, utilization and reduction of CO molecule. Herein, by employing computational simulations, we have developed and investigated an innovated intramolecular metal-free frustrated Lewis pairs (FLPs) as a catalyst for the CO reduction reactions. By applying nitrogen heterocycles and organoboron structure, the FLP catalyst is able to hydrogenate CO directly from dihydrogen and produce methanol as nal product. The mechanism and reaction path of the CO reduction reaction have been investigated using density functional theory. The simulation data indicate that the proposed catalyst may greatly reduce the activation energy barrier and hold promise in developing metal-free catalyst for the CO reduction reactions.

Presented by: Ankai Wang (Graduate, Physical Chemistry)

Topological magnetic textures in cubic nanoparticles

Magnetic topological spin textures are promising for fundamental physics, next-generation devices, and dense data storage. There is a unique coupling between the electronic and the magnetic structure, which can be e ciently manipulated by electromagnetic external elds, such as laser light. We study the magnetic structures from the trivial ferromagnetic state to the highly sought-after topological spin texture, i.e., skyrmions. We take an innovative approach by tackling nite-size cubic nanoparticles where we minimize the Gibbs free energy due to the competitions of the Heisenberg exchange, Dzyaloshinskii-Moriya Interaction (DMI) applied only at the surfaces of the nanoparticles, and various other magnetic interactions. We show that the spin eld has a non-trivial topology with bounded regions of high topological charge which can be associated with skyrmions. Our analytical results are compared with that of spin-dynamic simulations.

Presented by: Herrmann Antoine (Graduate, Physical Chemistry)

Oral Presentation Abstracts (Morning Session C)

New 1-(3-(2-Amino-2-oxoethoxy) phenyl) piperidine-3-carboxamide Derivatives as Small-Molecule Inhibitors for the -Catenin/BCL9 ProteinProtein Interaction

A series of 1-(3-(2-amino-2-oxoethoxy)phenyl)piperidine-3-carboxamide derivatives was reported as new small molecule -catenin/B-cell lymphoma 9 (BCL9) proteinprotein interaction (PPI) inhibitors. Compounds 1821 were found to disrupt the -catenin/BCL9 PPI with IC50s of 0.852.7 M in competitive inhibition assays. The disruption e ects of 21 on the -catenin/BCL9 PPI in cellular context were demonstrated by pulldown inhibition experiments using SW480 cell lysates. A series of cell-based studies revealed that 21 dose-dependently suppressed transactivation of Wnt/-catenin signaling, downregulated expression of Wnt target genes, and inhibited growth of cancer cells with hyperactive -catenin signaling. 21 was also more potent than previously reported analogue ZW4864

in suppressing transcription and expression of Wnt target genes and Wnt-dependent cancer cell survival. All in all, 21 represents a promising starting point for further optimization of -catenin/BCL9 PPI inhibitors.

Presented by: Harriet Thompson (Undergraduate, Biochemistry)

Selpercatinib Protac derivatives with di erent linkers act as RET degraders

Selpercatinib(LOXO-292) is a 2020 FDA approved highly potent drug for rearranged during transfection (RET) altered thyroid cancers and non-small-cell lung cancers(NSCLC). However, resistances were found RET G810C/S mutations at solvent front region and RETY806C/N mutation the hinge region. With these two mutations, resistance is developed and selpercatinib can't show good potent e cacy. Here, based on the patent WO 2018/071447 Al, we choose several potent structures that are di erent from Selpercatinib at the solvent exposed area and test them against wild type RET cell and mutated RET cell. From the cell results, these structures do not show good potency towards both wild type RET cells and mutated RET cells. Alternatively, now we are trying to develop selpercatinib based protac derivatives. The hydrophobic binding part of Selpercatinib and di erent E3 ligases are joined by several kinds of linkers. From western blotting results, two compounds can degrade P-RET and RET protein as low as 50nM. However, these two compounds can't kill cells after 3 or 5 days even if much higher concentration is used.

Presented by: Yafeng Wang (Graduate, Organic Chemistry)

Antibiotic Activity Driven Natural Product Discovery from Mangrove Endophytic Fungi

With the emergence of multi-drug resistant bacteria, natural product researchers are using more advanced techniques to discover novel drugs. Following prior success of fungal secondary metabolites as antibacterial agents, the expression of silent biosynthetic gene clusters (BGCs) may provide such innovation. Mangrove endophytic fungi were cultured in the presence of the DNA modi ers HDACi or DMNTi and subsequently screened for bioactivity against the ESKAPE pathogens. Using the global natural product social molecular networking (GNPS) software of LC-MS/MS fragmentation patterns resulted in the dereplication of several known compounds, as well as identi ed three new derivatives which were isolated and characterized using 1D and 2D nuclear magnetic resonance (NMR) spectroscopy and electrospray ionization mass spectrometry ESIMS). The lead compound bears structural similarity to a known compound with increased activity against Enterococcus faecium and Staphylococcus aureus pathogens.

Presented by: Benjamin Smith (Graduate, Organic Chemistry)

Oral Presentation Abstracts (Afternoon Session D)

E orts toward the enantioselective total syntheses of various marine natural products

Today, we are seeing tremendous issues with the presence of multi-drug resistant bacterial infections

Potential New Synthetic Ketogenic Molecules: Ester Derivatives

Ketone bodies are produced in our liver during prolong fasting and carbohydrate restricted diet, in a process called ketosis. Ketosis has already been proven as e ective tool for medical uses as it showed in uences on treating epilepsy, type 2 diabetes and weight loss. Ketone bodies are produced by metabolism of molecules called Long chain triglycerides (LCTs) which we gain from

context. Based on favorable Glide scores of the docked protein-ligand poses, the results reveal that a portion of the original antiviral compounds are potentially viable as inhibitors of the virus.

Presented by: Rose Pittman (Graduate, Physical Chemistry)

A high dimensional parameter search method to determine force eld mixing terms in molecular simulations

Molecular simulations depend on parameter sets for molecules that are developed independently of one another for use with water models. These parameters are often assumed to be transferrable; however, in many recent works this has been shown to work poorly for cases, especially when ions are involved. We have developed a method, using the ParOpt software from our group, to optimize Lennard-Jones cross-terms between cations and small-molecule representatives of lipids to ensure accurate reproduction of gas-phase geometries and energies from ab initial calculations. This method is a generic method that can be applied to mix any two independently developed MM force- elds.

Presented by: Matthew Saunders (Graduate, Physical Chemistry)

Inclusion of high- eld target data in AMOEBAs calibration improves predictions of protein-ion interactions

The reliability of molecular mechanics simulations to predict ion binding to proteins depends on their accuracy in describing protein-water, ion-water and ion-protein interactions. Protein and ion force elds are typically constructed independently of each other, and in simulations consisting of both proteins and ions, protein-ion interaction energies are estimated using some prede ned set of force eld mixing rules. This, however, does not guarantee the reliability of predicted ion-protein interactions and in fact yield large errors. Here we use the polarizable AMOEBA force eld to demonstrate that errors in ion-protein interactions can be reduced systematically by incorporating high electric eld target data during calibration of protein parameters. Recalibration of descriptors for peptide backbones and side chains consisting of carbonyls, hydroxyls and carboxylates reduces the error from 8.7 to 5.3 kcal/mol and 9.6 to 6.3 kcal/mol for interactions with Na^+ and K^+.

Presented by: Julian Melendez (Graduate, Biochemistry)

Sequence e ects of uracil damaged DNA

Uracil is a common type of lesion in DNA that arises from either spontaneous deamination of cytosine or errors in the replication process. DNA containing uracil is excised from the gen5 (e)-14deamination

Optimizing Protocols for Computing NMR Chemical Shifts for Saccharide-like Species

Cellulose is a readily abundant polymer in nature that is being investigated as an alternative fuel source. Computational methods can aid experimentalists by providing chemical shifts related to cellulosic biomass. As a prelude to future work, we conduct an investigative benchmark with a set of small carbohydrate analogs to identify which quantum-mechanical/molecular-mechanical (QM/MM) methods are the most accurate and the least computationally expensive when computing carbon-13 (13C) NMR chemical shifts. We nd that 13C root mean square error converges when a QM solvent sphere of 4 or more about a solute is used, showing a selection of method/basis set pairings that yield errors less than 3.0 parts per million. We also show that computational time can be greatly reduced while retaining and, in some cases, improving accuracy by employing a mixed basis set approach, wherein the QM region is partitioned into large basis set (inner) and small basis set (outer) regions.

Presented by: Nicole A Miller (Graduate, Physical Chemistry)

Poster Presentation Abstracts (Midday Session)

Electrochemical Detection of Cd(II) Ions in Environmental Samples Using Nanoelectrodes

Heavy metal contamination is a rising global concern and bioaccumulation of toxic metals in the

dopamine to enhance the detection of Cu^{2+}. We characterized our sensor with dopamine and Cu^{2+} with fast-scan cyclic voltammetry and optimized electrodeposition time through comparison and chose the best one. We performed all experiments in a buffer solution that mimics artificial CSF, showcasing the ability of our sensors for the in vivo detection of Cu^{2+} with high sensitivity and excellent biocompatibility.

Presented by: Noel Manring (Graduate, Analytical Chemistry)

are explored at a variety of "twist" angles between the two layers, which exhibit curious electrical/ quantum mechanical properties such as room-temperature superconductivity.

Presented by: Marcus Harvison (Undergraduate, Inorganic Chemistry)

Creation and Analysis of Novel Lead and Lead-Free Pervoskites

Perovskites are a class of inorganic materials most useful in the elds of solar cell technology and exible electronics, due to their ability to conduct electricity well while maintaining it under applied forces. Though commonly formulated using lead, recent experiments search for lead-free alternatives to more positively impact the environment. Newly discovered linkers are used in this experiment along with lead and lead-free metal combinations to form perovskite crystals which are then analyzed with powder x-ray di raction (PXRD), single crystal x-ray di raction (SXD) and then with various photochemical and thermal analysis tools to determine the properties of the perovskites and their possibility for application.

Presented by: Leah Lepore (Undergraduate, Inorganic Chemistry)

Evaluation and Identi cation of Antifungal Activity of Mangrove Endophyte against Candida Sp.

The wide range of adverse e ects that Candida Sp. can demonstrate in humans and the ever-growing multi-drug resistance pro les of the certain strains can result in life-threatening infections that remain uninhibited due to the limited clinical treatment available. Mangrove endophytes have shown signi cant promise in the development of new treatments because they can synthesize bioactive secondary metabolites. Secondary metabolites are especially interesting to scientists because these compounds typically demonstrate biologically active properties that can be used in antibiotics and antifungal treatments. With the limited antifungal treatments and the growing resistance of C. albicans and C. auris, the production of new secondary metabolites. The objectives of this paper are to isolate a bioactive compound through bioassay-guided fractionation as well as conduct DNA sequencing to determine the identity of fungal compound HF14-16C-2A-HDAC to assist in the development of new treatments.

Presented by: Jessica Bay (Undergraduate, Organic Chemistry)

Anti-plasmodial activity of Gardenia imperialis

Malaria is a widespread disease by female anopheles mosquito. There are 5 parasite species that cause malaria in humans with P. falciparum and P. vivax posing the greatest threat. In 2020, nearly half of the worlds population was at risk of malaria. Previous malaria research has resulted in combating the deadly disease using various drug discovery techniques. Natural products have played crucial roles in the ght against malaria from the discovery of artemisinin, quinine, and lapachol. Gardenia imperialis is a small plant found in Tropical Africa. Fungus living on the plant generate secondary metabolites known to have anti-plasmodial activity against PfDd2 species of Plasmodium and has antileishmanial potency. As part of this research project, fungal extracts were

desired macrocyclic -AApeptides were found to be e ective for ligand identi cation. This new approach of macrocyclic peptidomimetic library may lead to a novel platform which provides unique source of ligands for biomacromolecular surface recognition and function modulation.

Presented by: Meng Gu (Graduate, Organic Chemistry)

E cient Synthesis of Cyclopropylacetylene, a Crucial Synthetic Intermediate for Efavirenz Using a Mild Chlorinating Reagent (Ph_3PCl_2)

Cyclopropylacetylene (CA) is a key intermediate in the synthesis for the HIV reverse transcriptase inhibitor Efavirenz, an antiviral drug used to treat HIV. CA is an expensive raw material, di cult to obtain, employed in the preparation of medicaments to combat AIDS. The e cient process for the preparation of CA is described, in which cyclopropyl methyl ketone is chlorinated with PCl5. The resulting 1,1-dichloro-1-cyclopropylethane is isolated and then dehydrochlorinated with potassium tert-butoxide in toluene to form CA. However, the chlorination protocol has been found to take place with appreciable cyclopropyl ring opening. A mild chlorinating reagent is predicted to reduce ring-opening side products. For this, a one-pot synthesis was employed using dichlorotriphenylphosphorane|Ph_3PCl_2

The identi cation of new Suberitenones from the Antarctic sponge Suberites sp.

Natural products have been used as medicine to treat humans since ancient times due to their therapeutic properties. The secondary metabolites derived from terrestrial and marine sources have the potential to be novel, bioactive compounds, which can potentially be used as new drug candidates. I have recently worked on the Antarctic sponge Suberites sp. to identify new chemical compounds. During my research, I extracted, isolated, and puri ed a new Suberitenone from the Suberites sponge collected in Antarctica in 2018 with the goal to nd new, bioactive metabolites.

Extraction, Fractionation, and Metabolomic Analysis of Endophytic Fungal Sample EG12-41E-2

Healthcare facilities are haunted by a myriad of virulent and drug-resistant bacterial strains. In 2019, the Word Health Organization released a report revealing that such diseases are responsible for 700,000 annual deaths around the world. Among these bacteria can be found the infamous ESKAPE pathogens: Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa, and Enterobacter spp. Here, we attempt to inhibit the growths of the ESKAPE pathogens by utilizing the secondary metabolites found within the endophytic fungal sample EG12-41E-2. Liquid chromatography was used to fractionate the fungal sample. The resulting fractions were evaluated using NMR, QTOF-LC/MS, and bioassays. The results of the assays revealed which fractions were bioactive. These fractions were further deconstructed using HPLC to isolate the bioactive molecules. Attempts were made to elucidate the isolated compounds in hopes of discovering novel metabolites.

Presented by: Samuel Sarratt (Undergraduate, Organic Chemistry)

Con rming Stereochemistry of Sch725674 Using X-Ray Crystallography

Natural products chemistry o ers an area for novel biologically active molecules in hopes for use in the pharmaceutical/medicinal industry. The fungal sample Ive been working on, named TAP14-279b-5b, was collected from Tapachula Chiapas, Mexico in 2014. It has activity against the ESKAPE pathogens, but through isolation and puri cation techniques, I can determine which compound is responsible for this. So far, I have puri ed one compound - Sch725674, isolated from various fungi - which crystallized out of my MPLC fraction F. Running 1H NMR, 13C NMR, and HSQC along with using SMART NMR, we con rmed the structure of the compound. After completing some literature search, this compound has bioactivity against Saccharomyces cerevisiae and Candida albicans. Using x-ray crystallography, I was able to run a 1H NMR to con rm that the stereochemistry of the four carbinol protons is (4R, 5S, 7R, 13R), which which has not been previously reported.

Presented by: Stephanie Paola Suarez (Graduate, Organic Chemistry)

Design and Synthesis of Stable Four-Coordinated Benzotriazole-Borane with Tunable Fluorescence Emission

A new class of stable four-coordinated benzotriazole-borane compounds was developed via gold-catalyzed alkyne hydroboration. The application of polymeric (BH2CN)n reagent gave the formation of cyano-amine-boranes (CAB) complexes with less basic N-heterocyclic amines and anilines. Various new CABs were investigated in catalytic hydroboration to synthesize N-B cycles. The 1,2,3-benzotriazoles were identi ed as the only feasible N-source, giving the four coordinated borane N-B cycles (BTAB) in excellent yields (up to 90%) with good functional group tolerability. This new class of polycyclic N-B compounds showed excellent stability toward acid, base, high temperature, and photo-irradiation. The facile synthesis, excellent stability, strong and tunable uorescence emission make BTAB interesting new uorescent probes for future chemical and biological applications.

Presented by: Qi Tang (Graduate, Organic Chemistry)

Synthesis of Thiazole Derivatives with Hantzsch Condensation

By performing a Hantzsch condensation reaction on thiocyanates of acetophenone or propiophenone with several aniline derivatives, a library of N-Substituted 2-aminothiazole compounds have been synthesized. Improved synthesis of these compounds is a focus in medicinal chemistry due to unique biological activities exhibited by these molecules, including use as antimicrobial agents, anti-cancer or anti-tumor agents, and potential activity in combating neurodegenerative diseases. The library of aminothiazoles synthesized in this work is also being evaluated to prevent neural cell death and stop the progression of Alzheimer's disease.

Presented by: John Tatum (Undergraduate, Organic Chemistry)

One-pot reductive acylation and silylation of various benzoquinones, naphthoquinones and anthraquinones

The reversible reduction of quinone compounds to their hydroquinones is commonly seen in nature and is associated with the built-in triggering mechanisms of various potent antibiotics such as mitomycin C and daunomycin. Regulating this process can be challenging due to the relative ease of oxidation of the reduced hydroquinones, often yielding other unwanted products. The use of oxygen-protecting groups as a means of trapping the hydroquinone reduction products, is a strategy our lab is studying. Our goal is to execute the one-pot reductive acylation or silylation of photo-sensitive biologically active quinones to their hydroquinone forms. We aim to use this strategy to access otherwise unstable hydroquinones and study their enzymatic cleavage properties and capabilities to serve as pre-reduced, O-protected prodrugs.

Presented by: Katrinah Tirado (Graduate, Organic Chemistry)

Facile Synthesis of Hetero Polyaromatic Hydrocarbons (PAH) via Styryl Diels-Alder Reaction with Conjugated Diynes

The styryl dehydro-Diels|Alder reaction with conjugated diyne is reported. While typical alkyne-styrene condensation required elevated temperature> (160 C), the application of conjugated diyne allowed e ective transformation under milder condition (80 C). Thermal stable triazole-gold catalyst further improved the reaction performance (up to 90% yield), giving the desired alkynyl-naphthalene in one step with molecular oxygen as the oxidant. Sequential alkyne activation gave various polyaromatic hydrocarbons (PAHs) in excellent overall yields, highlighting the e ciency of this new strategy for the preparation of PAHs with good functional group tolerability and structural diversity.

Presented by: Jingwen Wei (Graduate, Organic Chemistry)

Mass spectrometry-guided isolation of polyketide macrolides from the Antarctic tunicate Synoicum adareanum

Defenseless against predation and subject to competitive ecosystems, marine invertebrates rely on an evolutionary mechanism to promote survival: secondary metabolites, also known as natural products (NPs). NPs act as species-speci c chemical defenses. Bioactive by design, many NPs derived

from marine invertebrates display cytotoxic and antimicrobial properties. NPs of particular interest are a class of macrolides known as palmerolides, found in Synoicum adareanum. This project aimed at the isolation of palmerolides from S. adareanum for downstream bioassays. Fractionation was achieved via a progression of separations: column chromatography followed by HPLC (high pressure liquid chromatography). Analysis of each fraction used quadrupole time-of- ight mass spectrometry (QTOF MS) to identify palmerolide-like fragmentation. The hits underwent further HPLC to achieve pure isolates. Structural veri cation of the palmerolide isolates was performed using via 1H NMR and mass spectrum data.

Presented by: Jennifer Williams (Undergraduate, Organic Chemistry)

Benzotriazole as a novel directing group to facilitate C-H functionalizations

C-H bond functionalization has been a long-standing problem, for its selectivity and reactivity. For the last two decades, directing group strategies have stands out, showing its power in precise and high-yielding functionalizations on C-H bonds. C-H bond functionalization catalyzed by palladium could go through Pd(0)-Pd(II) cycle and Pd(II)-Pd(IV) cycle, while the Pd(II)-Pd(IV) cycle is compatible for both C-C and C-X formations. Herein we report a new series of benzotriazole directing groups, with three coordination site to interact with the metal atom, which can accelerate C-H Bond functionalization through Pd(II)-Pd(IV) catalytic cycle, achieving C-C and C-X bond formation reaction.

Presented by: Chengkai Xu (Graduate, Organic Chemistry)

Synthesis and development of biodegradable antimicrobial guanylated polycarbonate polymers

The increasing resistance of antibiotics become a major concern in public health. Substantial interest has been devoted to the development of biodegradable antimicrobial polymers as a solution for combating antibiotic resistance. Herein, we report the design and synthesis of biodegradable antimicrobial random guanylated polycarbonate copolymers initiated by carbon chain that containing guanidium derived monomers and hydrophobic monomers. With di erent equivalence of monomers and di erent length of carbon chain, a series of antimicrobial polymers were synthesized. The antimicrobial activities against both Gram-negative and Gram-positive bacteria of these polymers are reported, as well as the hemolytic activity. The time kill assay show these polymers have low tendency to derivate the resistance. Other bacterial studies were also involved for drug-resistance determination, that suggest these polymers antimicrobial via membrane disruptions.

Presented by: Menglin Xue (Graduate, Organic Chemistry)

Diastereoselective phospha-Michael addition of aryl phosphinates catalyzed by a phase transfer agent

We are engaged in the development of a catalytic diastereoselective approach to the construction of organophosphinate compounds that are valued in the inhibitor design of metallo proteinases. Our strategy involves the phospha-Michael addition of aryl phosphinates to -disubstituted vinyl ketones under the action of phase transfer catalysts (PTCs). Reaction conditions using crown ethers as

PTCs led to high diastereoselectivities in most cases and when the phosphinates nucleophile contains a non-racemic menthyl substituent, additions led to enantiopure phosphinate adducts. A closed transition state model is proposed to explain the stereoselectivity in these addition reactions with the observed selectivity rationalized as preferential attack of phosphinate on vinyl ketones in the S-cis conformation.

Presented by: Krishna Yadavalli (Graduate, Organic Chemistry)

Investigating the e ects of linker substitution on H2 adsorption between two isostructural Metal-organic Frameworks (MOFs)

The e ects of linker substitution on the H2 adsorption mechanism between two isostructural metalorganic frameworks (MOFs), MOF-505 and NOTT-101, were investigated using grand canonical Monte Carlo simulations. Three potential energy functions of increasing complexity for the H2 were used for the simulations. Simulations of H2 adsorption in both MOFs resulted in isotherms that are in reasonable agreement with the experimenta32 (the)-331ganu80.00greem9 (with)77e nn phosp369.9

Judges

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