

8th Raymond N. Castle Student Research Conference

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Welcome from the Castle Committee

Dear Colleagues and Friends,

Welcome to the 8th Raymond N. Castle Student Research Conference. In honor of Dr. Raymond N. Castle, this conference was created to promote his goals of scientific collaboration and science education.

The Raymond N. Castle Student Research Conference continues to be organized by students for students as an excellent opportunity for undergraduate and graduate chemistry students to share scientific ideas and research progress. Students are encouraged to not only gain presentation experience, but to use the conference as a chance to further their research endeavors by gaining valuable feedback from other members of the chemistry community. It is this interaction and the sharing of ideas that makes the Raymond N Castle Student Research Conference a worthwhile experience and a continued success.

We are especially proud of the research done by all students in the department, both graduate and undergraduate. Today, we have an opportunity to hear from over 100 students and our special guest, Dr. Lyle W. Castle. We encourage everyone to take advantage of this occasion and attend both the poster and oral presentations, especially the Plenary Lecture. We are honored and greatly appreciative that Dr. Lyle W. Castle is able to return to USF and speak at the conference in honor of his father.

Lastly, we would like to thank all members of the Chemistry Department that chose to volunteer their time and efforts, particularly the judges and Dr. Patricia Muisener and Dr. Brian Space for helping us plan and coordinate this year's conference. We are grateful for the financial support that allows us to host this conference and owe special thanks to the University of South Florida College of Arts and Sciences, the Tampa Bay Section of the American Chemical Society, and the multiple sponsors and affiliates who have generously contributed to this event. Most importantly, this conference would not exist without the efforts of those of you presenting your research today. Therefore, we gratefully acknowledge you and your research advisors, as well as all in attendance. Thank you all, and we hope you enjoy and learn from the 8th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

8th Raymond N. Castle Student Research Conference Committee

Committee Members:

Todd Gatlin (Co-Chair) Christi Whittington Young (Co-Chair) **Biplob Bhattacharya** Christian Cioce **Kimberly Fields** Joseph Gill Priyesh Jain Chungsik Kim Wiliam Maza Sreya Mukherjee Meagan Small Melissa (Missy) Topper Carissa Vetromile Justin White Tarah Word Xue (Snow) Xu Mingzhou Zhou

Faculty Advisors:

Dr Patricia Muisener Dr Brian Space

Web Support:

Tony Green

Schedule of Events Saturday, April 17, 2010

<u>Time</u>	<u>Event</u>
8:00-8:30	Welcome Session - Registration and Breakfast NES Lobby
8:30-8:45	Castle Conference Introduction CHE 100
8:45-11:30	Morning Session – Graduate Student Oral Presentations CHE 100
11:30-11:45	Break
11:45-12:45	Plenary Speaker – Dr Lyle W Castle CHE 100
12:45-1:45	Lunch NES Lobby
1:15-2:45	Poster Session – Graduate and Undergraduate Presentations NES Hall and Classrooms
2:45-3:00	Break
3:00-5:45	Afternoon Session – Graduate Student Oral Presentations CHE 100
5:45-6:00	Break
6:00-6:15	Awards Ceremony CHE 100



Tampa Bay Local Section

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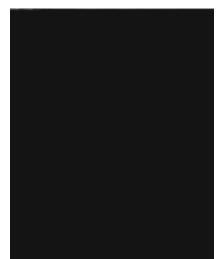
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Professor Raymond N. Castle

1916 – 1999



Raymond N. Castle was born on June 24, 1916 in Boise, Idaho where he attended Boise High School and Boise Junior College. A 1938 graduate in Pharmacy from the University of Idaho, Southern Branch in Pocatello, he completed the M.A. degree in Chemistry at the University of Colorado at Boulder in 1941. Shortly thereafter, he became a Chemistry instructor at the University of Idaho and then in 1943, returned to the University of Colorado in Boulder for a Ph.D. in Chemistry with a minor in Microbiology. After two years as a research chemist at the Battelle Memorial Institute in Columbus, Ohio, Dr. Castle accepted a position at the University of New Mexico as an Assistant Professor of Chemistry. He served as Chairman of the Chemistry Department from 1963 until 1970 before moving to Brigham Young University as Professor of Chemistry.

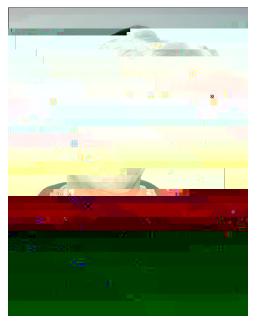
In 1981, Dr. Castle joined the faculty at University of South Florida as a Distinguished Research Professor. He and his wife, Ada, were a vibrant part of the Chemistry Department and for many years sponsored the Castle Lecture Series, which brought in numerous prominent scientists for lectures at USF.

A prolific researcher, Dr. Castle was an internationally recognized father figure in heterocyclic chemistry, both for his research and his involvement in meetings, symposia, and editorial boards. In 1964, he founded the Journal of Heterocyclic Chemistry and served as its editor. He also edited the Lectures in Heterocyclic Chemistry series, a publication of plenary lectures given at the International Congresses of Heterocyclic Chemistry, and was the American advisory editor for

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Dr. Lyle W. Castle

Plenary Speaker



Dr. Lyle Castle earned a Bachelor's degree in Chemistry from Southern Utah University, a Master's degree from the University of Nebraska and a Doctoral degree in Organic Chemistry from the University of South Florida in 1992, working under the direction of Dr. Milton Johnston Jr. Dr. Castle joined the Chemistry Faculty at Idaho State University in 1994, and currently serves as Professor and Dean of Academic Programs at Idaho State University – Idaho Falls. He was appointed Dean of Academic Programs in Spring 2008. ISU – Idaho Falls currently serves nearly 3,000 students and places strong emphasis on science and engineering programs.

Throughout his career, Dr. Castle's research has largely focused on organic and organometallic synthesis, with special interest in the synthesis of heterocyclic compounds. Recent work involved the synthesis and characterization of heterocyclic compounds with potential application as photosensitizes for

solar energy conversion devises. He has published numerous works in the field of heterocyclic chemistry and was named Cambridge's Who's Who in Professional of the year in Heterocyclic Chemistry in 2006.

Along with research, Dr. Castle has dedicated much time and effort towards teaching and preparing students for future careers in the sciences. He previously acted as Principal Investigator for an NSF funded grant to introduce FTNMR techniques and experiences into the general chemistry curriculum.

In September 1999, Dr. Castle took over as CEO and President of Hetero Corporation, and Editor-in-chief

Ylide Chemistry via Co(III) Corroles: Axial Ligand Effect of N-H Insertion Reactions with Diverse Diazocompounds

9:00- 9:15 AM Mingzhou Zhou

The Design and Synthesis of Non-Peptidic α -helix Mimics Targeting MDM2-P53 Protein-Protein Interaction

9:15- 9:30 AM Mike McIntosh

Elucidating the Reaction Mechanism and Electrochemical Behavior of Ellagic Acid, a Natural Polyphenolic Antioxidant

9:30- 9:45 AM Sridhar Reddy Kaulagari

Design and Synthesis of Novel Phospho-Tyrosine Mimetics

9:45-10:00 AM Jingran Tao Cobalt(II) Porphyrin Catalyzed Intramolecular C-H Amination Reaction with Carbonyl Azides

10:00-10:15 AM Break

10:15-10:30 AM Priyesh Jain Design and Synthesis of Novel Cyclic III Peptide as β1 Integrin Inhibitor

10:30-10:45 AM Seongmin Hong Gold Nanoparticles, Effect Substrates of Surface Enhanced Raman Spectroscopy

10:45-11:00 AM Jeremy Beau Investigations of Antimalarial and Antibiotic Compounds from Mangrove Endophytes

11:00-11:15 AM Gajendra Ingle

Graduate Talks Afternoon Session (CHE 100) Session Chair: William Maza

3:00- 3:15 PM Roger Bass Self-Healing Shape-Memp(a.4n..iT/P (430)

<u>M-08 10:45-11:00</u>

Jeremy Beau¹, Hoangmy Chau¹, Nida Mahid¹, Lindsey Shaw², Tina Mutka³, Dennis E. Kyle³, and Bill J. Baker³

¹Department of Chemistry, University of South Florida; ²Department of Biology CVIM, University of South Florida; ³Department of Global Health, University of South Florida

Investigations of Antimalarial and Antibiotic Compounds from Mangrove Endophytes

Recent studies have shown that within the leaves, bark, roots and seeds of mangroves exists an immense world of endophytic organisms. These microscopic communities are complex, providing a great diversity of secondary metabolites with special functions that combat the microbe-plentiful seawater. These secondary metabolites have the potential to be potent and highly selective drugs. As part of our screening program for drug leads against drug-resistant bacteria and protozoan parasites, we developed a collection of mangrove-endophytic microbes. This talk will present the results of the bioassay-guided fractionation of the extracts of several endophytes, that yielded a series of compounds bearing both anti-plasmodial and antibiotic activity.

<u>M-09</u> 11:00-11:15 Gajendra Ingle¹, Y Liang¹, M Mormino¹, Jon Antilla¹ ¹Department of Chemistry, University of South Florida

Chiral BIF4.2 13.10rida

frameworks. Here, we present a novel method to fit atomic point charges for the purposes of classical simulation that reproduces the fully periodic electrostatic potential.

thermal stability study of this category can reveal vital information such as the range of the temperature where reactions can be planned, knowledge of subsequent rearrangements, cyclization reactions, melting point, energy of decomposition and safety precautions for an exothermic process. Hence the knowledge of thermal stability is considered as an important tool in organic chemistry for various reactions involving azides. Here we present the thermal stability studies of three different types of azides namely sulfonyl, carbonyl and phosphonyl azides in terms of decomposition temperature, energy of decomposition and T_{max} . The effect of substituent groups on their thermal stability for the azides is also studied using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA).

<u>A-09 5:15-5:30</u>

Mu Seong Kim¹, Julie Harmon¹ ¹Department of Chemistry, University of South Florida

Dielectric Anylsis of PHEMA and PMMA Composites with OC12 Nanoball

A self assembled nanostructure with OC₁₂ functionality has been incorporated into two polymeric systems: poly(1-hydroxyethyl methacrylate) (PHEMA) and poly(methylmethacrylate) (PMMA). This nanoparticle is rhombihexahedral in shape and possesses 24 saturated 12 carbon chains on the surface. The effect of interactions between OH nanoballs with above mentioned polymers on dielectric properties was studied earlier. The present work deals with the interactions of OC₁₂ nanoballs with polymers and that there is an effect on dielectric properties. The dielectric permittivity (ϵ) and loss factor (ϵ ") measured via Dielectric Analysis (DEA) in the frequency range 1Hz to 100 kHz and between the temperatures -150 to 150°C. The electric modulus formalism was used to reveal α , β , γ and conductivity relaxations. The activation energies for the relaxations are presented. Nanocomposites were also characterized by differential scanning calorimetry (DSC) to determine glass transition temperatures.

<u>A-10 5:30-5:45</u>

William Maza¹, Xin Cui¹, Chungsik Kim¹, X Peter Zhang¹, Randy W Larsen¹ ¹Department of Chemistry, University of South Florida

Ion Sensing Using a Novel Functionalized Metalloporphyrin: Spectroscopic Studies of Nitrite/Nitrate Binding to Zn(II)[3,5-DitBu-IbuPhyrin]

The development of effective sensor elements relies on the ability of a chromophore to bind an analyte selectively and then report the binding through a change in spectroscopic signal. In this report the ability of Zn(II)[3,5-DitBu-IbuPorphyrin] (ZnDtBIP) to selectively bind nitrite ions over nitrate ions is examined. The results of Benesi-Hildebrand analysis reveals that ZnDtBIP binds nitrite ions with an association constant of 101.0 M¹ versus 80.9 M¹ for nitrate ions. In contrast, the association constants for nitrite and nitrite ion binding to unsubstituted Zn(II)tetraphenyl porphyrin (ZnTPP) are found to be 739.4 M¹ and 133.9 M¹, respectively. Interestingly, nitrogenous ligands in the fifth coordination site of the Zn(II) center enhance both the binding and selectivity of nitrite ions with bulkier N-heterocycles providing the most significant enhancement. These results will be discussed within the context of both steric flexibility of the substituted porphyrin as well as electron factors associated with the central Zn(II) ion.

The Barbara and Dean F Martin Graduate Poster Session

Analytical, Chemical Education, and Physical (NES North Hall)

<u>GP-01</u> Christi Young¹, Alfredo Cardenas²

¹Department of Chemistry, University of South Florida; ²Center for Computational Life Sciences and Biology, Institute for Computational Engineering and Sciences, University of Texas at Austin

Analysis of Molecular Dynamics Simulations of Influenza A NS1 RNA Binding Domain

The RNA binding domain of the Non-structural protein 1 (NS1) of influenza A virus, a homodimer, was studied using molecular dynamics simulations. The simulations were performed with NAVID at 298K in explicit water with force field CHARMIV22. The effect of a salt solution on the domain was determined by comparison of five explicit water and nine 0.1M explicit KCl and water simulations. Flexibility of key residues in the RNA binding cavity was studied. There are eighteen possible initial structures for the simulations, of which the first NIVIR PDB structure was chosen. RMSD values for the possible structures were compared against average structures from the simulations and structures from normal mode analysis.

<u>GP-02</u> Todd Gatlin¹, Santiago Sandi-Ureña¹

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improve the physical properties of polymers is the dispersion of a nano material. In this case, functionalized carbon nanotubes (FCNT) were dispersed in the polymer poly(4-methyl-1-pentene), PMP. However, dispersion of the nanotubes can be tricky. Previously techniques such as sonication have been used but this resulted in only a temporary solution as the tubes would agglomerate after only a short time. This limitation can be overcome by covalently bonding organic side chains to the FCNT with the process of reductive alkylation. Once functionalized these FCNT dissolve easily in common organic solvents and stay in solution making their dispersion in a polymer easy to achieve.

<u>GP-04</u> Wen-shan Chang¹, Megan Small¹, Dean F Martin¹ ¹Department of Chemistry, University of South Florida

Use of Model Compounds to Study Removal of Pharmaceuticals Using Octolig®

The existence of pharmaceuticals in the environment has some adverse effects, and may pose threat to the organisms in the environment. The possibility of removing certain pharmaceuticals from wastewater was tested using Octolig® commercially available material with polyethyldiamine moieties covalently attached to high-surface area silica gel. Selected drug models compounds were subjected to column chromatography in efforts to effect removal by means of ion encapsulation, the effectiveness of which would depend upon having appropriate anionic functional groups. The experimental results suggested that the model compounds, Rose Bengal, Eosin Y, Erythrosine and ZPS, were success to be encapsulated by Octolig®. Methylene Blue with quatemary ammonium groups was (statistically) unsuccessful. In contrast, complete success was attained for removal of each of three xanthenylbenzenes (Rose Bengal, Eosin Y, Erythrosine) that have both phenolic and carboxylic acid groups. In addition complete success was attained for ZPS (zinc phthalocyaninetetrasulfonate) and Lissamine Green B with sulfonate anions present. In addition, test of real pharmaceutical compound had been applied on Amoxicillin, and the result indicates that Octolig® can be used to remove this compound.

<u>GP-05</u> Cynthia Nwachukwu^{1,3}, Nathan Gallant^{2,3}

¹Department of Chemical and Biomedical Engineering, University of South Florida; ²Department of Mechanical Engineering, University of South Florida; ³Cellular Mechanotransduction and Biomaterials laboratory, University of South Florida

Electrospun BSA Nanofibers: Integrin Binding with Fibronectin, Focal Adhesion Component and Cell Adhesion Strength

The structural and mechanical properties of a surface often play an integral part in the determination of the cell adhesion strength and design parameters for creating a biodegradable electrospun scaffold. This electrospun protein scaffold serves as an extracellular matrix to which adhesion interaction exist with cells via cell surface integrins. This interaction is vital in regulation cell differentiation, growth and migration. Nanofibers composed of the globular proteins bovine serum albumin (BSA) and fibronectin were produced by electrospinning from a solution consisting of 10% BSA, β -mercaptoethanol, trifluoroethanol (TFE), deionized water (dH₂O)₂, and various concentrations of fibronectin. Fibers based on BSA were selected due to its abundance in blood and its non-adhesive nature. Therefore, the nanofibers produced via the

fibronectin which when viewed during immunofluorescence analysis should show the specific binding site to which integrins can bind and finally control and the...

<u>GP-06</u> Parul Jain¹, Niloofar Ghazi-Moghaddam¹, Julie P Harmon¹ ¹Department of Chemistry, University of South Florida

Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF) is a accurate and sensitive technique for the identification of biomolecules. Analysis of proteins and peptides by MALDI-TOF is affected by sample formulation and spotting onto a MALDI target. Here we used a novel technique, induction based fluidics (IBF), to analyze its effectiveness during sample preparation. It is a simple and contact free technology that offers a method of spotting samples kinetically by delivering precise volumes. We have produced bovine serum albumin samples with increased uniformity and a greater signal to noise ration by depositing in an electric field. In this study, the common "dried droplet" method is compared to electric field enhancement (EFE) sample preparation technique. Transmission electron microscopy and a polarizing optical microscope were used to contrast the EFE and dried droplet method. In addition, we used surface profilometry to demonstrate the evenness of the EFE samples.

conventional coatings in the preconcentration of analytes, problems arise due to their cracking tendency. Crack free sol-gel germania PEG monolithic beds were successfully immobilized within fused silica capillaries through extension of sol-gel condensation reaction to the capillary walls. This monolith was very porous and able to withstand liquid-phase operations involving elevated pressures. Detection limits in the nanogram/liter range were accomplished with CME sol-gel germania PEG monolithic capillaries coupled to

Bioorganic, Natural, and Organic (NES South Hall)

<u>GO-01</u> Wai Sheung Ma¹, Tina Mutka², Dennis E Kyle^{2,3}, Lilian Vrijmoed⁴, Bill J Baker^{1,3} ¹Department of Chemistry, University of South Florida; scaffold. The design, synthesis, incorporation of proline-based bicyclic core structure into potential Akt inhibitors, and their preliminary biological activity will be presented.

<u>GO-04</u> Tao Liang¹, Jon Antilla¹ ¹Department of Chemistry, University of South Florida

Brønsted Acid Catalyzed Enantioselective Pinacol Rearrangement

The first example of chiral phosphoric acid catalyzed enantioselective pinacol rearrangement of indole derivatives with up to 90% yield and 95% ee.

<u>GO-05</u> Biplob Bhattacharya¹, Silvia Robles¹, Edward Turos¹ ¹Department of Chemistry, University of South Florida

N-Thiolated β-Lactams: Altering Microbiological Activity and Bacterial Cell Targeting with C3 Ring Functionality

The main objective of this project is to check any change in inhibitor activity if the side chains were watersoluble polar groups like amino acids. This project also includes studying the effect of side chain structure and polarity at the C3 position of N-Thiolated β -Lactams on solubility and antibacterial activity. Our primary objective is to see if there is a correlation between chain length and polarity at the C3 position of N-Thiolated β -Lactams on the antibacterial activity. The project started to diverge and now we are looking at different moieties like carbohydrates and PEG attached to N-Thiolated β -Lactams.

<u>GO-06</u>

<u>GO-07</u> Sameer Kulkarni¹, Niranjan Namelikonda¹, Xiangdong Hu¹, Kenichiro Doi², Hong-Gang Wang², Roman Manetsch¹

¹Department of Chemistry, University of South Florida; ²Department of Pharmacology, Penn State College of Medicine

Kinetic Target Guided Synthesis for the Identification of BcI-XL-protein Interaction Modulators

In the recent years, protein-protein interactions have been identified to possess significant biological importance and targeting certain protein-protein interactions has been shown to have therapeutic effects. The discovery of numerous small molecules interfering with Bd-XL-protein complexes has introduced a practicable route for inducing apoptosis in cancer cells. Herein, we report our progress towards the development of a novel drug discovery method that generates only biologically active compounds, an approach known as kinetic target guided synthesis (TGS). We discovered that an amidation reaction between thio acids and sulfonyl azides can be employed for Bd-XL-templated screening to identify inhibitors of Bd-XL itself. The target protein, Bd-XL, displayed selective formation of bidentate compounds from different libra2sf4TC3T0 1 Tf-0.00f93.000 527.22 471 13.89000 527.22 471 151

<u>GO-10</u> Kurt Van Horn¹, Anuradha Srivastava¹, Dennis Kyle², Roman Manetsch¹ ¹Department of Chemistry, University of South Florida; ²College of Public Health, University of South Florida

Anti-leishmanial Activity of a New Series of Quinazolines

A new series of 2,4-disubstituted quinazolines has been synthesized and tested for in vitro activity against Leishmania mexicana axenic amastigotes and L. donovani intracellular amastigotes. The Topliss scheme was loosely followed in order to see if an accurate structure activity relationship (SAR) study could be evaluated to bring to fruition a usable lead compound. This study led to several compounds in the low micromolar range for EC₅₀ in the L. donovani intracellular amastigote assay.

nis Kyle²,

Roman Manetsch¹

Florida

The Development and Use of an HPLC-based Assay to Determine Aqueous SolubiCollege/TT0 1 Tf-0.0005 Tc 044.ellular

The Clear Springs Land Undergraduate Poster Session

Analytical and Biochemical (NES 106)

<u>AB-01</u> Rebecca Burt¹, Kimberly Fields¹, Whittney Burda², Natasa Dragicevic², Cynthia Bucher³, Alberto van Olphen³, Patrick Bradshaw², Lindsey Shaw², Peter Zhang¹ ¹Department of Chemistry, University of South Florida; ²Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida; ³Department of Global Health, University of South Florida

Biomedical Applications of Porphyrins and Small Molecules

Porphyrins are organic compounds commonly found in nature and in the human body. Heme containing proteins, such as hemoglobin, myoglobin, and cytochromes, are a few examples of porphyrins in the human body. The focus of this project is the possible biomedical uses of lab synthesized porphyrins in the treatment of disease and infections; particularly Methycillin Resistant Staphylococcus aureus (MRSA) infections, Alzheimer's disease, and influenza. For each disease specific porphyrins and porpyhrin derivatives were selected based on chemical properties and structures. The compounds were then diluted in DMSO and delivered for testing. A total of about 250 different porphyrins and related organic compounds were screened. Approximately 50 porphyrins and related compounds have shown to inhibit the growth of several strains of Staphylococcus aureus. Further testing is underway to determine the mechanism of action of these compounds. The preliminary testing of the compounds in the Alzheimer's lab show that approximately 15 porphyrins and related compounds are effective in treating mitochondrial cells that express the β

<u>AB-03</u> Nishal Patel¹, Erica B Turner¹, Abdul Malik¹ ¹Department of Chemistry, University of South Florida

Sol-Gel Mixed Germania-Silica Poly(ethylene glycol) Monoliths for Capillary Microextraction Coupled to

<u>AB-06</u> Christopher Lizardi¹, Eileen Schulman¹, Bryan Vo¹, Darius Wynn¹, Dean F Martin¹ ¹Department of Chemistry, University of South Florida

Removal of Selected Nuisance Anions by Octolig®

Octolig®, a commercially available immobilized ligand (IMLIG), has been studied for its effectiveness in removing nuisance anions. The material consists of polyethylenediamines covalently linked to high surfacearea silica, and has a high affinity for transition metal ions. Previous research indicated that anions could be removed quantitatively from aqueous solutions using the metal derivatives of Octolig® as packing in column chromatography. The present study focused on the results with Octolig® alone. Quantitative removals (>99%) were obtained for arsenate, chromate, paramolybdate, selenious acid, and fluoride. Boric acid was not removed by under similar conditions, but previously the copper(II) derivative of Octolig® had been partially successful. A mechanism of removal is proposed.

<u>AB-07</u> Robin Fulton¹, Abdullah Alhendal¹, Abdul Malik¹ ¹Department of Chemistry, University of South Florida

Preparation of a Polar Hybrid Organic-Inorganic Germania-based Coating for Capillary Microextraction by Sol-gel Chemistry

<u>AB-09</u> Lorenzo Rodriguez¹, Dean F Martin¹ ¹Department of Chemistry, University of South Florida

Removal of Lithium from Solutions Using Octolig®

TEEDA (tetraethylethylenediamine) has been used before to remove lithium cations from tandem organic reactions. An attempt was made to achieve a similar feat using a commercial product called Octolig® that consists of polyethylenediamine moieties covalently bound to silica gel. Octolig®'s polyethylenediamine units are similar in structure to TEEDA. The hypothesis was that Octolig® should be able to remove lithium cations from solution as well. Our initial attempt used water as the solvent because water is environmentally-safe. Three solutions were prepared with a concentration of 100 ppm Li: LiNO₃ and LiCl in deionized water, and LiCl in well water. Each solution was passed through a chromatography column (dimensions 2 cm x 30 cm) packed with 62.8 cm3 of Octolig®. The lithium concentrations of both composite effluent samples and the standard solutions were determined indicating 0% removal. Presumably the lithium cation has too much affinity for water, preventing it from interacting with the Octolig®. Future work will involve trying non-aqueous solvents such as ethers. Given the growing need for lithium in electric and hybrid-electric vehicles, finding a method to remove lithium is of critical importance.

<u>AB-10</u> Jorge Vega¹, Sharon Spencer¹, Brent Hilker¹, Julie P Harmon¹ Department ClicClinetry, iStriy, University of South Florida

Blister Agent Analog Sequestration using Porphyrins and Polymer Hydrogels

Polymer hydrogel systems are investigated as a media to make a useful composite with meso-tetra(mhydroxy phenyl)porphyrin (4(m-OHP)P) to sequester and ultimately photo-catalytically destroy sulfur and nitrogen mustards. Hydroxyethyl methacrylate (HEMA), vinylpyrrolidinone (VP), ethylene glycol

<u>AB-12</u> Sibel Demirel¹, Daniel Leyva¹, Ruben Durand¹, Vicky Lykourinou¹, Li-June Ming¹ ¹Department of Chemistry, University of South Florida

Mechanistic Studies of Catalytic Activity of Cu(II)-Bound Copolymers in Oxidation of Catechols, DNA Cleavage and Modeling of Antioxidant Activity of Natural Products

Copper (II)-bound copolymers can catalyze the oxidation of catechol, mimicking enzymes such as tyrosinase and catechol oxidase. The catalytic behavior of these copper-bound copolymers has been attributed to the functional groups in the polymeric chain namely pyridine and amide or phenyl. We investigate the catalytic activity of two linear copolymers containing a hydrophobic or a hydrophilic functional group (from styrene or acrylamide) and a metal binding functional group (e.g. vinylpyridine). The 1:1 Cu(II) complexes of these copolymers exhibit a significant catalytic activity in oxidation of catechol derivatives in air and H_2O_2 and toward DNA cleavage with H_2O_2 or O_2 (under reduction conditions). Our

eukaryotes, and is part of hormones activation system, since ~50% of all mammalian peptide hormones are

ascertain if cocrystals can be formed between lithium chloride and six different neutral amino acids. The amino acids, L-valine, L-alanine, L-leucine, L-isoleucine, N,N-dimethylglycine, and betaine are all neutral amino acids that become zwitterions in solution. Lithium chloride is being targeted because it does not cause suicidality as a side effect as compared to other commercially available antidepressant drugs. Due to lithium's narrow therapeutic index, it is desired to make cocrystals of lithium chloride in order to modulate the concentration of lithium cations in solution (solubilityw-am(h)1(milato52.225 (e))]TJEMC ET1 g70.52 13418 471 13.74 reference.

including hydrogen or carbon dioxide, both used for energy storage and sequestration, respectively. H₄BIPA-TC was synthesized by cocrystal controlled solid-state synthesis (C3S3) and was used to construct a porous 3-periodic framework with copper. Initial results suggest the material retains its structure after the removal of solvent molecules and allows for the absorption of nitrogen gas at 77 K for surface area analysis.

<u>IP-10</u> Anna Cardwell¹ ¹Department of Chemistry, University of South Florida

Natural Product Cocrystals

To further comprehend the concept of the supramolecular synthon, a research plan involving an extensive amount of cocrystal formers was devised. The two different types of synthons are heterosynthons and homosynthons. A supramolecular heterosynthon involves two different functional groups hydrogen bonding. Melatonin, a naturally occurring hormone produced by the pineal gland in mammals has been proven to improve sleep quality, is the chosen compound to bind with a list of various cocrystals formers. A supramolecular homosynthon involves two identical functional groups hydrogen bonding to one another. Lactic acid is an ingredient found in yogurt, cottage cheese and butter and has beneficial effects on the skin as a cleanser. Lactic acid is the chosen compound to demonstrate a homosynthon containing carboxylic acid functional groups. Lactic acid was ball milled with glutaric acid on a 1:1 ratio and provided different experimental data from the starting carboxylic acid compounds.

Organic (NES 104)

<u>O-01</u> Petoria Gayle¹, Sameer Kulkarni¹, Xiangdong Hu¹, Hong-Gang Wang², Roman Manetsch¹

¹Department of Chemistry, University of South Florida; ²Department of Pharmacology, Penn State College of Medicine

Protein-Protein Interaction Modulators & Role of Target Guided Synthesis

Protein-protein interactions are necessary for basic biological functions. However, modulators to certain protein-protein interactions can have therapeutic effects. We are focusing on the disruption of the interactions between anti-apoptotic proteins, such as Bd-XL and pro-apoptotic proteins. Bd-XL is the main regulator of apoptosis, or programmed cell death. Over expression of anti-apoptotic proteins has been commonly observed in cancer cells. This over-expression results in the suppression of apoptosis, leading to uncontrolled growth of cells, a phenomenon known as tumor growth. We are targeting the anti-apoptotic protein Bd-XL using a fragment-based drug discovery approach known as Target-Guided Synthesis (TGS). In this approach, the biological target (Bcl-XL in this case) acts as a template onto which the fragments can bind and form a covalent bond, leading to a potential inhibitor of that target itself. These fragments generally consist of complimentary reactive functional groups. After investigating various reactions, an amidation reaction between sulfonyl azides and thio acids was employed for this purpose. So far, several acyl sulfonamides have been identified as potential inhibitors of Bd-XL, using this approach. We believe that this approach will be ut9T0 1 Tf3crm0.000004srogramm

O-08

<u>O-11</u> Mijal Guevara¹, Carolina Lopez¹, Ali Hussain¹ ¹Department of Chemistry, University of South Florida

Formation of Bridged-Resorcinarene: Tetrabromoresorcinarene

The synthesis of the bridged resorcinareme was accomplished in three steps. To begin with, condensation of 2-methyl-resorcinol and one equivalent of heptaldehyde catalyzed by hydrochloric acid in ethanol led to the octahydroxyresorcinarene. The product, a white solid, was filtered and washed with cold ethanol and water. The resulting product was then treated with dibromomethane/ K_2OO_3 in DMF as a solvent to form the bridged resorcinarene product. The bridged resorcinarene was then brominated (using NBS as a reagent, and AIBN as an initiator) in benzene to yield the tetr

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Isolation and Further Chemical Investigation of Ecdysteroids from Synoicum Adareanum

Ecdysteroids, hormones responsible in the regulation of molting, metamorphosis, reproduction, and diapauses in crustaceans, were first isolated in the 1950's. Evidence suggests that some of these compounds possess pharmacological properties. In fact, there are several plant species among traditional medicines that contain ecdysteroids. The tunicate Synoicum adareanum, contains six known ecdysteroids and represents first tunicate reported to yield ecdysteroids. Previous studies have shown that the S. adareanum ecdysteroid abeohyousterone exhibits considerable cytotoxicity against leukemia, colon, and lung cancer cell lines. This paper describes the isolation of the six known ecdysteroids from S. adareanum as the basis of continuing studies of their pharmacological activity.

<u>N-04</u> Hoangmy Chau¹, Jeremy Beau¹, Bill Baker¹ ¹Department of Chemistry, University of South Florida

Isolation and Chemical Extraction of Endophytes from Rhizophora Mangle for Bioactivity against S. aureus

Rhizophora Mangle are plants that grow around salty bodies of water. They are unique because they are able to flourish in soil that is unstable and low in oxygen. R. mangle depend on chemical and biological defenses in order to protect themselves from pathogens. They do this through a symbiotic relationship with endophytes. Endophytes are bacteria and fungi that live symbiotically within the R. mangle. The endophytes benefit from the R. mangle because the R. mangle provide the endophytes with nutrients. The endophytes, in turn, provide the R. mangle with protec

<u>N-06</u> Ryan Baker¹, Charles Harter¹, Matt Lebar¹, Raymond Chowmond³, Tina Mutka², Dennis Kyle², Cedric Pearce⁴, Lilian Vrijmoed³, Bill Baker¹

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Antimalarial Constituents of Fungi

Malaria, a vector borne plasmodium parasite, is responsible for 200-300 million infections each year in mostly developing nations according the The World Health Organization. The two most common species, Plasmodium falciparum and Plasmodium vivax, are becoming resistant to all forms of treatment. Thus a need exists for new drug therapies. The chemical constituents of approximately 70,000 fungi were extracted in methanol and bioassayed at a 30µg/ml concentration to determine which microbes were producing anti-malarial compounds. The extracts showing the highest level of activity were then separated into fractions based on polarity using Medium Pressure Liquid Chromatography with a gradient solvent system (hexane to ethyl acetate to methanol). The resulting fractions were assayed again. The fractions that remained active against malaria were further purified using High Pressure Liquid Chromatography. The resulting pure compounds were identified via Nuclear Magnetic Resonance spectroscopy, Mass Spectroscopy and re-screened against malaria.

<u>N-07</u> Jayesh Gopal¹, Bill J Baker¹, Matthew Lebar¹ ¹Department of Chemistry, University of South Florida

Florida Marine Tunicates

Antarctic marine tunicates have been previously studied, with special note being given to their ability to sequester metals such as vanadium, manganese, and nickel. The environment of Antarctica is known for being one of the most pure, pollution-free areas in the world, making it a possibility that its marine tunicates store metals differently from tunicates found elsewhere. For this reason Florida tunicates must also be studied and their mechanism of storage compared to that of Antarctic tunicates. The tunicates are freeze-dried and their minerals extracted using

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Isolation of Endophytic Fungi from Exostema Cari

<u>N-12</u> Steven Austin¹, Jeremy Beau¹, Bill J Baker¹