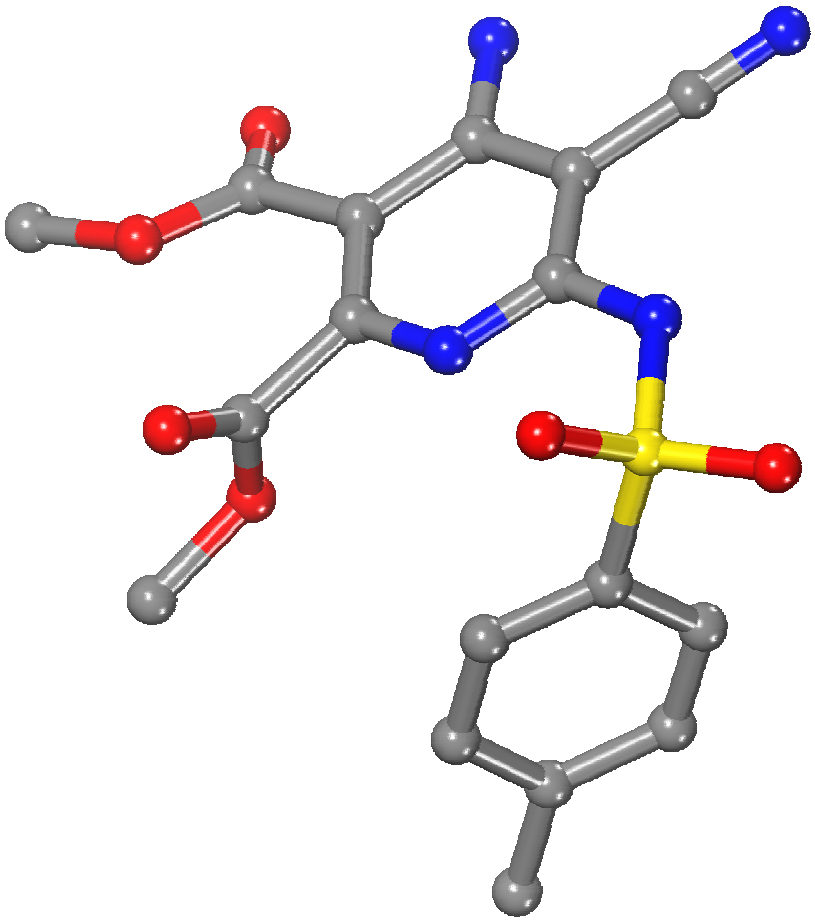
Fifth Annual
Raymond N. Castle
Student Research Conference



Department of Chemistry

University of South Florida

2006

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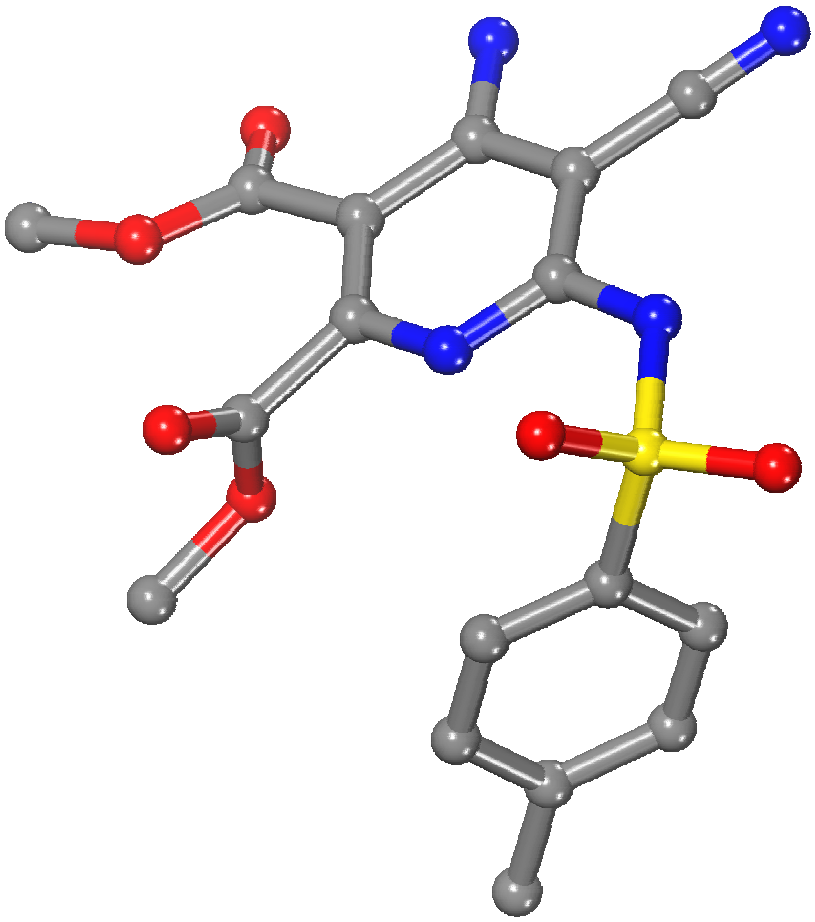
Raymond N. Castle
Student Research Conference



Department of Chemistry

University of South Florida

2006

Welcome

Dear Colleagues,

歡迎, 欢迎, Bienvenue, Willkommen, Υποδοχή, Swagat, Benvenuto, 歓迎, 환영, Boas-vindas, مرحبا, Bine ati venit, Добро пожаловать, Bienvenidos, and Welcome to the Fifth Annual 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. A pioneer in the synthesis of heterocyclic compounds, Dr. Castle published well over 200 articles, including collaborations with other USF Department of Chemistry researchers, Andrew S. Zektzer, Milton Johnston, and Ron Federspiel, as well as chemists from Japan. On this year's cover, Dr. Castle's synthetic efforts are illustrated through his heterocyclic molecule, dimethyl 2-(p-toluenesulfonylamino)-3-cyano-4-imino-1,4-dihydropyridine-5,6-dicarboxylate.

The Raymond N. Castle Conference was designed to be organized by students for students as an excellent opportunity for both undergraduate and graduate students to present their scientific research in a familiar, amiable environment, as well as provide leadership experience for those interested in the conference organization. Students within the department are encouraged to not only gain presentation experience and hone their communication skills to effectively convey their results to a broad audience, but also to discover more about their colleagues' research. We encourage everyone to take advantage of this opportunity and attend both the poster and oral presentations. Additionally, we are all excited to attend our plenary lecture, and we are particularly grateful to have Dr. William Wulff, Professor of Chemistry at Michigan State University as our plenary speaker and distinguished guest.

Lastly, I would like to personally thank all of the committee members involved for their help in the coordination of this year's event. Likewise, we, the committee, would not have been able to organize such an event without the assistance of our faculty advisor, Dr. Mohamed Eddaoudi. In addition, any conference could not be successful without financial support, and as such we are grateful to our sponsors and the University of South Florida Department of Chemistry, who have generously contributed to our event. Most importantly, this conference would not exist without the efforts of those of you presenting research today, graduate and undergraduate alike. Therefore, we gratefully acknowledge you and your major professors, as well as all in attendance. Thank you all, and I hope you enjoy the Fifth Annual Raymond N. Castle Student Research Conference.

Sincerely,
Jarrod F. Eubank
Jarrod F. Eubank
'06 Castle Conference Chair

Raymond N. Castle Research Conference Committee

Faculty Advisor:
Dr. Mohamed Eddaoudi

Chair:
Jarrod F. Eubank

Committee Members:
Jacilynn Brant
Richard (Matt) Cross
Giordano da Silva
John J. Perry IV
Dorina Sava
Tanise Shattock

Web Support:
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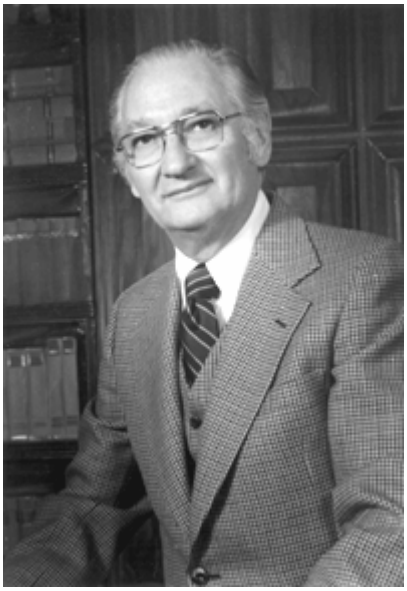
SCHEDULE OF EVENTS

Saturday, April 29th, 2006

Time	Event
8:30 - 9:00 A.M.	Registration and Breakfast
9:00 - 11:40 A.M.	**Morning Session** – Oral presentations (Graduate students)
11:40am – 12:40 P.M.	**Plenary Speaker** - Dr. William Wulff – *Catalyse Asymetrique Inspire´Au Naturel*
12:40 – 2:40 P.M.	Lunch / Posters
2:40 – 5:30 P.M.	**Afternoon Session** – Oral Presentations (Graduate Students)
5:30 P.M.	Awards Ceremony

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, 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, have been 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 as the American advisory editor for the English translation of the Russian Journal of Heterocyclic Compounds. He was in great demand as a speaker, lecturing at hundreds of institutions worldwide. He was general chairman of the First International Congress of Heterocyclic Chemistry held in Albuquerque (1967), secretary of the Second International Congress held in Montpellier, France (1969), vice-president of subsequent congresses held in Sendai, Japan, Salt Lake City, Utah, Ljubljana, Yugoslavia, and Tehran, Iran. He was chairman and committee member for the American Chemical Society. In addition, he was cofounder of the International Society of Heterocyclic Chemistry, which he served as chairman of the executive committee, and president (1973-1975). Professor Castle received numerous awards and honors, including the prestigious International Award in Heterocyclic Chemistry (1983) for outstanding contributions to the field of heterocyclic chemistry, presented in Tokyo, Japan. Dr. Castle was listed in the first edition of Who's Who in World Science and in Who's Who in the World.

The Chemistry Department remains deeply indebted to Professor Castle for his many outstanding contributions to the Department, and to science overall. He would have been a strong supporter of this student symposium, and thus, it is fitting that we dedicate this and future symposia to his memory.

Dr. Dean F. Martin, Special Thanks

Dean F. Martin is Distinguished Service Professor and Director of the Institute for Environmental Studies at the University of South Florida, where he has been a member of the faculty since 1964. Dr. Martin received his B.A., with Honors, from Grinnell College (1955), where he met his future wife Barbara while both were chemistry majors. They were married in 1956 while both attended Pennsylvania State University as graduate students and in 1958 Dr. Martin received his Ph.D. and Mrs. Martin her Masters degree. In 1958-59, he was a National Science Foundation Post-Doctoral Fellow at University College, London after which he returned to the States and accepted a faculty position at the University of Illinois, Urbana-Champaign, as Instructor and Assistant Professor of Inorganic Chemistry (1959-1964). He received (1969-1974) a Career Development Award from the Division of General Medical Sciences, NIH, to study the chemistry and chemical environment of algal toxins. In 1970-71, he was a Visiting Professor of Physiology and Pharmacology at Duke University Medical Center.

Dr. Martin and his wife share research interests concerned with the coordination chemistry of natural water systems, including problems of red tide and aquatic weeds and they have collaborated in research involving the properties of coordination compounds, as well as aspects of environmental chemistry. Currently, they are investigating the removal of arsenic by means of supported chelated iron compounds. Dean Martin is the author or co-author of over 300 publications, including four books. He was the recipient of the 1975 Florida Award and the 1987 Civic Service Award of the Florida Section, ACS; in 1978, he received the F. J. Zimmermann Award in Environmental Science from the Central Wisconsin Section, sponsored by Zimpro Inc.; and in 1983, he was elected Fellow of the American Association for the Advancement of Science. Dean and Barbara Martin were the co-recipients of the 1994 Medalist Award of the Florida Academy of Sciences, its highest award. Dean Martin has been active in the Florida Section of the American Chemical Society (Chairman,1986), and he has held several positions in the Aquatic Plant Management Society (President,1986-87). Both of the Martins have received the Alumni Award of Grinnell College.

The Martins have personally funded the George Bursa Award given annually to a deserving graduate student within the Chemistry Department who has demonstrated notable professional dedication and consideration for others, as well as a Graduate Student Travel Award the past two years. In addition, they have been the benefactors of the annual Barbara and Dean Martin Lecture Series. Together the Martins have edited *Florida Scientist* since January 1984. Dr. Martin initiated and continues to edit the departmental newsletter and has written a departmental history to coincide with the 40th Anniversary of the founding of the department.

The Martins have six children; Diane, Bruce, John, Paul, Brian, and Eric, and four grandchildren.

PLENARY SPEAKER

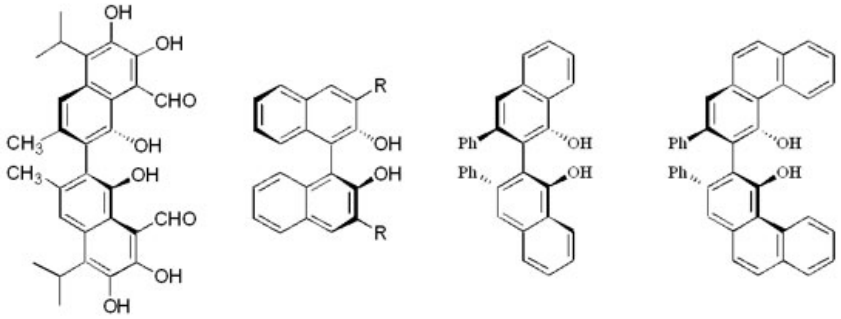
William Dean Wulff
Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA

Prof. Wulff is currently a Professor of Chemistry at Michigan State University. He finished his B.S. at the University of Wisconsin-Eau Claire in 1971, and obtained his Ph.D. in organic chemistry from Iowa State University in 1979. He was granted an NIH Postdoctoral Fellowship to Princeton, and then he accepted his first Assistant Professor position in 1980 at the University of Chicago. Since then, he has moved to Michigan State University, and has developed diverse research interests, including methodology development, macrocyclic chemistry, organometallic chemistry, the total synthesis of natural products, supramolecular chemistry, and the design and development of new asymmetric catalysts.

PLENARY SEMINAR

"CATALYSE ASYMETRIQUE INSPIRE´AU NATUREL"

This talk will describe a new chiral catalyst (chemzyme) for the formation of aziridines from the reaction of imines with diazo compounds and the formation of dihydropyridinones from a hetero Diels-Alder reaction of imines with dienes. The development of the chiral catalysts used in these reaction was inspired by the natural product gossypol. Gossypol is a natural product that is isolated from cotton seeds and exists in optically pure form. It is related in structure to the widely used and successful chiral ligand BINOL. The difference is that in gossypol the biaryl linkage is at the 2 and 2'-positions of the naphthalene core whereas, in BINOL, it is at the 1 and 1'-positions. Inspired by this natural product, we set out to prepare and evaluate the two ligands VANOL and VAPOL as ligands in asymmetric synthesis and these results will be presented.



Gossypol (S)-BINOL (*S*)-VANOL (*S*)-VAPOL

Session Schedule

9:00 – 9:20 Matt Lebar
"Chemical transformations of tylosin, an antibiotic agent"

9:20 – 9:40 Surbhi Bhatt
"Chemo-enzymatic syntheses of Glycolipid analogs"

9:40 – 10:00 Miranda L. Cheney
"Solid-State Synthesis of Imides via Mechanochemistry"

10:00 – 10:20 Giordano da Silva
"A 'Moonlighting' Dinuclear Hydrolase: Activities toward Phosphoester Hydrolysis and Catechol Oxidation"

10:20 – 10:30 Break

10:50 – 11:10 Jaime Heimbegner
"Chemical Investigation of Synoicum adareanum"

11:10 – 11:30 Kashmir Juneja
"Natural Antioxidant Inhibition of Copper Induced Neurodegenerative Diseases"

11:30 – 11:40 Break
Afternoon Session (CHE 100)

2:40 – 3:00 Pasha Khan
" Chemoenzymatic synthesis of bicycle[3.1.0]hexane ring compounds"

3:00 – 3:20 Sampath Abeylath
" Sugar-Coated Nanobiotics"

3:20 – 3:40 Vasiliki Lykourinou
" Phenol Hydroxylation and Oxidation by a Copper(II) Complex of a Pyridyl-Containing Copolymer in Aqueous Medium

3:40 – 4:00 Christine Neipert
" Theoretical Development and Application of a Computationally Amenable Sum Vibrational Frequency Theory (SVF)"

4:00 – 4:10 Break

4:10 – 4:30 Sumedh Parulekar
" Novel Approach to manipulate the Cavity Size in Resorcinarenes"

4:30 – 4:50 Praveen Ramaraju
"Penicillin bound nanoparticles: A potential way to overcome drug resistance in bacteria"

4:50 – 5:10 William Tay
"Binding of the Flavonoid Quercetin: Implications in Drug Design toward Prevention and Treatment of Alzheimer's Disease"

5:10 – 5:30 Chien-yi (Erin) Wu
"Nickel Derivative of Streptomyces griseus Aminopeptidase: The Importance of Metals in Bio-Hydrolysis"

5:30 Awards Ceremony

The Barbara and Dean F. Martin Academic Research Experience for Undergraduates Poster Session
(NES First Floor)

1. Kenny Aristide; Alfredo Cardenas
"Computational Study of Folding Pathways of Oxygen Sensing Heme Proteins"

2. Kyle Belknap; Monica Elmashat; Saira Gardezi; Matthew Hight; Tiffany Mueller; Tyler Sexton; Kenneth Caswell
"An Antigen-Presenting Device for a Bio-Nano Vaccine"

3. Kyle Belknap; Monica Elmashat; Saira Gardezi; Matthew Hight; Tiffany Mueller; Tyler Sexton; Kenneth Caswell
"Metal CdS nanosphere formation in presence of zeolite-like metal organic frameworks (ZMOFs)"

4. Ryan Centko; Bill Baker
"Possible Biosynthetic Pathways for Isocyanides"

5. Casey Cosner
"Selective Thiolate Labeling Agents"

6. Vedad Delic; Cairns, Amy; Mohamed Eddaoudi
" Metal-Organic Frameworks (MOFs)"

7. Christina Drenberg; Marianne Fatica; Ellen Verdel
"Development of a Quick Field Assay for Africanized Honey Bees based on Africanized Honey Bee Specific Proteins"

8. Andrew Gerges; Tanise Shattock; Michael J. Zaworotko
"The Effect of Solvent and Impurity on the Solid State Synthesis of Polymorphic 2:3 Co-Crystals of Trimesic Acid and 1,2-Bis(4-pyridyl)ethane"

9. Edward Gerges; Marian N. Farag; Miranda L. Cheney; Michael J. Zaworotko
"The Effects of Solvent and Impurity on the Solid State Preparation of Imides Utilizing Green Chemistry Techniques"

10. Glenn Harris; Anne Shearrow; Abdul Malik
" Investigative study on the use of Ionic Liquids as solvents for sol-gel preparation"

11. Diondra Hill; M. Acevedo-Duncan
"Down regulation of PKC-ι decreases the proliferation of breast cancer cells"

12. Majdouline Leroy; Bill Baker
"Biological Activity of Three Antarctic Invertebrates"

13. William Maza; Audrey Mokdad; Randy L. Larsen
"Photoinduced Intermolecular Electron Transfer Dynamics between Perylenetetracarboxylic Acid and Cytochrome C"

14. Lidija Milisav; Dean F. Martin
"Properties of Nitrilotriacetic Acid (NTA) Condensed with Silica Gel"

15. Theresa Minoudakis; Kristen Wheeler; Ellen Verdel
"Africanization of Honey Bees"

16. Lauren O'Donnell; Dean F. Martin
"REMOVAL OF AQUEOUS ARSENIC USING IRON ATTACHED TO IMMOBILIZED LIGANDS (IMLIGS)"

17. John O'Leary; Li-June Ming
"Inhibition Studies of Prolidase by Anthracycline Anti-Cancer Drugs"

18. Fernando Ortiz; Nicholas Orletsky; Albert Alguadich, Jr.; Joseph White; Noel Dickson
"The PMD Project"

19. Jimmy Rodriguez, Jr.; Alfredo Cardenas
"Molecular Simulation of HemAT"

20. Mohammed Shafiq; Dean F. Martin
"Extraction of Heavy Metals by Silica Gel Composites with EDTA, NTA, 2-Mercaptoethanol"

21. Ekta Shah; Bill Baker
"Bioactivity of Antarctic Sponges"

22. Misbahuddin Syed; Mark McLaughlin
"Synthesis of Alpha-Helical Amphipathic Peptides with Links to Anti-cancer Activity"

23. Phoebe Zito; David J. Merkler
"The PAM catalyzed cleavage of a carbon-sulfur bond"

Graduate Posters (NES First Floor)

24. Jonathan Belof
"Volume determination of globular proteins by molecular dynamics"

25. Amy Cairns
"Assembly of Lanthanide based Metal-Organic Frameworks"

26. Adam Clarke
"Effects of Mutations on the Folding Pathways of a Cold Shock Protein"

27. Richard Cross
"Synthesis of IBTZ6PA2: A Potential Acetylcholinesterase Inhibitor with Improved Species Specificity"

28. Kerrian Greenhalgh
"Mechanical Properties of Biocompatible Smart Films for Burn Wound Applications"

29. Dijana Lekic
"PHOTOTHERMAL STUDIES OF THE COIL TO HELIX TRANSITION IN POLY-GLU20"

30. Neil McIntyre
"The Imino-Oxy Acetic Acids as Substrates for Peptidylglycine alpha-Amidating Monooxygenase (PAM): Product Analysis, Steady-State Kinetics, and Deuterium Isotope Effects"

31. Audrey Mokdad
"Photothermal and transient optical studies of CO binding to HemAT from Bacillus subtilis"

32. Divya Ramamoorthy
"Preparation of Small molecule inhibitors of BCl-XL-Bax"

33. Kevin Revell
"N-Alkylthio beta-lactams Inhibit the Growth of Methicillin-Resistant Staphylococcus aureus (MRSA) through a Novel Mode of Action Involving Type II Fatty Acid Synthesis"

34. Emily Rowland
"Catalytic Asymmetric Imine Amidation"

35. Dorina Sava
"Molecular-building block approach for the design and synthesis of MOFs"

36. Anne Shearrow
"Microchip-based electrochromatography system with sol-gel stationary phase to study physiological processes at the skin-interface"

37. Hla Win
"Role of Atypical Protein Kinase C-iota in Prostate Cancer Cell Cycle, Proliferation, and Apoptosis"

Session Abstracts

Saturday, April 29th, 2006

Morning Session (CHE 100)

9:00 – 9:20 **Matt Lebar**
"Chemical transformations of tylosin, an antibiotic agent"

Tylosin is a chemical with antibiotic properties originally isolated from bacteria (Streptomyces fradiae). This antibiotic is used to treat mainly livestock and other animals. Tylosin has been subjected to many different chemical transformations. Each product of these reactions has been analyzed to determine its structure.
Tylosin shares similar structural characteristics with a new compound isolated in our lab, palmerolide A. Palmerolide A, however, is only obtained in small quantities. Because tylosin mimics certain functionalities of palmerolide A, it should react similarly and thus can be used as a predictive tool. Techniques will be perfected on tylosin, and then performed with confidence on palmerolide A.

9:20 – 9:40 **Surbhi Bhatt**
"Chemo-enzymatic syntheses of Glycolipid analogs"

In search of a environment friendly compounds and synthetic routes, The stress has been given on chemo-enzymatic synthesis of glycolipid analogs. These analogs were synthesized using common disaccharides (Maltose, Lactose, mellibiose and cellobiose) as starting material and exploiting the regioselectivity of lipases.

9:40 – 10:00 **Miranda L. Cheney**
"Solid-State Synthesis of Imides via Mechanochemistry"

The emergence of green chemistry in the early 1990's has lead to the development of many new methods for synthetic chemistry. The focus of this contribution will be to explore the use of mechanochemistry and other "green" techniques for solid-state synthesis with particular emphasis upon generation of the imide moiety. The significance of the utilization of co-crystals in solid-state synthesis via crystal engineering will be established as well as the potential applications of imides as active pharmaceutical ingredients (API's).

10:00 – 10:20 **Giordano da Silva**
"A 'Moonlighting' Dinuclear Hydrolase: Activities toward Phosphoester Hydrolysis and Catechol Oxidation"

The aminopeptidase from Streptomyces griseus (SgAP) is a hydrophobic-specific dinuclear metalloenzyme. Recently, it has been found to perform interesting alternative catalyses, with the ability to hydrolyze the phosphodiester bis(p-nitrophenyl) phosphate (BNPP) and the phosphonatoester p-nitrophenylphenyl phosphonate with enormous catalytic proficiencies in terms of the first-order rate constant (kcat/k0= 0.94–67 billion and 0.043–0.29 million, respectively). Study of the alternative catalyses of SgAP may provide further insight into its mechanism that is otherwise not obtainable by the use of the regular peptide substrates. To demonstrated this concept further, we have investigated the di-Cu(II) derivative of this enzyme toward the oxidation of a prototypical catechol oxidase substrate, 3,5-di-t-butyl-catechol. Significant activity was observed with rate constants of kcat = 1.45 s–1, Km = 0.44 mM, and kcat/Km = 3,300 M–1 s–1.

10:20 – 10:30 **Break**

10:30 – 10:50 **Julio Garay**
" 'Surfactant-free' Nanoparticles for Delivery of Antibiotics"

Recent research in our laboratory has centered on the development of polyacrylate and polyacrylamide nanoparticles prepared in water emulsions. Our goal is to use these nanoparticle emulsions for treatment of life-threatening bacterial infections such as those caused by methicillin-resistant Staphylococcus aureus and Bacillus anthracis. One of the problems we have encountered with these polymeric antibiotics is that the surfactant used for the polymerizations can leach away from the nanoparticle in high enough concentrations to cause cytotoxic effects in human fibroblast cells. To circumvent this, we are investigating the development of new types of nanoparticles in which the surfactant molecule is covalently attached to the backbone of the polymer. The synthesis and characterization of these "surfactant-free" nanoparticle systems, and their application to drug delivery, will be discussed.

10:50 – 11:10 **Jaime Heimbegner**
"Chemical Investigation of Synoicum adareanum"

Many plants and animals that lack the ability to flee in response to predatory attack have evolved chemical defense systems. These chemical substances, which are often toxic or noxious to predators, have been of interest in biomedical studies since many of them have been shown to be effective in the treatment of human diseases. We have been studying Antarctic marine invertebrates for the presence of such natural products. Synoicum adareanum is a sea squirt (tunicate) endemic to the waters of Antarctica and can be found in abundance near the U.S. research station (Palmer Station) on the Antarctic Peninsula. Chemical investigation of this marine invertebrate has revealed that its natural product diversity is broad, including polyketide macrolides (more commonly familiar as the antibiotic erythromycin), glucoshpingolipids (structurally related to fats), and steroids (structurally related to cholesterol), all of which have very different structural features as well as functions within the organism. This paper reports on our chemical investigation of Synoicum adareanum, more specifically focusing on the description of these three structurally diverse series of natural products, the majority of which are new compounds to science.

11:10 – 11:30 **Kashmir Juneja**
"Natural Antioxidant Inhibition of Copper Induced Neurodegenerative Diseases"

Many plants and animals that lack the ability to flee in response to predatory attack have evolved chemical defense systems. These chemical substances, which are often toxic or noxious to predators, have been of interest in biomedical studies since many of them have been shown to be effective in the treatment of human diseases. We have been studying Antarctic marine invertebrates for the presence of such natural products. Synoicum adareanum is a sea squirt (tunicate) endemic to the waters of Antarctica and can be found in abundance near the U.S. research station (Palmer Station) on the Antarctic Peninsula. Chemical investigation of this marine invertebrate has revealed that its natural product diversity is broad, including polyketide macrolides (more commonly familiar as the antibiotic erythromycin), glucoshpingolipids (structurally related to fats), and steroids (structurally related to cholesterol), all of which have very different structural features as well as functions within the organism. This paper reports on our chemical investigation of Synoicum adareanum, more specifically focusing on the description of these three structurally diverse series of natural products, the majority of which are new compounds to science.

11:30 – 11:40 **Break**

Afternoon Session (CHE 100)

2:40 – 3:00 **Pasha Khan**

" Chemoenzymatic synthesis of bicycle[3.1.0]hexane ring compounds"

Bicyclic compounds such as bicyclo[3.1.0]hexene and its analogs have always fascinated organic chemists by virtue of the inherent strain in the molecule and thereby the challenges involved in their synthesis. We have accomplished synthesis of bicyclo[3.1.0]hexene systems using much milder chemoenzymatic method involving lipase catalyzed dissymmetrization and Pd catalyzed allylation to produce the title compounds in high enantiomeric excess (> 97%). Compounds containing these bicyclic rings are known to inhibit alpha-mannosidase, an enzyme involved in oligosaccharide processing and are present in carboxycyclopropyl glycines that have shown to have antipsychotic effects in animal models. Unlike methods describing assembly of such system mainly via Simmons-Smith reaction or its modification or via Rh-catalyzed carbene insertion reaction, which are difficult because of the toxic and explosive nature of the reagents, the chemoenzymatic strategy developed in our laboratories utilizes mild reactions conditions and non toxic catalysts.

3:00 – 3:20 **Sampath Abeylath**

" Sugar-Coated Nanobiotics"

Carbohydrate-containing polyacrylate nanoparticles were prepared by emulsion polymerization and studied by a number of methods. The effect of different sugar groups and linker units on the physical and microbiological properties of these new drug delivery vehicles will be discussed.

3:20 – 3:40 **Vasiliki Lykourinou**

" Phenol Hydroxylation and Oxidation by a Copper(II) Complex of a Pyridyl-Containing Copolymer in Aqueous Medium

A Cu^{2+} -polymer system exhibits a very effective activity toward phenol hydroxylation/oxidation to yield o-quinone in 50% aqueous methanol solution at pH 8.0 and 25 °C, showing first-order rate acceleration of 6.0 ´ 105 and 7.8´ 104 folds. The catalyst is active in presence of oxygen and in presence of hydrogen peroxide. The catalytic efficiency towards various phenolic substrates will be presented along with the proposed mechanism of action based on kinetic studies performed

3:40 – 4:00 **Christine Neipert**

" Theoretical Development and Application of a Computationally Amenable Sum Vibrational Frequency Theory (SVF)"

SVF is a second order spectroscopy that is dipole forbidden in bulk media, and hence is a useful tool for probing exclusively interfacial molecular species in the condensed phase. By considering only the dominant terms of the second order susceptibility that will become resonant with the applied fields, a correlation function approach can be developed to calculate the resulting interfacial spectra. Using this correlation function approach, we determine the spectra of an air/water interface, and compare our result to extant experiment.

4:00 – 4:10 **Break**

4:10 – 4:30 **Sumedh Parulekar**

" Novel Approach to manipulate the Cavity Size in Resorcinarenes"

Resorcinarenes have been used as metal complexing agents, sensors, receptors, molecular reaction vessels and catalytic chambers. They are able to encapsulate small neutral molecules, drug molecules. Such cavitands offer unique molecular platforms for host–guest chemistries, as well as new polymers and self-assembled systems. A facile and efficient synthesis of these novel resorcinarenes containing hydroxyl groups and allyl groups can be accomplished in few steps beginning from commercially available resorcinols and the corresponding aldehydes followed by chromatographic separations and recrystallization. Their structures are confirmed by spectroscopic techniques. Ring Closing Metathesis in the presence of Grubbs' catalyst has been used as an efficient approach to synthesize allyloxy resorcinarene in the cone conformation with upper rim allyl substituents. Octaallyl cavitands may undergo conformational changes in all direction, but ring formation of allyl group gives rigid enforced concave cavity to hold neutral molecule in it.

4:30 – 4:50 **Praveen Ramaraju**

"Penicillin bound nanoparticles: A potential way to overcome drug resistance in bacteria"

Penicillin is a beta-lactam antibiotic commonly used for the treatment of bacterial infections. However, antibiotic-resistant bacteria have emerged in hospitals throughout the world that are able to destroy penicillin, and thus cause lethal infections. This resistance is due to the production of beta-lactamase proteins, enzymes which hydrolyze the beta-lactam ring of penicillin to render the drug inactive. We are developing an approach to recover the effectiveness of penicillin through the use of polyacrylate nanoparticles. These nanoparticle penicillins, or nanopenicillins, serve as delivery vehicles that also protect the sensitive drug within its interior, enabling us to rejuvenate these important, life-saving antibiotics for use against dangerous drug-resistant bacteria.

4:50 – 5:10 **William Tay**

"Binding of the Flavonoid Quercetin: Implications in Drug Design toward Prevention and Treatment of Alzheimer's Disease"

Penicillin is a beta-lactam antibiotic commonly used for the treatment of bacterial infections. However, antibiotic-resistant bacteria have emerged in hospitals throughout the world that are able to destroy penicillin, and thus cause lethal infections. This resistance is due to the production of beta-lactamase proteins, enzymes which hydrolyze the beta-lactam ring of penicillin to render the drug inactive. We are developing an approach to recover the effectiveness of penicillin through the use of polyacrylate nanoparticles. These nanoparticle penicillins, or nanopenicillins, serve as delivery vehicles that also protect the sensitive drug within its interior, enabling us to rejuvenate these important, life-saving antibiotics for use against dangerous drug-resistant bacteria.

5:10 – 5:30 **Chien-yi (Erin) Wu**

"Nickel Derivative of Streptomyces griseus Aminopeptidase: The Importance of Metals in Bio-Hydrolysis"

Metalloenzymes are a unique family of enzymes which contain various metal ions involved in catalysis. This unique structural feature allows us to gain further insight into how different metal ions interact with proteins. The aminopeptidase from Streptomyces griseus (SgAP) contain a di-Zn(II) center in the active site. By comparing the native form of SgAP with its di-metal derivatives afford more information about the action of this enzyme, such as substrate specificity. Moreover, further investigation of the metal derivatives will also provide insight into the catalytic promiscuity of this enzyme and its metal derivatives. Thus, we can use SgAP as a model system to gain further understanding about how metal ions change catalytic properties of metalloenzyme.

5:30 **Awards Ceremony**

POSTER EXHIBIT ABSTRACTS

The Barbara and Dean F. Martin Academic Research Experience for Undergraduates Poster Session

(NES First Floor)

1. Kenny Aristide; Alfredo Cardenas
"Computational Study of Folding Pathways of Oxygen Sensing Heme Proteins"

The objective of our research is to determine the conformational changes upon ligand unbinding of the Dos protein of the bacterium Escherichia coli (EcDos). Structurally resolved recently, EcDos is a heme-based signal protein responsible for phosphodiesterase activity. We examined two forms of EcDos, the oxygen-bound form and the deoxy form (Protein Data Bank ID 1V9Z and 1VB6 respectively).
Using Moil9, a molecular modeling software, and specifically the Stochastic Difference Equation in length algorithm (SDEL), we were able to attain trajectories connecting these two forms of the natural protein.
Our present study provides dynamical structure information for the conformational changes of EcDos that the one simply revealed for the experimental static structures. Our results could provide insight as to how exactly this protein transmit signals to other proteins.

2. Kyle Belknap; Monica Elmashat; Saira Gardezi; Matthew Hight; Tiffany Mueller; Tyler Sexton; Kenneth Caswell
"An Antigen-Presenting Device for a Bio-Nano Vaccine"

Traditional vaccines invoke an immune response and establish memory by introducing whole live or weakened pathogens into the body. This effective method is inherently hazardous, especially for weakened or compromised immune systems. This research introduces only the disease-causing vector's signature on antigen-presenting devices. These templates are composed of protein-coated nano-sized particles. Particle size-controlled syntheses allow investigation of the strongest immune recognition and response induction. Surface proteins are strategically modified, which readily attach to surfaces. The vector's identifying tags are presented by binding in surface proteins. Verification and characterization of protein binding will include spectroscopy and antibody assays. Non-cell to cell interactions of the antigen-presenting devices will be investigated for their ability to arm the body with the requisite immune response memory. Effective bio-nano-vaccines can be dried, are not temperature dependent, and can be safely used as cocktails to compensate for particularly virulent viruses (HIV) that rapidly mutate their protein coats.

3. **Kyle Belknap; Monica Elmashat; Saira Gardezi; Matthew Hight; Tiffany Mueller; Tyler Sexton; Kenneth Caswell**
"Metal CdS nanosphere formation in presence of zeolite-like metal organic frameworks (ZMOFs)"

Metal nanospheres have been synthesized in the presence of porous, three-dimensional, zeolite-like metal organic frameworks (ZMOFS). These frameworks are based on the same topology as the corresponding zeolites, but have larger cavities because they substitute the oxygen linkers of rho-ZMOF (the MOF presently in use, which can fit spheres of maximum diameter 18.2 Å) with organic ones.1 Cadmium cations are left to exchange into the anionic rho-ZMOF over a 24-hour period. Particle formation occurs with sodium sulfide addition. UV-visible spectroscopy suggests that cadmium nanoparticles of appropriate size have been formed. Electron microscopy will be used to determine whether the particles have been formed outside or inside the ZMOF. Ideal conditions and ratios of cadmium, sulfide, and rho-ZMOF are being determined for nanoparticle formation within the MOF. Possible applications include but are not limited to technologies that require regularly patterned nanoparticles (such as smart surfaces, biosensors, storage, etc.)

[1] Liu, Yunling, Victor C. Kravstov, Randy Larsen, and Mohamed Eddaoudi. "Molecular Building Blocks Approach to the Assembly of Zeolite-Like Metal-Organic Frameworks (ZMOFs) with Extra-Large Cavities." Chemical Communications (2006). Royal Society of Chemistry. Tampa. 20 Mar. 2006.

4. **Ryan Centko; Bill Baker**
"Possible Biosynthetic Pathways for Isocyanides"

The isocyano functional group (R-NC) is rare in nature and possibly important in cancer treatment research. However, the biosynthesis of marine isocyanides is as of yet unknown to chemists and its occurrence in several bioactive secondary metabolites makes it an important and exciting functional group to study. The particular compounds that are of interest in this study are 9- and 2-isocyanopupuakeanane. A sponge native to Hawaii in the genus Ciocalypta produces these compounds. The sponges were collected and using feeding experiments, chemical markers were added so that possible biosynthetic pathways of the sponge could be discovered.

5. Casey Cosner
"Selective Thiolate Labeling Agents"

Utilizing well-known chemical reactions, a new class of selective thiolate labeling agents have been synthesized. The reaction and class itself is general, allowing for a multitude of fluorescent/UV-active agents to be prepared on a large scale in good yields. The agents prepared react selectively with thiolate even in the presence of alcohols or amine containing nucleophiles.

6. Vedad Delic; Cairns, Amy; Mohamed Eddaoudi
" Metal-Organic Frameworks (MOFs)"

Metal-Organic Frameworks (MOFs) represent an important class of solid crystalline materials. Within recent years, they have gained considerable attention for their applications in catalysis, magnetism, and gas storage. The design strategy of these frameworks focuses on a rational approach utilizing pre-designed molecular building blocks with metal ions and/or clusters linked by organic units. In this project a rigid, multifunctional carboxylate linker was chosen namely, 2,4,6-pyridine-tricarboxylic acid (H3PTC). Its reaction with Ni2+ has permitted the assembly of an extended network, 1. Assembly of second network with Co2+ and the same carboxylate linker was also achieved 2. Characterization of 1 and 2 was done using infrared spectroscopy (IR) and X-ray Powder Diffraction (XRPD); further studies are underway such as sorption properties.

7. Christina Drenberg; Marianne Fatica; Ellen Verdel
"Development of a Quick Field Assay for Africanized Honey Bees based on Africanized Honey Bee Specific Proteins"

The north bound migration of Africanized Honey Bees (AHB) has caused economic and ecological problems in Texas and Florida. Most AHB posses one or more Africanized Honey Bee Specific Proteins (AHBSP) termed A1, A2, and B1. The purpose of this research is to create an ELISA based assay for identification of these bees in the field. Sample proteins from bees in the Tampa area are screened by 2-D gel electrophoresis in order to determine their degree of Africanization. The AHBSP are purified and tested using an assay developed at UT Austin by Dr. Verdel, in which monoclonal antibodies recognize the AHBSP from the Florida bees. Thus far, the research indicates 92% of the tested protein samples are AHBSP. Further research will contribute to the development of a dipstick assay for field identification of AHB in Florida.

8. Andrew Gerges; Tanise Shattock; Michael J. Zaworotko
"The Effect of Solvent and Impurity on the Solid State Synthesis of Polymorphic 2:3 Co-Crystals of Trimesic Acid and 1,2-Bis(4-pyridyl)ethane"

Co-crystals are multiple-component crystals that consist of two or more molecules that are solids under ambient conditions and coexist through intermolecular interactions. Co-crystallization offers attractive opportunities to modify the chemical and/or physical properties of an active pharmaceutical ingredient without the need to make or break covalent bonds. Polymorphism is the existence of more than one crystalline form of a compound. The discovery and selective production of a particular crystalline form is of great industrial relevance, especially in the pharmaceutical industry. The concomitant polymorphic co-crystals of trimesic acid and 1,2-bis(4-pyridyl) ethane exhibit two forms. Form I exhibits (10,3)-a networks that display an unprecedented 18-fold interpenetration whereas Form II exhibits hexagonal networks. The potential impact of solvents and impurities in the context of the solid state preparation and polymorph selection in this system was studied via solvent drop grinding and the addition of a 5% impurity that mimic the co-crystal former. The solvent drop grinding screen involved 16 different solvents that range in polarities. Infrared spectroscopy and powder X-ray diffraction were the primary characterization techniques employed. The result of this study will be presented herein.

9. Edward Gerges; Marian N. Farag; Miranda L. Cheney; Michael J. Zaworotko
"The Effects of Solvent and Impurity on the Solid State Preparation of Imides Utilizing Green Chemistry Techniques"

The emergence of green chemistry has lead to the development of many new synthetic techniques resulting in a reduction of hazardous waste. Solvent-drop grinding has proven to be a novel approach in utilizing green chemistry for the generation of many co-crystals. By applying this technique with a wide range of solvents of various polarities and introducing an impurity, one can study their effects on co-crystal formation. Multiple solvents were employed to initiate the co-crystal formation while a 5% impurity was added to mimic one of the reactants. The impurity was chosen for its ability to potentially generate a co-crystal which, once formed, acts as a catalyst causing the remaining material to form a co-crystal. The mechanism for the condensation reaction that occurs in solution between the primary amine and acid anhydride has been well studied. In the solid state, however, the mechanism is still unclear. It is likely that the condensation reaction occurs in the solid state due to the intermolecular interactions between the acid anhydride and primary amine moieties resulting in imide formation. The material was analyzed using Infrared Spectroscopy and X-ray Powder Diffraction.

10. Glenn Harris; Anne Shearrow; Abdul Malik

" Investigative study on the use of Ionic Liquids as solvents for sol-gel preparation"

A principal problem facing chemical processing involves the replacement of modern environmentally damaging solvents for "greener" and safer solvents in chemical processes. Traditional solvents are harmful to the environment because they are commonly volatile and are used in high quantities. Ionic liquids are thermally stable and have low vapor pressures. These properties lower the environmental and detrimental impacts to human health. Substitution of conventional solvents with ionic liquids will provide a greener form of synthesis while still maintaining the integrity of the sol-gel system. Various ionic liquids were studied to synthesize novel hybrid organic-inorganic sol-gels.

11. Diondra Hill; M. Acevedo-Duncan

"Down regulation of PKC-ι decreases the proliferation of breast cancer cells"

Breast cancers are highly lethal tumors and are one of the leading causes of death among women. The aim of this study was to identify PKC isozymes and cell cycle markers in the breast cancer cell line, MD-468. Additionally, we wished to determine if PKCs are involved in the proliferation of these breast cancer cells. Western blot analysis shows the presence of PKC-ι, α, β1, γ, ε, θ, ζ, μ, δ, η, Cdk7, Cdk2, Parp1, MAT 1, and Cyclin-H in the MD-468 breast cancer cell line. In addition, immunoprecipitation of anti-Cdk7 with rabbit polyclonal shows that PKC-ι is associated with Cdk7 in the MD-468 breast cancer cells. Inhibition of PKC- ι with small interfering RNA (SiRNA) decreased the proliferation of MD-468 cells; thereby suggest that PKC- ι is involved in regulating the proliferation of these breast caner cells.

12. Majdouline Leroy; Bill Baker

"Biological Activity of Three Antarctic Invertebrates"

The sponge Phorbus sp., the tunicate Distaplia cylindrica, and a yet to be classified yellow sponge were collected from the benthos around Palmer Station, Antarctica. In ongoing studies of natural products chemistry of Antarctic invertebrates, these organisms were extracted and subject to bioassay for antibiotic activity and cytotoxic activity. Bioactivity studies will be discussed.

13. William Maza; Audrey Mokdad; Randy L. Larsen
"Photoinduced Intermolecular Electron Transfer Dynamics between Perylenetetracarboxylic Acid and Cytochrome C"

Biological electron transfer (ET) systems are an important area of research considering these reactions play critical roles in cellular respiration, metabolism, photosynthesis, etc. Such ET reactions can occur between cofactors imbedded within a protein matrix with fixed distance and orientation (intra-molecular ET) or between cofactors contained within separate protein complexes (inter-molecular ET). In the case of intermolecular ET, the interface between electron donor/acceptor proteins plays an important role in modulating the reaction. The present study aims to better understand the dynamics involved with the intermolecular transfer of electrons between self-assembled, non-covalent complexes of cytochrome c (Cc) and the probe molecule 3,4,9,10-perylenetetracarboxylic acid (PTCA). PTCA is a chromophoric molecule containing carboxylic moieties at approximately congruent dimensions allowing for electrostatic association with lysine groups forming a docking site located on the surface of Cc. Observing lifetimes, quenching dynamics, calculated and experimental ET efficiency, fluorescence emission and polarization we hope to gain insight into these mechanisms occurring at the PTCA:Cc interface subsequent to photoinduced transfer of electrons affording a biomimetic model of intermolecular ET.

14. Lidija Milisav; Dean F. Martin
"Properties of Nitrilotriacetic Acid (NTA) Condensed with Silica Gel"

Nitrilotriacetic acid (NTA) and silica gel were suspended in toluene and refluxed using a condenser and a Dean-Stark tube. Water was removed by azeotropic distillation, and the progress of the reaction could be followed by noting the volume of water produced. Presumably, the NTA condensed by elimination of water between silica and the carboxyl group and a quadridentate ligand (O,O,N,O coordination) was converted to a tridentate one (O,N,O coordination). The NTA/silica gel weight ratio was varied to obtain an optimum loading value. The properties of the composite are being explored. These include the proton availability, and the ability to remove toxic metal ions from aqueous solutions. Among toxic metals investigated were nickel and copper which have been known to cause health problems such as kidney damage. We are grateful for a generous gift of silica gel from Metre-General, Inc.

15. Theresa Minoudakis; Kristen Wheeler; Ellen Verdel
"Africanization of Honey Bees"

The Africanized honey bee (AHB) poses potential economic, environmental and health problems. They interbreed with local European (EHB) bees and they produce hybrid offspring that possess the characteristics of the Africanized bees, not the gentler European bees. Our research goal is to provide an inexpensive, rapid field
test to accurately identify the Africanized phenotype. This assay is based upon the existence of three Africanized honey bee specific proteins (AHBSP), A1, A2, and B1 that are present in Africanized honey bees and not present in European honey bees. These proteins were isolated using 2-dimensional gel electrophoresis.
These proteins have been used to develop a monoclonal antibody based assay for AHBSP in Texas. We are currently screening bee swarms trapped in the Tampa,
FL area. AHBSP from these bees are being purified for use in testing the existing ELISA and fine-tuning it for use with Florida.

16. Lauren O'Donnell; Dean F. Martin
"REMOVAL OF AQUEOUS ARSENIC USING IRON ATTACHED TO IMMOBILIZED LIGANDS (IMLIGS)"

Lauren O'Donnell, Dean F. Martin(1), Barbara B. Martin(1), and Robert Alldredge (2). (1) IES/Department of Chemistry, University of South Florida, 4202 East Fowler Avenue, Tampa, FL 33620, (2) Metre-General, Inc., P.O. Box 1149, Frederick, CO 80530. Arsenic contamination of groundwater has grown to an international problem due to its toxic and carcinogenic properties. The problem is especially serious in Bangladesh where the use of shallow tube wells is said to have contributed to the "largest mass poisoning of a population in history" (Smith et al., 2002). The present study describes the synthesis of an iron(III) salt of a commercial IMLIG, Octolig®-21, and its use to remove arsenic from aqueous solutions.

17. John O'Leary; Li-June Ming
"Inhibition Studies of Prolidase by Anthracycline Anti-Cancer Drugs"

The proline-specific metalloenzyme prolidase is of considerable biochemical importance in tissue remodeling. The di-Co derivative of Altermonas prolidase serves as a model system for the eukaryotic enzyme in studies pertinent to the side-effects of anti-cancer drugs. Herein we present inhibition studies of di-Co prolidase by anthracyline anti-cancer drugs that shed inshight into the mechanism of the cardiomyopathy side-effects of this class of drugs.

18. Fernando Ortiz; Nicholas Orletsky; Albert Alguadich, Jr.; Joseph White; Noel Dickson

"The PMD Project"

The PMD (p-menthane-3, 8-diol) molecule is a natural product, which is secreted from the Eucalyptus citriodora plant, and is found to inhibit seed germination and successfully repel insects, such as mosquitoes. The overall objective of this experiment is the manipulation of the PMD molecule's functional groups to observe any change in the effectiveness of the molecule as either a seed germination inhibiter or insect repellant. This will be accomplished by simple organic reaction in the laboratory, such as oxidation of the secondary alcohol functional group. These new synthesized molecules will be tested by various methods in the laboratory to see if there are any changes in the overall efficacy of the molecule's aforementioned properties.

19. Jimmy Rodriguez, Jr.; Alfredo Cardenas

"Molecular Simulation of HemAT"

In this study, a molecular simulation of the specific conformational changes associated with ligand binding and unbinding of the protein HemAT will be characterized and analyzed to produce theoretical assistance for further research concerning this protein. Data will be extrapolated from a series of simulations that will utilize characteristics of the protein in its initial and final conformations to see the relationship between this conformational change and signaling processes initiated by the protein.

More explicitly, the molecular simulations conducted will: compute potential energies for the liganded and unliganded forms of the protein, find a global potential energy minimum for these two conformations, find the minimum energy path, further extrapolate characteristics of molecular dynamics, and ultimately find the thermally excited path between the two conformations.

Computational results of this molecular analysis will provide structural insight into the signaling process of HemAT that has been obtained experimentally by other researchers.

20. Mohammed Shafiq; Dean F. Martin
"Extraction of Heavy Metals by Silica Gel Composites with EDTA, NTA, 2-Mercaptoethanol"

Extraction of Heavy Metals by Silica Gel Composites with EDTA, NTA, 2-Mercaptoethanol
Mohammed Shafiq and Dean F. Martin*
Institute for Environmental Studies, Department of Chemistry, University of South Florida, Tampa, FL 33620.

Abstract
Removal of heavy metals will allow elimination of toxic substances from environmental samples or will prevent their introduction into the environment. Silica gel will be used to form a complex with other compounds such as nitrilitriacetic acid (NTA), ethylenediaminetetraacetic acid (EDTA) and 2-mercaptoethanol by an acid catalyzed condensation. Compounds such as NTA were suspended with silica gel in toluene and refluxed using a condenser and a Dean-Stark tube. Water was removed by azeotropic distillation, and the progress of the reaction could be followed by noting the volume of water produced. Presumably, the NTA condensed by elimination of water between silica and the carboxyl group and a quadridentate ligand was converted to a tridentate one (O, N, O coordination). The complex would be used to remove nickel (II) and other metal from standard solutions. Atomic spectrometer would be used to detect the removal of nickel (II) compounds. The complex is expected to remove most of the heavy metals from the solutions. Since, this will be a cheaper alternative to remove metals than the other compounds available in market; it could be used at large scale. We are grateful for a generous gift of silica gel from Metre-General, Inc.

21. Ekta Shah; Bill Baker
"Bioactivity of Antarctic Sponges"

An orange/tan membranous sponge was collected from the benthos around Palmer Station, Antarctica. In ongoing studies of natural products chemistry of Antarctic invertebrates, this organism was extracted and subject to bioassay for antibiotic activity and cytotoxic activity. Bioactivity studies will be discussed.

22. Misbahuddin Syed; Mark McLaughlin

*"*Synthesis of Alpha-Helical Amphipathic Peptides with Links to Anti-cancer Activity*"*

The B-cell lymphoma (Bcl-2) family contains proteins that are comprised of anti-apoptotic and pro-apoptotic members, which in conjunction with the p53, a tumor suppressor protein, decides whether a cell undergoes a programmed cell death or not. Studies indicate that oncogenic mutations induce apoptotic defects through the Bcl-2-dependent pathway.1 The Bcl-xL/Bak BH3 domain complex indicates an improved quality of inhibition and an induction of apoptosis. It is believed that the amphipathic terephthalamide scaffold, a small group of Bcl-xL inhibitors mimics the alpha-helical region of the Bak peptide, thereby inhibiting the anti-apoptotic members of the complex. Recent experiments via multi-step synthetic reactions and verification of the product using NMR analyses have led to progress in the development of these highly amphipathic alpha-helical peptides based on the terephthalamide scaffold to use in anti-cancer studies.

1 Yin, Hang, et al. "Terephthalamide Derivatives as Mimetics of Helical Peptides: Disruption of the Bcl-xL/Bak Interaction." Journal of American Chemical Society 127 (2005): 5463-5468.

23. Phoebe Zito; David J. Merkler

"The PAM catalyzed cleavage of a carbon-sulfur bond"

Peptidylglycine α-amidating monooxygenase (PAM) is a bi-functional copper and zinc dependent protein consisting of two separate catalytic components: peptidyl α-hydroxylating monooxygenase (PHM) and peptidylamidoglycolate (PAL). PHM hydroxylates (adds an -OH group) the α-carbon and PAL cleaves the bond between the carbon and nitrogen releasing the free amide and glyoxylate. The substrates for PAM, in vivo, have the general formula: R-CO-NH-CO2-COOH. The R-groups are either peptides or fatty acids yielding the α-amidated peptide or fatty acid amide hormones with the general formula: R-CO-NH2 and glyoxylates. In order to investigate whether PAM is capable of cleaving a sulfur-carbon bond, we tested thio-acetic acids (R-S-CH2-COOH) as PAM substrates. Oxygen consumption was detected with a number of thio-acetic acids indicating that the enzyme is able to hydroxylate these compounds. Presence of glyoxylate was confirmed through a glyoxylate assay indicating that the reaction proceeded beyond the hydroxylation and that the second step i.e. the S-C cleavage occurred. Further studies will include full characterization of the products of these reactions and the outcome of these studies may provide a better understanding of PAM chemistry to facilitate the rational design of anticancer PAM inhibitors.

Graduate Posters (NES First Floor)

24. Jonathan Belof
"Volume determination of globular proteins by molecular dynamics"

Methods utilizing molecular dynamics in the isobaric/isothermal ensemble have been developed to determine the partial specific volume of globular proteins in solution and provided results that are in quantitative agreement with experiment. The volumetric contributions due to the electrostatic and van der Waals forces, elements that provide insight into the dynamics of protein hydration, are presented. The methodology presented makes the case that analysis of MD trajectories can correlate experimentally-determined volumetric fluctuations with specific conformational states indicative of protein folding events.

25. Amy Cairns
"Assembly of Lanthanide based Metal-Organic Frameworks"

Metal-organic frameworks (MOFs) represent an important class of solid state materials. The design strategy focuses on a rational approach utilizing pre-designed molecular building blocks with metal ions and/or clusters connected by organic linkers. Lanthanide metals are of particular interest because of their ability to achieve higher coordination numbers. The 4-connected rectangular organic linker used in this study is, 3,5-dicarboxyl-(3',5'-dicarboxylazophenyl)benzene (shown below). The building block assembly, characterization, and potential applications of these materials will be shown.

26. Adam Clarke
"Effects of Mutations on the Folding Pathways of a Cold Shock Protein"

Cold shock proteins are a small single-domain protein family with a five-stranded anti-parallel beta-sheet structure. In this work, atomically detailed simulations are used to describe the folding mechanisms of three Cold Shock protein mutants. For each protein, the Stochastic Difference Equation in Length (SDEL) was used to obtain multiple trajectories of 400 slices at room temperature. These trajectories are computed from the unfolded state to the native state as a boundary value problem with the integration step in the arc length. These trajectories are analyzed and compared to study the effect of the mutations on strand-strand interaction, turn formation, and collapse dynamics. Finally these results are compared against recent experimental evidence that suggests a two-state folding path with a rapid collapse.

27. Richard Cross

"Synthesis of IBTZ6PA2: A Potential Acetylcholinesterase Inhibitor with Improved Species Specificity"

In situ click chemistry is a novel target-guided synthesis approach that aims at creating a shortcut in certain aspects of lead discovery applications. It relies solely on the protein target's ability to bind azide and acetylene reagents and hold them together in close proximity until they become connected via the arranged [1,3]-dipolar cycloaddition reaction yielding 1,2,3-triazoles. The concept of in situ click chemistry was initially exploited using the enzyme acetylcholinesterase (AChE). Incubation of AChE with libraries of azides and acetylenes led to the formation of eight tacrine-derived 1,2,3-triazoles, which turned out to be highly potent AChE inhibitors with dissociation constants in the femto- and picomolar range. Although these eight inhibitors have been proven to be the most potent noncovalent inhibitors of AChE to this date, they show a poor species specificity. Detailed binding studies revealed that these eight triazoles show similar inhibitory activity towards mouse, eel and drosophila melanogaster AChE.
Herein we discuss our attempts to design and synthesize a modified tacrine-derived triazole, namely IBTZ6PA2. We anticipate that the affinity of IBTZ6PA2 towards drosophila melanogaster AChE to be significantly higher compared to mouse or eel AChE.

28. Kerrian Greenhalgh

"Mechanical Properties of Biocompatible Smart Films for Burn Wound Applications"

Biocompatible polymer films are of great utility in medical applications, specifically artificial skin for burn wound treatment. Polymer films containing differing ratios of butyl acrylate to styrene and butyl acrylate to methyl methacrylate were polymerized by emulsion polymerization and their physical and mechanical properties were analyzed, as well as their biocompatibility. Mechanical analysis determined that the films are a new form of smart materials that are able to return to ~50% of their nominal geometry after 1000% deformation under uni-axial tensile loads, and 100% of their original geometry after 700% displacement. It was concluded that different percentages of co-monomers, surfactant and initiator result in polymer films with different strengths, yet all retain the same degree of memory. Biocompatibility of the films was established in vitro against dermal fibroblast cells, which allows these smart films to be viewed as a promising new material for numerous biomedical applications.

29. Dijana Lekic

"PHOTOTHERMAL STUDIES OF THE COIL TO HELIX TRANSITION IN POLY-GLU20"

The time-resolved photo acoustic calorimetry (PAC) was used to investigate structural volume (ΔV) and enthalpic (ΔH) changes induced in aqueous solution (light-induced transfer reaction). This experiment consist of two parts. First part of experiment is laser induced pH jump reaction where a proton is photo detached from a photoactivable "caged" compound (o-nitrobezaldehyde (oNBA)) at different pH's (pH=6,7 and 8). Experiment was performed using Nd:YAG laser at λ=355nm It was found that ΔV (pH6)= -7.1 ml/mol, ΔH(pH=6)=-199.4 kcal/mol, ΔV(pH=7)=-2.7ml/mol, ΔH(pH=7)=-140.2 kcal/mol, ΔV(pH=8)=-4.9 ml/mol and ΔH (pH8)=-134.4 kcal/mol.Where, negative electrostricitive volume change indicates contraction of the medium resulting from the salvation of ions. This results in negative oscillation of the signal. Second part of the experiment was to investigate the structural response of carboxylates and polyGlu20 due to the protonation and their early events in acid induced protein folding/unfolding. This proton transfer from oNBA to polyGLu20 manifest itself into neutralization of carboxylates in aqueous solution of PolyGlu20, which removes electrostrictically unfavorable interactions). This neutralization of carboxylates results in expansion of the solution and it is displayed in positive oscillation of the photoacoustic signal (ΔV is positive).

30. Neil McIntyre

"The Imino-Oxy Acetic Acids as Substrates for Peptidylglycine alpha-Amidating Monooxygenase (PAM): Product Analysis, Steady-State Kinetics, and Deuterium Isotope Effects"

Peptidylglycine alpha-amidating monooxygenase (PAM) is a bifunctional enzyme consisting of two catalytically distinct domains, peptidylgycine alpha-hydroxylating monooxygenase (PHM) and peptidylglycine amidoglycolate lyase (PAL). PAM is of interest because of its role in the post-translational bioactivation of ~50% of all known peptide hormones. The two-step PAM reaction begins with a stereospecific copper- and ascorbate-dependent hydroxylation of the alpha-glycyl carbon in a C-terminal glycine extended substrate. The subsequent alpha-hydroxylated product (PHM) undergoes a zinc-dependent dealkylation yielding the alpha-amidated peptide and glyoxylate (PAL).
Among others, the May group has shown a variety of novel substrates for PAM that fail to posses a glycine termini, yet are still able to undergo PAM dependant alpha-hydroxylation. We have investigated both the aldehyde and ketone derivatives of the imino-oxy acetic acids (PhCX(NOCH2C(O)XOH; X=H or CH3) as novel substrates for PAM. Our results show that PAM oxidizes all synthesized analogues to their respective oximes and glyoxylate in a ratio of 1.05 ± 0.14. The stoichiometry of imino-oxy acetic acid oxidation to O2 consumption is 1.06 ± - amidated peptide catalysis, product formation (an oximeα0.07. In contrast to and glyoxylate) appear independent of PAL activity. Our hypothesis is that the

hydroxylated intermediate undergoes a rapid, non-enzymatic dealkylation. Measurement of steady state kinetic isotope effect for alpha-C-H cleavage indicates a steady-state ordered mechanism. These data suggest that O2 binds following the imino-oxy acetic acid, as the D(VMAX/KM)IAA is strongly dependant on the O2 concentration and D(VMAX/KM)oxygen remains constant through variation in IAA concentration.

31. Audrey Mokdad

"Photothermal and transient optical studies of CO binding to HemAT from Bacillus subtilis"

The ligand affinity and dynamics of a recently discovered aerotaxis heme proteins HemAT-Bs is described. This protein reversibly binds carbon monoxide resulting in a shift in the Soret band. The kinetic difference spectrum of the photolyzed minus unphotolyzed protein is significantly red-shifted relative to the equilibrium deoxy minus CO-bound spectrum. The rate of CO recombination (1.3x105M-1s-1) is found for HemAT-Bs relative to horse heart myoglobin (4.7x105M-1s-1). Using these rate constants along with the corresponding CO-dissociation rate constants the equilibrium constants for CO binding are found to be 1.4x106M-1 for HemAT-Bs which is similar to that of horse heart myoglobin (7.6x106M-1). Results of PhotoAcoustic calorimetry (PAC) studies demonstrate an increase in the molar volume (17mL.mol-1)and an enthalpy change (-33kcalmol-1) upon photolysis <50ns. Unlike other sensors FixL, EcDOS), no longer timescale dynamics are observed in PAC. These studies demonstrate that the dynamics associated with ligand dissociation are distinct between different classes of oxygen sensing proteins.

32. Divya Ramamoorthy

"Preparation of Small molecule inhibitors of BCl-XL-Bax"

Inhibiting the interaction of two proteins by a small organic molecule remains a challenging objective in chemical biology. The BCl2 family of anti-apoptotic proteins confer a survival advantage to many cancer cells. The ability of a cell to undergo apopotosis can be restored by binding of the BCl2 peptides to BH3 pro-apoptotic binding partners. This anticancer response can be mimicked by small drug-like molecules that effectively act as BH3 peptide surrogates.

We will describe the combinatorial synthesis of a small array of substituted isoquinolines that are potential inhibitors of the BCl-XL-Bax interaction. We will demonstrate that a versatile drug-like scaffold can be prepared rapidly by adapting an old isoquinoline synthesis. We show that microwave assisted synthesis is ideal for the rapid construction of this class of heterocycle. The library has been designed to be appropriate for screening against a number of other cancer related targets.

33. Kevin Revell

"N-Alkylthio beta-lactams Inhibit the Growth of Methicillin-Resistant Staphylococcus aureus (MRSA) through a Novel Mode of Action Involving Type II Fatty Acid Synthesis"

Recent work in the Turos group has focused on the development of N-alkylthio beta-lactams, which show antibacterial activity against Staphylococcus (including MRSA), Bacillus, and others. These compounds do not function in the manner of the traditional beta-lactam antibiotics, but were thought to undergo an intracellular thiol-transfer to coenzyme A. Although CoA acts as the thiol-redox buffer in the genera most susceptible to the N-alkylthio-beta-lactams, studies on Coenzyme A disulfide reductase (CoADR) show that the redox buffer is not affected by these compounds. However, the recent finding that fatty acid synthesis is affected by the N-alkylthio beta-lactams led to the discovery that these compounds act as prodrugs, and that the asymmetric CoA disulfides produced by intracellular thiol transfer are potent inhibitors of beta-Ketoacyl-acyl carrier protein synthase III (FabH) through a novel thiol-disulfide exchange with the active site cysteine.

34. Emily Rowland

"Catalytic Asymmetric Imine Amidation"

Bronsted acid catalysts were used to promote the addition of amides to Boc-protected imines. A wide range of amides and sulfonamides were utilized in the reaction to provide high yields of the aminal products (up to 99%). A chiral phosphoric acid derived from VAPOL was used in the addition of sulfonamides to imines resulting in the formation of aminal products with up to 99% yield and 99% enantioselectivity.

35. Dorina Sava

"Molecular-building block approach for the design and synthesis of MOFs"

The quest for improving the properties of materials has been enhanced in recent years by conducting intense studies for the synthesis of hybrid organic-inorganic materials, in which case the cumulative effects emerging from both components can be taken advantage of. Metal-Organic Frameworks (MOFs) are a subset of this new class of compounds hold great promise for applications in gas storage, ion exchange, catalysis, separation and molecular magnetism. Herein we describe the synthesis and characterization of novel structures derived from thiophene-based carboxylic acids coordinated to metal centers. There are highlighted differences and resemblances between networks obtained from very similar starting reagents. The unique character of this work includes the frameworks' unprecedented or rare topologies, as well as interesting magnetic properties that could favor potential applications in the area of molecular magnetism.

36. Anne Shearrow

"Microchip-based electrochromatography system with sol-gel stationary phase to study physiological processes at the skin-interface"

The objective of the proposed research is to develop an integrated microchip-based electrochromatography (μ-EC) system utilizing the attributes of microelectromechanical systems (MEMS) and sol-gel technology. The novel idea underlying the goal is to use the μ-EC to separate and quantify chemical/biological species quickly and efficiently at the outermost layer of the skin. Towards this goal novel biocompatible poly (ethylene glycol) (PEG) sol-gels have been developed and studied. These sol-gels employed non-traditional solvents, and they have been optimized for their use as stationary phases in the u-EC. The separation ability of these sol-gel PEG stationary phases will be tested using typical sweat components from an artificially prepared sweat-like solution. A glass chip will serve as the u-EC. Microfluidic channels of multiple configurations have been etched in glass. Once the etching process is optimized, the novel sol-gel PEG stationary phase will be loaded into the micro channels.

37. Hla Win

"Role of Atypical Protein Kinase C-iota in Prostate Cancer Cell Cycle, Proliferation, and Apoptosis"

Prostate cancers are highly lethal tumors and, excluding skin cancers, is the leading type of cancers among men in the United States. It's been well documented that protein kinase C (PKC) play a critical role in cell survival, differentiation, proliferation, and cell polarity. However, the role of PKC-iota (PKC-i) in prostate cancer is largely unexplored. We hypothesized that PKC-i plays a critical role in cell proliferation and cell survival in prostate cancer cells. We found that in malignant cancer cells such as in the androgen-dependent prostate cancer cell line, LNCaP and androgen independent prostate cancer cell line, DU145 there is an overexpression of PKC-i compare to normal prostate cells, RWPE-1. In normal prostate cells, RWPE-1, PKC-i is associated with cyclin dependent kinase activating kinase (CAK/cdk-7). Cdk7 contributes to the cell cycle progression as part of the trimeric CAK complex that phosphorylates and activates cdk-2/cyclin A to ensure the G1/S transition. Treatment of RWPE-1 cells with PKC-i short interference RNA (siRNA) reduced cell proliferation and resulted in decreases in phosphorylation of phospho-cdk2 (p-cdk2; Ther160). Similar to normal cells, PKC-i temporally associated with CAK/cdk7 at 30 hours post serum addition in LNCaP cells but not in DU145. However, both LNCaP and DU145 undergo apoptosis when treated with PKC-i siRNA. In DU145, PKC-i siRNA treatment provokes cytochrome C release from mitorchondria into the cytoplasm leading to Caspase activation followed by poly (ADP-ribose) polymerase (PARP) cleavage and apoptosis.

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Amendment

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In addition, we would like to acknowledge all of the judges for their wisdom and guidance in selecting today's most outstanding presentations. Again, we want to graciously thank our plenary speaker, Dr. William Wulff, for agreeing to present at this year's conference, and Dr. Jon Antilla for his help in making it possible.