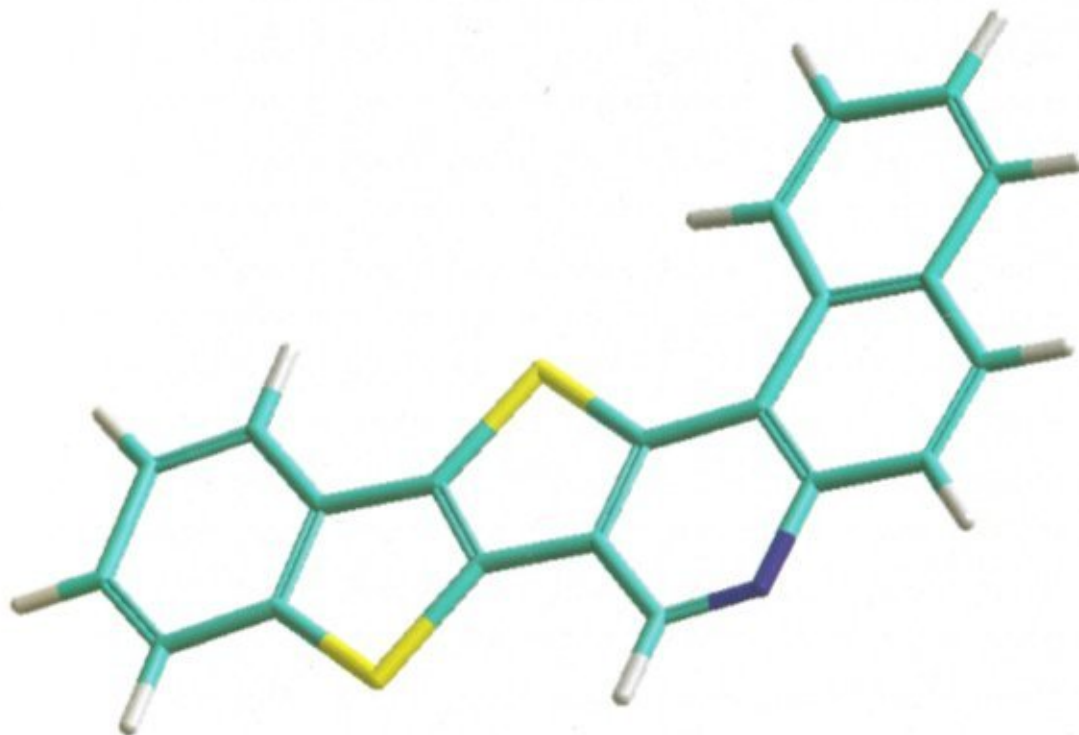


Seventh Annual Raymond N. Castle Student Research Conference



**University of South Florida
Department of Chemistry**

2009



ACS
Chemistry for Life™

Tampa Bay Local Section

Welcome

Dear Colleagues,

Welcome to the Seventh 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, 6-aminobenzo[b]naphtho[2,1-d]thiophene.

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 are especially proud of the research done by all the students in the department both graduate and undergraduate. Our department hosts over seventy undergraduate students conducting research in all disciplines of chemistry, accounting for over ten percent of students performing undergraduate at the university. We encourage everyone to take advantage of this opportunity and attend both the poster and oral presentations, especially our plenary speaker Dr. John Shelnut. We thank Dr. Shelnut for visiting us and speaking at the conference.

Lastly, we would like to personally thank all of the members of the Chemistry Department involved for their help on this year's event, particularly Drs. Jon Antilla, Patricia Muisener, and Dean Martin for helping to coordinate the Castle Conference. In addition, any conference could not be successful without financial support, and as such we are grateful to the Tampa Bay Section of the American Chemical Society and the University Of South Florida College Of Arts and Sciences and our sponsors and affiliates 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 we hope you enjoy the Sixth Annual Raymond N. Castle Student Research Conference.

Sincerely,
The Castle Conference Committee

Raymond N. Castle Research Conference Committee

Faculty Advisors:

Dr. Jon Antilla
Dr. Patricia Muisener

Chair:

Jason Cuce

Committee Members:

Michelle Cortes-Salva
Sumit Handa
Rosemary Persaud
Chung Sik Kim
Wai Sheung Ma
William Maza
Carissa Vetromile
Meagan Small
Christi Young

Web Support:

Tony Green

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We would like to thank our sponsors and affiliates.

Schedule of Events

Saturday, April 18th, 2009

Time	Event
8:00 – 8:45 A.M.	Welcome Session - Registration and Breakfast NES Lobby
8:45 – 9:00 A.M.	Castle Conference Introduction CHE100
9:00 – 11:15 A.M.	Morning Session – Oral Presentations (Graduate Students) CHE100
11:30 A.M. – 12:30 P.M.	Plenary Speaker – Dr. John Shelnett CHE100
12:30 – 2:15 P.M.	Poster Session – Posters and Lunch NES First Floor Hallway and Classrooms
2:30 – 5:15 P.M.	Afternoon Session – Oral Presentations (Graduate Students) CHE100
5:30 P.M.	Awards Ceremony CHE100

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.

Plenary Speaker – John Shelnut



Dr. John Shelnut, earned his Bachelor's degree in physics from the Georgia Institute of Technology. He then went on to obtain his Master's and Doctoral degrees, also from Georgia Institute of Technology, in 1971 and 1975, respectively. After earning his Bachelor's, Dr. Shelnut served as a Systems Analyst at the Naval Weapons Center in China Lake, CA. Upon completion of his Ph.D., he became a Research Assistant Professor at the Georgia Institute of Technology, and was a Consultant for AT&T Bell Laboratories. In 1979, he joined Sandia National Laboratories, where he remains a Distinguished Member of Technical Staff. He has also been a Professor of Chemistry at the University of New

Mexico from 1989 to 2002, and is currently an Adjunct Professor of Chemistry at the University of Georgia. During his time at Sandia, he has received numerous awards, including 6 Sandia National Laboratories Awards for Excellence.

Dr. Shelnut's current research interests include:

- Solar energy and electronic applications of porphyrin nanotubes and other porphyrin nanostructures.
- Photocatalytic growth of metal and semiconductor nanostructures and nanostructured materials.
- Molecular mechanics and quantum chemical theoretical methods applied to designing molecular optical switches, catalysts, photomediators, chemical sensors, and nanostructured materials.
- Fundamental studies of tetrapyrrole-containing proteins using computational and experimental methods, in particular, molecular mechanics, Normal-Coordinate Structural Decomposition (NSD), and resonance Raman spectroscopy.
- Experimental and theoretical studies of basic photophysical processes in biomolecular systems and their biomimes; theory of vibronic molecular states and resonance Raman scattering.

Dr. Dean F. Martin, Special Thanks



Dean F. Martin is Distinguished University Professor Emeritus 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 endowed six chemistry funds, including 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. 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.

Session Schedule

Graduate Talks Morning Session (CHE100)

Session Chair: William Maza

8:45-9:00 AM Introduction

9:00-9:15 AM **Wai Sheung Ma**

“Norselic Acid A-E, Five New Anti-Leishmanial Steroids Isolated From Antarctic Sponge Crella sp.”

9:15-9:30 AM **Jason Cuce**

“Mass Spectrometry Screening for Palmerolide A in Cultures of Synoicum adareanum”

9:30-9:45 AM **Xue Xu**

“Donor-Acceptor Carbene Transfer Reaction on Cyclopropanation towards electron deficient olefins”

9:45-10:00 AM **Michelle Cortes-Salva**

“A Novel Route for the Synthesis of N, N’-Disubstituted Guanidines using Copper Catalyzed Cross Coupling Reactions”

10:00-10:15 AM Break

10:15-10:30 AM **Jeremy Beau**

“Drug Discovery from Floridian Mangrove Endophytes”

10:30-10:45 AM **Shawn Larson**

“The Organocatalytic Ring-Opening of Aziridines”

10:45-11:00 AM **J. Alan Maschek**

“Isolation of Protein with Strong Anti-Influenza Activity from the Antarctic Red Marine Algae Gigartina skottsbergii”

11:00-11:15 AM **Chungsik Kim**

“Stereoselective Synthesis of Expoxides from Diazoacetates via Ylide Intermediates using Co(III)corroles”

11:30 AM Plenary Speaker- Dr. John Shelnutt

12:30 PM Lunch/Poster Session

Graduate Talks Afternoon Session (CHE100)

Session Chair: Meagan Small

2:30-2:45 PM **Emma Farrel**

“How the body makes primary fatty acid amides”

2:45-3:00 PM **Christi Young**

“Molecular Dynamics Simulations of the Influenza A Non-structural Protein 1 (NS1) RNA Binding Domain”

3:00-3:15 PM **Justin Moses**

“Catalytic Promiscuity of SgAP and the Potential for Decontamination”

3:15-3:30 PM **Brent Hilker**

“Electric Field Enhanced Sample Preparation for Synthetic Polymer MALDI-TOF Mass Spectrometry via Induction Based Fluidics (IBF)”

3:30-3:45 PM **Ramakanth Ananthoji**

“Controlled Drug Delivery in Novel Zeolite-net-like Metal-organic Frameworks (rho-ZMOFs) - Hydrogel Composites”

3:45-4:00 PM Break

4:00-4:15 PM **Alaa Hashim**

“Oxidative Activities of Catalytic Metallopeptides”

4:15-4:30 PM **Roger Bass**

“Polymer-Carbon Nanotube Interface within Shape Memory Polymer”

4:30-4:45 PM **Sumit Handa**

“Synthesis and Photophysical Studies of Photocaged N-Protected Glycine for Peptidyl α -Amidating Monooxygenase (PAM)”

4:45-5:00 PM **Mohamed H. Alkordi**

“Insight into the Directed Assembly of Metal–Organic Materials”

5:00-5:15 PM **Zhenming An**

“Amidated Peptides Found in Mouse Pituitary Cell Line ATT-20 Using a New Mass Spectrometry Based Screening Method”

5:30 PM Awards Ceremony

The Barbara and Dean F. Martin Poster Session (NES First Floor)

Graduate Posters (NES North Hallway)

P-1. **Meghanath Gali and Kirpal S. Bisht**

“Enantioselective Synthesis of Phosphodiesterase Inhibitor Rolipram via Enzymatic Desymmetrization”

P-2. **Laura Anderson , MingZhou Zhou, Vasudha Sharma, Jillian McLaughlin, and Mark L. McLaughlin**

“Design, Synthesis, and Bioactivity of Non-peptidic α -Helix Mimetics”

P-3. **Parul Jain, Selma Hokenek, Julie Harmon, and Norma A. Alcantar**

“Characterization of Transparent Conducting Films for Vapor Sensors”

P-4. **Mike McIntosh and Xiao Li**

“Enhancing Quantitative Measurements of Traditional Electrochemical Techniques by Employing Ultramicroelectrodes for the Detection of Biomolecules”

P-5. **Deniz Ozer and Serpil Takaç**

“Effects of Solvent Type, Aqueous Phase/Solvent Volume Ratio and Temperature on the Hydrolytic Activity of Candida rugosa Lipase in a Biphasic Medium Designed for S-Naproxen Production”

P-6. **Mu-Seong Kim and Julie Harmon**

“Effect of Silica Nanowire on Dielectric Properties of Polyurethane Composite”

P-7. **Katherine Parra and Alfredo Cardenas**

“Conformational Changes and Ligand Behavior after CO Dissociation of the Oxygen Sensor bjFixLH: a Study by Molecular Dynamics”

P-8. **Sai Lakshmana Vankayala, Anthony E. Pegg, Wayne C. Guida, Gary T. Pauly, Natalia Loktionova, and Qingming Fang**

“Computational Correlation Studies Towards Inactivation of O6-alkylguanine-DNA Alkyltransferase by O6-benzylguanine Analogs”

P-9. **Matt D. Lebar, Sridevi Ankisetty, and Bill J. Baker**

“A Synthetic Study of Meridianin A and Psammopemmin A, Pyrimidine Containing Indoles from Antarctic Marine Invertebrates”

P-10. **Maryam Babaie and Hassan Sheibani**

“Synthesis of Novel Fused Heterocycles by High surface area MgO as a highly effective heterogeneous base catalyst”

P-11. Daniel N. Santiago, Wesley H. Brooks, MinhPhuong Tran, Ashley A. Tillette, Robin Scherer, Shen-Shu Sung, Kenyon G. Daniel, and Wayne C. Guida
“Virtual Counter Screening: Recycling of Old Molecules for New Uses”

P-12. Butch Knudsen and Julie Harmon
“The Functionalization and Dispersion of Nanotubes in Poly (4-methyl-1-pentene)”

P-13. Kurt Van Horn and Roman Manetsch
“Templated Assembly of DNA Fragments via Complimentary Reactive Functionalities”

P-14. Sebastian Gutmann, Matthaeus A. Wolak, Martin M. Beerbom, and Rudy Schlaf
“Effect of UV and X-ray Radiation on the Work Function of Nanocrystalline TiO₂ Thin Films”

P-15. Shikha Mahajan, David Merkler, and Roman Manetsch
“Synthesis of Biotinylated Azido-Adenine-Ribose Derivatives: Potential Activity-Based Protein Profiling Probes”

P-16. Seongmin Hong and Xiao Li
“SERS Detection of Dopamine”

P-17. Arun Babu Kumar and Roman Manetsch
“Development of a Labeling Probe for the Discovery and Identification of Saccharide-Binding Proteins”

P-18. Ranjani Muralidharan and Xiao Li
“Study of the Electrooxidation of Formic Acid and Methanol”

Undergraduate Posters – Organic Chemistry (NES 103)

- S-1. **John Markantonis, Ruizhi Wu, and Kirpal Bisht**
“Stereo-controlled Synthesis of Organic Molecules”
- S-2. **Hiondy Polanco, Yuxue Liang, Gajendra Ingle, and Jon C. Antilla**
“Organocatalytic Asymmetric Addition of Diphenylphosphine Oxide to Imines”
- S-3. **Beata Kaminski and Ted Gauthier**
“Synthesis and Characterization of 1400W and 1400W-azide”
- S-4. **Mario Martinez and Roman Manetsch**
“LC/MS–Based Drug Discovery: Fragment Screening for the Development of Potential Bcl-XL Protein-Protein Interaction Modulators”
- S-5. **Kristopher Hahn, Matt Lebar, and Bill J. Baker**
“Synthesis of the C16 – C25 Portion of Palmerolide A”
- S-6. **Petoria Gayle, Sameer Kulkarni, Xiangdong Hu, Hong-Gang Wang, and Roman Manetsch**
“Protein-Protein Interaction Modulators & Role of Target Guided Synthesis”
- S-7. **Joseph Gill, Chungsik Kim, and X. Peter Zhang**
“Design and Synthesis of Chiral Corroles”
- S-8. **Corey Garvin, Michelle Cortes-Salva, and Jon C. Antilla**
“Copper Catalyzed Reactions of Amidines”
- S-9. **Erin Coke, John Struss, Eleanor Clements, and Martha Bromfield**
“A Green Bromination/Oxidation Reaction – The Conversion of Simple Non-Aromatic Heterocycles to Lactones, Lactams and Thiophenones”
- S-10. **Charles Myers, Meghanath Gali and Kirpal S. Bisht**
“Synthesis of A Prochiral Diol, 2-(3'-cyclopentyloxy-4'-methoxy phenyl)propyl-1,3-diol, for Enzymatic Desymmetrization”
- S-11. **Sahir Quraeshi, Sridhar Kaulagari, Priyesh Jain, and Mark Mclaughlin**
“PNAs: Structure, Synthesis, and Application”
- S-12. **Kirk McDoneld, Pasha M. Khan, and Kirpal S. Bisht**
“Pd catalyzed Allylic Alkylation- Application Towards Synthesis of New Anti-HIV and Anti-viral Carbocyclic Nucleosides”
- S-13. **Cynthia Lichorowic and Edward Turos**
“Water Soluble N-Thiolated β -lactam Antibacterials”

Undergraduate Posters – Analytical Chemistry (NES South Hallway)

- A-1. **Lieu Huynh, Fang Li, and Abdul Malik**
“Pre-concentration and Analysis of Haloacetic Acids in Drinking Water”
- A-2. **Nicole Rubin and Dean Martin**
“A Study of Copper Complexes Associated with Cuprilig Synthesis”
- A-3. **Maria Parra, Fang Li, and Abdul Malik**
“Sol-Gel Capillary Macroextraction”
- A-4. **Farzana Shaik, Mike McIntosh, and Xiao Li**
“Establishing Quantitative Parameters for the Electrochemical Detection of Curcumin using Platinum Ultramicroelectrodes”
- A-5. **Jessica Hoffman, Scott Segro, and Abdul Malik**
“Quantitative Analysis of Oligonucleotide Class Compounds via Sol-Gel CME-HPLC”
- A-6. **Frederick Stull and Dean Martin**
“A Comparison of the Ease of Separation of Sulfate, Phosphate, Nitrate, and Nitrite from Aqueous Solutions using Octolig®”
- A-7. **Ronelle Bailey, Minhphuong Tran, and Abdul Malik**
“Extraction of Biomolecules Using Silica-based Sol-gel Coated Fused Silica Capillaries”
- A-8. **Karin Thatcher and Dean Martin**
“Effect of Octolig® Treatment on the Growth of Lyngbya Majuscula”
- A-9. **Judy Triplett, Scott Segro, and Abdul Malik**
“Tri-block Copolymer/Germania Sol-gel Coating for HPLC-CME”
- A-10. **Agnes Prospere, S. Hong, and Xiao Li**
“Synthesis of Silver And Gold Colloidal Solutions for Use in Surface Enhanced Raman Spectroscopy (SERS)”
- A-11. **Darius Wynn and Dean F. Martin**
“Separation of Aqueous Borates with Octolig and Selected Metalloids”
- A-12. **Tarik Elmohd, Carey Boudreau, Erica Turner, and Abdul Malik**
“Sol-gel Germania Sorbents for Capillary Microextraction On-line Coupled to Gas Chromatography”
- A-13. **Christopher Lee Lizardi and Dean F. Martin**
“Selenium Removal Through the Use of Octolig and Its Copper (II) Derivative Cuprilig”

A-14. **Christopher Cook, Fang Li, and Abdul Malik**
“Sol-Gel Column Technology”

A-15. **Bryan Vo and Dean Martin**
“Removal of Fluoride from Drinking Water using Octilig®”

Undergraduate Posters – Biochemistry, Polymer, Physical, and Computational Chemistry (NES 104)

- B-1. Arjun Rammohandas, Peguy Gaboton, and My Lien Dao**
“Biochemical Detection of Microsporidemia”
Cell Biology, microbiology, molecular biology, University of South Florida
- B-2. John Rodriguez, Dean F. Martin, and Ted Gauthier**
“Mathematical Treatment to the Production of TAGs by A Green Alga, Chlorella Vulgaris”
- B-3. Revika Matuknauth, Gabriela Wright, Haikou Bian, Steve Enkemann, Bernadette Sosa, Pedro Santiago and Doug Cress**
“Transcriptional Repression of the Ret Oncogene by RB”
- B-4. Mary Falatek, Courtney Duboulay and Wayne C. Guida**
“Computational Studies of MDM2 Interactions”
- B-5. Felipe O. Cameroamortegui, Muna H. Barazanji, Emma K. Farrell and David J. Merkler**
“GC-MS of Primary Fatty Acid Amide Metabolites from Mammalian Cell”
- B-6. Emma Kathleen Carter, Carissa Vetromile, and Randy W. Larsen**
“Towards the Formation of Novel Hybrid Biological Metal Organic Materials”
- B-7. Sibel Demirel, Ruben Durand, Daniel Leyva, Mrunal Tailor, Vasiliki Lykourinou, and Li-June Ming**
“Cu(II)-Bound Copolymers as Catalysts in Oxidation of Catechols and Oxidative DNA”
- B-8. Timothy Backus, William A. Maza, and Randy W. Larsen**
“Synthesis, Structure, and Characterization of A New Crystal Involving a 4,4'-bipyridine Dimer and p-aminobenzoic Acid”
- B-9. Isaac Dodd, Jason Cuce, and Bill J. Baker**
“Systematic Management of Research Data Using a Relational DBMS”
- B-10. Amanda Preece, Parul Jain, and Julie Harmon**
“Conductive Polymer Films”
- B-11. Christian Cioce, Jon Belof, Brian Space, and X. Peter Zhang**
“Determination of the Reaction Mechanism of Cobalt-Catalyzed Asymmetric Z-Cyclopropanation of Alkenes via Quantum Computation”

B-12. George Rhoden, Christi Young, and Alfredo Cardenas

“A Study of the Influenza A Virus Non-structural Protein 1 (NS1) RNA Binding Domain in A Water Box using the NAMD Program for Molecular Dynamics”

B-13. Pamela Castro, Brent Hilker, and Julie Harmon

“Characterization of Polymers”

Undergraduate Posters – Inorganic and Natural Products Chemistry (NES 108)

I-1. **Rosemary Persaud, Jaime H. Noguez, Tina S. Mutka, Dennis E. Kyle, and Bill J. Baker**

“The Chemical Investigation of Antarctic Marine Organisms for Anti-Malarial and Anti-Leishmanial Compounds”

I-2. **Jennifer Drozd, Catherine Geiser, and Mike Zaworotko**

“Melatonin Co-crystals”

I-3. **Lisha Luttenton, Matt D. Lebar and Bill J. Baker**

“Accumulation of Vanadium, Manganese, and Nickel in Antarctic Tunicates”

I-4. **Kevin Dubois, Jason A. Perman, and Michael J. Zaworotko**

“Synthesis and Characterization of a Series of Isostructural Metal-Organic Frameworks”

I-5. **Ryan Baker, Jackie Salm, Samantha Landolf, Roberto Lopez, Tiffany Lanham, Minh Cong Nguyen, Anangamanjari Pedapudi, Michele Summerville, Hoangmy Chau, Elisa Herrera, Matt Lebar, Charles Harter, Tina S. Mutka, Dennis E. Kyle, and Bill J. Baker**

“New Malarial Drugs; Screening Microbes to Treat Malaria”

I-6. **Mary-Ellen Edmiston, Hiren Shah, Mohamed Alkordi, and Mohamed Eddaoudi**

“A Zeolite-like Metal-Organic Framework as a Platform for the Oxidation and Epoxidation of Alkenes”

I-7. **Garrett Craft, Wai Sheung Ma, Tina Mutka, Dennis Kyle, and Lilian L. P. Vrijmoed, and Bill J. Baker**

“Anti-Malarial Bioassay Guided Fractionation of Hong Kong Endophytic Fungal Extracts”

I-8. **Alyssa Kennedy, Heather Clarke, and Michael J. Zaworotko**

“Designing Cocrystals using the Carboxylate-phenol Supramolecular Heterosynthon”

I-9. **Emily E. Mevers, Rebecca J. Gridley, John A. Maschek, Nerida G. Wilson, Sydney K. Pierce, James B. McClintock, Charles D. Amsler, and Bill J. Baker**

“A Chemical Investigation into Austrodoris Kerguelenensis, an Antarctic Nudibranch and Elysia Clarki, A Saccoglossan from the Florida Keys”

I-10. **Hiren Shah, Mary-Ellen Edmiston, Mohamed Alkordi, and Mohamed Eddaoudi**

“Zeolite-like Metal-Organic Frameworks: Platforms Encapsulating Lewis Acid Catalysts”

I-11. Franka Co, Uma Hannubal, Jackie Wood, Natalie Wright, Jeremy Beau, and Bill Baker

“Drug Discovery from Floridian Mangrove Endophytes”

I-12. Nicholas Zoumberos, Ryan Luebke, and Mohamed Eddaoudi

“Targeted Synthesis of Metal Organic Frameworks Featuring Single-Ion Molecular Building Blocks”

Session Abstracts
Saturday, April 18th, 2009

Graduate Talks Morning Session (CHE100)

O-1 9:00-9:15 AM

Wai Sheung Ma¹, Bill J. Baker¹, Dennis Kyle¹, Brian Vesley¹, James B. McClintock², and Charles D. Amsler²

“Norselic Acid A-E, Five New Anti-Leishmanial Steroids Isolated from Antarctic Sponge Crellasp.”

¹Department of Chemistry and Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida, Tampa, FL 33620,

²Department of Biological Science, University of Alabama at Birmingham, Birmingham, AL 35294

Five new steroids, norselic acid A-E (1-5), were isolated from *Crella sp.* collected in Antarctica. The structures of the norselic acids were established by NMR and MS. The absolute stereochemistry of norselic acid A was elucidated by SXRD. The antimicrobial and anti-leishmania activities of norselic acid A have been studied. Compound 1 displays antimicrobial activities against methicillin-resistant *S. aureus* (MRSA), *S. aureus*, *E. faecium*, and *C. albicans*. Compounds 2-5 exhibit mild antimicrobial activities. Compounds 1-5 exhibit strong cytotoxicity against leishmania.

O-2. 9:00-9:15 AM

Jason Cuce¹, Christian S. Riesenfeld², Alison E. Murray², and Bill J. Baker¹

“Mass Spectrometry Screening for Palmerolide A in Cultures of Synoicum adareanum”

¹Department of Chemistry and Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida, 4202 E. Fowler Ave, Tampa, FL 33620,

²Division of Earth & Ecosystem Sciences, Desert Research Institute, 2215 Raggio Parkway Reno, NV 89512

Palmerolide A, a polyketide macrolide from the Antarctic tunicate *Synoicum adareanum*, is selectively cytotoxic toward melanoma in vitro. Due to the remote location of the source organism, resupply of palmerolide A for preclinical or clinical development could be hampered. Therefore, we have undertaken a study of the microbial component of *S. adareanum* to search for a potential renewable producer. Toward this goal, selected bacterial isolates have been obtained and cultivated using a variety of microbiological conditions. The cultures have been analyzed by liquid chromatography/mass spectrometry for the presences of palmerolide A. This paper reports the findings of these analyses.

O-3. 9:15-9:30 AM

Xue Xu and Peter Zhang

“Donor-Acceptor Carbene Transfer Reaction on Cyclopropanation towards electron deficient olefins”

Department of Chemistry, University of South Florida

Use metal catalyzed carbene transfer reaction on cyclopropanation was commonly used as a efficient way to synthesis three member ring structure, however electron deficient olefin is still an undeveloped embranchment due to the electrophilic nature of the metal-carbene intermediates in the catalytic cycles. Cobalt (II) carbene, because of its unique radical character, shows high reactivity toward electron deficient olefin. It was proposed that, increase the electron density on the carbene center will further enhance the reactivity.

O-4. 9:45-10:00 AM

Michelle Cortes-Salva¹, Adam Behensky², Craig Ajmo², Keith Pennypacker², Javier Cuevas², and Jon Antilla¹

“A Novel Route for the Synthesis of N, N’-Disubstituted Guanidines using Copper Catalyzed Cross Coupling Reactions”

¹Department of Chemistry, University of South Florida

²Department of Molecular Pharmacology and Physiology, College of Medicine, University of South Florida

Our research involves the development of guanidine analogues to be used as therapeutic agents for the treatment of ischemic stroke. The synthesis of guanidines uses a copper-catalyzed cross coupling reaction between an inexpensive guanidine salt and substituted aryl iodides. Ligand studies have shown that the presence of N,N'-diethylsalicylamide has a dramatic effect on the overall reaction yields. Electron donating aryl iodides gave the highest yields for the cross coupling reaction. After the synthesis of various symmetrical guanidines was accomplished by this new methodology, sigma receptor studies on cortical neuron cells were performed. Our preliminary results show that N, N'-di-*p*-bromophenyl guanidine (*p*-BrDPhG) exhibited a higher Ca⁺² inhibition than the current therapeutic agent N,N-di-*o*-tolyl guandine (*o*-DTG). Middle cerebral occlusion tests were performed on rats. Subsequent injections of *p*-BrDPhG at 24, 48, and 72 hours proved to reduce the ischemic volume in the brain more effectively than *o*-DTG.

O-5. 10:15-10:30 AM

Jeremy Beau and Bill Baker

“Drug Discovery from Floridian Mangrove Endophytes”

Department of Chemistry, University of South Florida

Recent studies have shown that within the leaves, bark, roots and seeds of mangroves exist 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 drug candidates. A collection of endophytes from Floridian mangroves is currently being developed. The microorganisms are cultured in the laboratory and then screened against various illnesses such as cancers, infectious diseases and common pathogenic microbes. This paper reports on the results of the active extracts and fractions.

O-6. 10:30-10:45 AM

Shawn Larson and Jon Antilla

“The Organocatalytic Ring-Opening of Aziridines”

Department of Chemistry, University of South Florida

In the field of asymmetric organo-catalysis, Chiral Brønsted Acids are an emerging tool for the synthetic organic chemistry. Enantioselective reactions to produce two neighboring chiral centers simultaneously have been found to be effectively catalyzed by Chiral Brønsted Acids. The reaction of thiophenol with aziridines can be catalyzed by a Brønsted acid catalyst in this manner. Aromatic thiols show excellent selectivity over a wide range of substitutions including electron withdrawing groups, electron donating groups and steric hindrance. Currently we have 14 examples of thiol nucleophiles ranging from 84 to 99 percent Yield and 80 to 96 percent enantiomeric excess.

O-7. 10:45-11:00 AM

J. Alan Maschek¹, Cindy Bucher², Alberto van Olphen² and Bill J Baker¹

*“Isolation of Protein with Strong Anti-Influenza Activity from the Antarctic Red Marine Algae *Gigartina skottsbergii*”*

¹University of South Florida, Department of Chemistry

²University of South Florida, Department of Global Health

With an estimated 3 to 5 million infections and as many as 500,000 deaths from the complications of influenza infections each year, there lies a critical need to identify novel drug classes and structures, which can be exploited for antiviral development. A bioassay-guided fractionation of extracts from the red marine algae *Gigartina skottsbergii*, collected near Anvers Island, Antarctica, significantly inhibited the reproduction of influenza virus A/Wyoming/3/2003 (H3N2) in MDCK cells in vitro with an IC₅₀ value of 4 µg/mL. The virus-inhibitory effect was selective, dose-dependent, strain-specific and the virus induced cytopathogenic effect (CPE) was reduced at non-toxic concentrations of the extract. SDS-Gel electrophoresis and sequencing of the active fraction reveals homology with lectins. Insight into the mechanism of action via hemagglutination assay suggests cell protection by interference of viral docking

O-8. 11:00-11:15 AM

Chungsik Kim¹, Joseph Gill¹, Jess E. Jones², and X. Peter Zhang¹

“Stereoselective Synthesis of Epoxides from Diazoacetates via Ylide Intermediates using Co(III)corroles”

¹Department of Chemistry, University of South Florida, ²University of Tampa

Corroles are aromatic tetrapyrrole macrocycles having one direct pyrrole-pyrrole linkage. Since 1999, corrole research has been dramatically increased as a result of improved synthetic methods as well as an intense interest in their applications in different areas, including catalysis, sensors, and medicine. In this oral presentation, we report the synthesis of diverse corroles and Co(III)corroles. These corroles have shown to be effective ligands in supporting metal-catalyzed reactions such as epoxidation. The reaction of donor/acceptor diazoacetate with aldehyde is confirmed to be a general and highly diastereoselective method for the synthesis of epoxides.

Graduate Talks Afternoon Session (CHE100)

C-1. 2:30-2:45 PM

Emma Farrell and David Merkler

“How the body makes primary fatty acid amides”

Department of Chemistry, University of South Florida

Primary fatty acid amides (PFAMs) have been discovered in many organisms from plants to mammals and have been shown to serve important roles as neural regulators. As of yet the in vivo mechanism of PFAM biosynthesis has not been determined. Working from the hypothetical model in which fatty acid \rightarrow acyl-CoA \rightarrow acylglycine \rightarrow PFAM, RT-PCR and western blotting were employed to determine which enzymes are expressed in several cell lines that produce oleamide from oleic acid.

The expression of Acyl CoA synthetase and peptidylglycine alpha-amidating monooxygenase, and not bile acid:amino acid transferase or acyl CoA:glycine N-acyltransferase (ACGNAT) in the cells supports the proposed biosynthetic pathway which involves an enzyme yet to be discovered: a long chain-specific ACGNAT. A metabolite quantification system has also been developed to monitor the flux of PFAMs. We show that these PFAMs are produced in N18TG2 mouse neuroblastoma and sheep choroid plexus (SCP) cells. Further, incubation with the corresponding fatty acid results in a marked increase in their production over time, both as a cell product and secreted into the media. Future directions of this project include developing an assay for the acylglycines and the use of RNAi to target these enzymes and show the accumulation of metabolic precursors.

C-2. 2:45-3:00 PM

Christi Young and Alfredo Cardenas

“Molecular Dynamics Simulations of the Influenza A Non-structural Protein 1 (NS1) RNA Binding Domain”

Department of Chemistry, University of South Florida

Nine molecular dynamics simulations of the RNA binding domain of the Non-structural protein 1 (NS1) of influenza A virus, a homodimer, were performed at 298K in explicit water and 0.1M KCl. We focused our analysis on helices 2 and 2', which are involved in RNA binding. A salt bridge displaying instability was identified between Aspartate-29 of chain A and Arginine-46 of chain B, breaking in half of the simulations. A recent experimental paper described the presence of a cavity in the surface of the side chains of helices 2 and 2'. In our simulations we observed a change in this cavity with time, correlated with the salt bridge motion. Principal component and normal mode analysis were done to support this correlation. Recently, five simulations were performed differing only in that no KCl was added. The same analysis steps were performed and the results compared to the simulations with KCl.

C-3. 3:00-3:15 PM

Justin Moses and Li-June Ming

“Catalytic Promiscuity of SgAP and the Potential for Decontamination”

Department of Chemistry, University of South Florida

Copper-substituted aminopeptidase from streptomyces griseus (CuCu-SgAP) exhibits several unexpected proficient enzymatic activities. The ability of this enzyme to perform peptide hydrolysis, phenol hydroxylation and oxidation, catechol oxidation, and phosphoester hydrolysis all within the same active site is unique. We have expanded our study of phenol hydroxylation, and have begun to explore the novel observation of oxidative dechlorination of chlorophenols which may prove beneficial to the design of artificial systems to break down halocarbon pollutants.

C-4. 3:15-3:30 PM

**Brent Hilker¹, Kevin J. Clifford¹, Andrew D. Sauter Jr², Andrew D. Sauter III²,
Ted Gauthier¹, and Julie P. Harmon¹**

“Electric Field Enhanced Sample Preparation for Synthetic Polymer MALDI-TOF Mass Spectrometry via Induction Based Fluidics (IBF)”

¹Department of Chemistry, University of South Florida

²Nanoliter LLC, 217 Garfield Drive, Henderson NV 89074.

MALDI-TOF mass spectroscopy is used in the characterization of synthetic polymers. MALDI allows for determination of: modal, most probable peak, (MP), molecular number average (MN), molecular weight average (MW), polydispersity (PD), and polymer spread (PSP). We evaluate a novel sample preparation method using Induction Based Fluidics (IBF) to kinetically launch and direct nanoliter volumes to a target without contact. IBF offers signal improvement via field enhanced crystallization. IBF increases signal/noise (S/N) and signal intensity for polystyrene (PS), poly(methyl methacrylate) (PMMA), and poly(ethylene glycol) (PEG) across a mass range of 2500 u to 92,000 u showing more accurate PSP. Increases in S/N range from 69-190% for PS, 115% for PMMA, and 410% for PEG. Signal intensities increased 128-303% for PS, 55% for PMMA, 130% for PEG. Cross polarization microscopy indicates dramatic morphology differences between IBF and micropipette. Finally, we speculate as to why IBF nanoliter depositions afford higher S/N.

C-5. 3:30-3:45 PM

Ramakanth Ananthoji¹, Farid Nouar², Mohamed Eddaoudi² and Julie P Harmon¹

“Controlled drug Delivery in Novel Zeolite-net-like Metal-organic Frameworks (rho-ZMOFs) - Hydrogel Composites”

¹Polymer Chemistry Research group, University of South Florida

²Inorganic Chemistry Research group, University of South Florida

Porous materials are of vital importance to the scientific world in many ways. One such class known as zeolites, aluminosilicates, has been widely used in applications such as catalysis, ion-exchange and separation. A novel class of this category, metal-organic frameworks based on zeolite topologies (rho-ZMOFs) opened the door for preparing novel polymer composites with enhanced mechanical properties. On the other hand bio-compatible hydrogels have a vital role in drug delivery. Here we present the novel hydrogel composites with zeolite-net-like organic framework, (rho-ZMOF) using 2-hydroxyethyl methacrylate (HEMA), 2,3-dihydroxypropyl methacrylate (DHPMA), N-vinyl-2-pyrrolidinone (VP) and ethyleneglycol dimethacrylate (EGDMA). Both neat and ZMOF composite hydrogels are tested for control delivery of procainamide hydrochloride, antiarrhythmic drug. The testing of drug release in phosphate buffer solution (PBS) is done using ultraviolet (UV) spectroscopy.

C-6. 4:00-4:15 PM

Alaa Hashim and Li-June Ming

“Oxidative Activities of Catalytic Metallopeptides”

Department of Chemistry, University of South Florida

A spectroscopic UV-vis study of Cu(II) binding to hepta peptides, one being hydrophobic, DHHNWHW, and another hydrophilic, DHHNKHA was performed. These studies suggest that each of the peptides bind two equivalence of Cu(II), mimicking the binding site of Cu(II) to bovine serum albumin, serve as catalysts for the oxidation of catechol and phenol type substrates, and exhibit double stranded oxidative plasmid DNA cleavage. The results also suggest that the hydrophobicity of the peptide may play a role in the oxidation of catechol containing substrates. The dependence of oxygen on the proposed mechanism of catechol oxidation by metallopeptides was also investigated by anaerobic studies.

C-7. 4:15-4:30 PM

Roger Bass¹, Julie Harmon¹, and Nathan Crane²

“Polymer-Carbon Nanotube Interface within Shape Memory Polymer”

¹Department of Chemistry, University of South Florida

²Department of Mechanical Engineering, University of South Florida

Current work focuses on an investigation of several polyurethane based shape memory polymers containing both single and multi-walled carbon nanotubes (CNT) in order to elucidate a more complete understanding of the interactions between polymer matrices and carbon nanotube interfaces. Efforts to incorporate CNTs in various polymer matrices have increased over the last several years due to the proven physical characteristics benefits including increases in strength and recovery; however the exact role CNTs play in the improved performance of the polymer is not yet fully understood. An induction-based fluidics (IBF) technique is used in an attempt to control CNT orientation within the polymer matrices as a basis to explore the interfaces between polymers and CNTs and to provide insight into the involvement of CNTs in the stress, strain and recovery process' of shape memory polymers. DSC data is shown as evidence in the manipulation of the polymer CNT interface.

C-8. 4:30-4:45 PM

Sumit Handa, Audrey Mokdad, Randy W. Larsen, and David J. Merkler

“Synthesis and Photophysical Studies of Photocaged N-Protected Glycine for Peptidyl α -Amidating Monooxygenase (PAM)”

Department of Chemistry, University of South Florida

Synthesis and photophysical properties of two photocaged derivative of N-protected Glycine (NPG) are been described. NPG are substrate for bi-functional enzyme peptidyl α -amidating monooxygenase (PAM), which catalyze the stepwise alpha hydroxylation followed by amidation. Many bioactive peptides possess a C-terminal α -amide group that is a critical determinant for their optimal bioactivities, explaining the biological importance of PAM. 2-Methoxy-5-nitrophenol (MNP) is used for caging the carboxylate group of NPG by esterification. The caged substrate are not substrate of PAM, while the photoreleased product is and the other photolytic product doesn't inhibit PAM. Photothermal methods such as photoacoustic calorimetry (PAC) are used to obtain the molar enthalpy and molar volume changes associated with the dissociation of the caged substrate to NPG and MNP. High quantum yield (0.53) was measured for the dissociation of photocaged substrate, such that the release of substrate is quantitative. Hence, these photocaged substrates are ideal molecules for elucidating the transient state mechanism of PAM.

C-9. 4:45-5:00 PM

Mohamed H. Alkordi, Edwin Rivera, Jonathan L. Belof, Lukasz Wojtas, Li-June Ming, and Mohamed Eddaoudi

“Insight into the Directed Assembly of Metal–Organic Materials”

Department of Chemistry, University of South Florida

Three novel Metal–Organic Materials (MOMs), 1-3, based on the assembly of 2,2'-(1H-imidazole-4,5-diyl)di-1,4,5,6-tetrahydropyrimidine, HL1, and octahedrally coordinated metal ions, $[\text{Co}_8(\text{C}_{11}\text{N}_6\text{H}_{15})_{12}]\text{Cl}_{12}\cdot(\text{H}_2\text{O})_x$ (1), $[\text{Ni}_4(\text{C}_{11}\text{N}_6\text{H}_{15})_4](\text{NO}_3)_4(\text{DMF})_2$ (2), and $[\text{Cd}(\text{C}_{11}\text{N}_6\text{H}_{15})(\text{NO}_3)]_n$ (3) were synthesized through solvothermal reactions and subsequently characterized using single crystal X-ray diffraction studies. Four different compounds, 1a-d, containing the same Metal–Organic Cube (MOC) as in 1, but with different counterions and in different packing arrangements, are also described. The assembly process of 1, a cobalt-based MOC, is investigated through solution NMR spectroscopy, UV–vis spectroscopy, and MALDI–TOF mass spectrometry. Aqueous dissolution of 1 resulted in solvated discrete MOCs, 1S, where integrity of solvated MOCs is maintained as evident from analysis of ^1H - and ^{13}C -NMR spectra of 1S. Stability of solvated MOCs under a wide range of solution pH (2~8) is assessed through solution ^1H NMR spectroscopy. The ability of MOCs to assemble at room temperature is evident from both NMR spectroscopy and single crystal X-ray diffraction studies. MALDI-TOF mass spectrum of 1 exhibits a molecular ion peak at $m/z = 3238.35$, $[1-12 \text{HCl}]^+$, along with several fragmentation products. Association of L1 to CoII in D₂O solution is monitored through observation of characteristic isotropically-shifted proton signals of coordinated L1 molecules in the D₂O ^1H NMR spectrum of the reaction mixture. Co-H relative distances, calculated through measurements of proton spin-lattice relaxation times (T₁), facilitate the construction of possible models for the solvated species. Computational models of several geometrically-optimized fragments of the MOC are constructed to better understand the observed experimental ^1H NMR spectra and to establish viability of proposed solvated species. Attempts are made to probe the assembly process of 1, in solution, as well as to investigate the effects and roles of several key parameters affecting assembly of 1, which include varying the metal ions, solvents, counterions, and reaction temperature, on the observed product(s) thus obtained.

C-10 5:00-5:15 PM

Zhenming An¹, Yudan Chen¹, John Koomen², and David Merkler¹

“Amidated Peptides Found in Mouse Pituitary Cell Line ATT-20 Using a New Mass Spectrometry Based Screening Method”

¹Department of Chemistry, University of South Florida

²H. Lee Moffitt Cancer Center & Research Institute

Peptide amidation is an important post-translational modification which has been argued as a “signature of bioactivity”. It was reported that about half of the bioactive peptides found in the nervous and endocrine -amidating monooxygenase (PAM; α systems were amidated.

Peptidylglycine E.C. 1.14.17.3) is the only known enzyme responsible for the biosynthesis of amidated peptides from their glycine-extended precursors. Inhibition of PAM will result in the accumulation of glycine-extended peptides.

This investigation reports an efficient method to screen and identify amidated peptides and their glycine-extended precursors in cultured cell lines. This method is based on the biosynthesis mechanism of amidated peptides and the high mass measurement accuracy of mass spectrometry. Using this method, a few amidated peptides were found and identified from mouse pituitary cell line Att-20, including a group of mouse joining peptide related peptides and a novel amidated peptide ELEGERPL-NH₂, as well as some known amidated peptides.

Graduate Posters (NES North Hallway)

P-1. Meghanath Gali and Kirpal S. Bisht

“Enantioselective Synthesis of Phosphodiesterase Inhibitor Rolipram via Enzymatic Desymmetrization”

Department of Chemistry, University of South Florida

A novel synthetic strategy involving green protocols such as enzymatic desymmetrization is discussed in the synthesis of (R)-rolipram, a potent and selective inhibitor of phosphodiesterase IV (PDE4). PDE4 is main enzyme regulating the concentration of secondary messenger cAMP (cyclic adenosine-3',5'-monophosphate) which in turn leads biochemical events to inflammatory processes. So a potent inhibitor is in need. In this strategy, starting intermediate 2-Aryl propyl-1,3-diol synthesis through palladium catalyzed cross coupling, reduction and various other methods such as resolution using pseudomonas cepacia enzyme, wittig reaction is explained.

P-2. Laura Anderson^{1,2}, MingZhou Zhou^{1,2}, Vasudha Sharma², Jillian McLaughlin², and Mark L. McLaughlin^{1,2}

“Design, Synthesis, and Bioactivity of Non-peptidic α -Helix Mimetics”

¹Department of Chemistry, University of South Florida

²Department of Drug Discovery, H. Lee Moffitt Cancer Center

The α -helix is the most common secondary structure found in proteins and many protein-protein interactions involve recognition of 3 or more side chains along a single face of an α -helix at the protein-protein interaction surface. Our studies have focused on the design and synthesis of semi-rigid scaffolds that hold individual side chain-like residues in orientations that mimic the orientations of i th, i th + 4, i th + 7, and i th + 11, etc. side chain residues of an α -helical protein domain. Our semi-rigid scaffolds are further designed to have drug-like physical properties to enhance the potential therapeutic applications of the resulting protein-protein interaction inhibitor. Our current studies focus on disrupting the protein-protein interactions between MDM family proteins with the N-terminal helical domain of the tumor suppressor p53 and the Bcl family of proteins with helical BH3 only pro-apoptotic proteins. We will report the synthesis of new oligomeric 2,5-pyrimidines with variable groups at the 4- or 4,6-position(s) and the biological activity of these α -helix mimics as MDM-p53 and Bcl-Bax disruptors.

P-3. Parul Jain², Selma Hokenek¹, Julie Harmon², and Norma A. Alcantar¹

“Characterization of Transparent Conducting Films for Vapor Sensors”

¹Department of Chemical and Biomedical Engineering

²Department of Chemistry, University of South Florida

Possibly the biggest challenge in polymer film fabrication is process control. We have synthesized films with the potential to be used as powerful surface sensors for chemical vapors. These films can also be used to investigate the relationship between structure, properties, and performance. To accomplish this, Bis(ethylenedioxy)-tetrathiafulvalene (BEDO-TTF) dye was incorporated into bisphenol A polycarbonate films at 2% wt and the films were doped with iodine at different concentrations with the aim of developing a method to make thin, flexible, transparent, and conductive films. The films were then characterized using AFM, TEM, transmission FTIR, UV-Visible spectroscopy, and conductivity-voltage measurements. Measured resistivities of the doped films range from 148 Ω -cm to 2.82 k Ω -cm. The film color correlates to film conductivity: metallic films have the best conductivity, and green films showed no conductivity. The variation of the film properties illustrates that the process conditions must be controlled carefully during fabrication.

P-4. Mike McIntosh and Xiao Li

“Enhancing Quantitative Measurements of Traditional Electrochemical Techniques by Employing Ultramicroelectrodes for the Detection of Biomolecules”

Department of Chemistry, University of South Florida

Amperometric techniques in Electrochemistry offer the advantage of low cost quantification and characterization of redox species important to biological systems. The development of Ultramicroelectrodes (UMEs) reduces the effects of noise and nonfaradaic processes that either inhibit micro and macroelectrodes' ability to produce quantitative information or limit their use to strictly qualitative information. Successful development of UMEs in the laboratory provides an alternative to using commercially available electrodes and offers a low cost methodology to design electrodes specifically for an intended study. Lab developed carbon fiber disk UMEs have been used to improve upon both previous electrochemical studies of (-)-Epigallocatechin gallate (EGCG), an antioxidant found in green and oolong teas. Determination of biological concentration in a rapid and reproducible manner would serve to corroborate biological research on EGCG's effects as they correlate to levels present in the body after ingestion. Bare surface carbon fiber disk UMEs have demonstrated an ability to quantify EGCG concentration over a linear range using Cyclic Voltammetry (CV), a precursor step to determining the viability of in vivo measurements that utilize polymeric membranes or surface modification to prevent electrode fouling.

P-5. Deniz Ozer and Serpil Takacı

“Effects of Solvent Type, Aqueous Phase/Solvent Volume Ratio and Temperature on the Hydrolytic Activity of Candida rugosa Lipase in a Biphasic Medium Designed for S-Naproxen Production”

Ankara University, Department of Chemical Engineering and Institute of Biotechnology

Candida rugosa lipase (CRL), which has a high specificity toward stereoisomers, is successfully used in nonsteroidal, anti-inflammatory drug S-Naproxen production through the hydrolysis of racemic Naproxen methyl ester. In this study, the variations in the hydrolytic activity of CRL (U) with some properties of the biphasic medium designed for the S-Naproxen production medium were investigated. Organic solvents of isooctane, hexane, cyclohexane and toluene (log P values are 4.7, 3.5, 3.2 and 2.5, respectively) in comparison with phosphate buffer, aqueous phase (phosphate buffer) /solvent volume ratios (A/O) of 1/2 and 2; and temperatures of 30, 37, 45 and 50°C were tested to improve the activity of CRL. Along 120h, in every 24h, samples were taken from the biphasic medium and measured for their CRL activity toward p-nitrophenol acetate spectrophotometrically by following the increase in the absorbance at 404 nm due to the liberation of p-nitrophenol in the hydrolysis of 0.005M p-nitrophenylacetate in 0.1 M sodium phosphate buffer at pH 7.5 and 25 °C. The CRL hydrolytic activity was found to decrease in the following order: For solvent type (U): isooctane > hexane > cyclohexane > toluene > phosphate buffer. For aqueous phase (phosphate buffer) /solvent volume ratio (U): A/O: 2 > A/O :1/2. For temperature (U): 37°C > 30°C > 45°C > 50°C. The results showed that hydrophobic forces were the major contributors to molecular interactions that altered the activity of CRL.

Acknowledgement

This study was supported by Ankara University Biotechnology Institute (Project No: 89)

P-6. Mu-Seong Kim and Julie Harmon

“Effect of Silica Nanowire on Dielectric Properties of Polyurethane Composite”

Department of Chemistry, University of South Florida

An aliphatic isocyanate, polyether, polyol thermoplastic polyurethane, Tecoflex® SG-85A, was solution processed with the varying amounts of silica nanowire. The dielectric permittivity (ϵ') and loss factor (ϵ'') were measured via Dielectric Analysis (DEA) in the frequency range 1Hz to 100 kHz and between the temperature -150 to 150. The electric modulus formalism was used to reveal alpha,beta 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. The onset of decomposition temperature was measured by thermogravimetric analysis (TGA). Scanning electron microscopy (SEM) provided images of the polymer-nanocomposites.

P-7. Katherine Parra and Alfredo Cardenas

“Conformational Changes and Ligand Behavior after CO Dissociation of the Oxygen Sensor bjFixLH: a Study by Molecular Dynamics”

Department of Chemistry, University of South Florida

FixL, a dimeric protein of *bradyrhizobia japonicum*, regulates the expression of genes responsible for nitrogen fixation and anaerobic respiration in response to molecular oxygen. It contains an N-terminal heme-bound PAS domain that controls the activity of the C-terminal histidine kinase domain depending on the heme ligation state. To investigate the ligand behavior after CO dissociation as well as the protein structural changes involved in the relaxation to the deoxy state, 10ns molecular dynamics simulations of the CO-bound and CO-unbound bjFixL heme domain in crystal and solution environments were performed. Crystallographic studies of CO photolysis in bjFixLH showed long-range conformational changes in the protein as well as changes in heme stereochemistry. However, details of CO diffusion after dissociation remained unclear. Comparing simulation to experimental data, it was shown that different environments affect the dynamics of the ligand and the structural changes within important protein regions.

P-8. Sai Lakshmana Vankayala³, Anthony E. Pegg², Wayne C. Guida³, Gary T. Pauly¹, Natalia Loktionova², and Qingming Fang²

“Computational Correlation Studies Towards Inactivation of O6-alkylguanine-DNA Alkyltransferase by O6-benzylguanine Analogs”

¹Laboratory of Comparative Carcinogenesis, National Cancer Institute at Frederick, MD; ²Penn State University, Hershey, PA ; ³University of South Florida, Tampa, FL

O6-alkylguanine-DNA alkyltransferase (AGT) is a DNA repair protein that acts in a single step to restore DNA with O6-Alkylguanine adducts, and thus prevents mutations and apoptosis arising from alkylated guanines. AGT irreversibly transfers the alkyl group to an active site cysteine in the acceptor site and provides resistance to alkylating therapeutic agents. So various analogs of benzyl guanine were synthesized and tested for activity as potential inhibitors. The nature and position of the substitutions -methyl and -aminomethyl profoundly affected their activity. Molecular modeling of their interactions with alkyltransferase provided a molecular explanation for these results. The square of the correlation coefficient (R²) obtained between E-model scores (obtained from GLIDE XP/QPLD docking calculations) vs. log(ED50) values via a linear regression analysis was 0.96. The models indicate that the ortho- substitution causes a steric clash interfering with binding whereas the meta- aminomethyl substitution allows an interaction of the amino group to generate an additional hydrogen bond with the protein.

P-9. **Matt D. Lebar¹, Sridevi Ankisetty², and Bill J. Baker¹**

“A Synthetic Study of Meridianin A and Psammopemmin A, Pyrimidine Containing Indoles from Antarctic Marine Invertebrates”

¹Department of Chemistry, University of South Florida

²School of Pharmacy, University of Mississippi, 443 Faser Hall, University, MS 38677

Our ongoing search for bioactive metabolites produced by Antarctic marine invertebrates has resulted in the isolation of several previously characterized aminopyrimidine substituted indole alkaloids. We have isolated these compounds, initially reported from the tunicate *Aplidium meridianum* and named meridianins, from the yellow top tunicate (*Synoicum* sp.) collected at Palmer Station, Antarctica. Meridianins display interesting bioactivity which includes protein kinase inhibition as well as toxicity toward murine tumor cell lines. Amongst the many syntheses of meridianins found in literature, only one synthesis of meridianin A has been reported to date. No reported syntheses or biological data exist for psammopemmins, structurally similar metabolites isolated from the Antarctic sponge *Psammopemma* sp. A synthetic route to both meridianin A and psammopemmin A from a common precursor would generate quantities of the metabolites suitable for further biological testing. Efforts toward the syntheses of meridianin A and psammopemmin A as well as analogs utilizing palladium cross coupling methodology will be discussed.

P-10. **Maryam Babaie Mahani and Hassan Sheibani**

“Synthesis of Novel Fused Heterocycles by High surface area MgO as a highly effective heterogeneous base catalyst”

Department of Chemistry, Shahid Bahonar University of Kerman, Kerman, Iran

In the last few decades, the chemistry of pyrrole and fused heterocyclic pyrrole derivatives has received considerable attention owing to their synthetic and effective biological and pharmacological properties. During the course of our investigations on the synthesis of heterocyclic compounds, we developed a novel method for preparing of 6-amino-4-aryl-5-cyano-1,4-dihydropyrano[2,3-c]pyrazole derivatives from three-component reaction of 3-methyl-1-phenyl-2-pyrazolin-5-one arylhydrazones, aromatic aldehydes and malononitrile in the presence of MgO as the base catalyst. This method offers several advantages including high yields, short reaction times, easy work-up and the catalyst is inexpensive and easily obtained, stable and storable, easily recycled and reused for several cycles with consistent activity.

P-11. Daniel N. Santiago, Wesley H. Brooks, MinhPhuong Tran, Ashley A. Tillette, Robin Scherer, Shen-Shu Sung, Kenyon G. Daniel, and Wayne C. Guida

“Virtual Counter Screening: Recycling of Old Molecules for New Uses”

Department of Chemistry, University of South Florida

In computer aided drug design, software simulates molecular docking (virtual screening) of a 3D database of small molecules against a single protein target to find potential hits for drug discovery. In virtual counter screening (VCS) a small molecule of interest is docked against a protein structure library. The VCS approach is potentially useful for identifying new targets for known compounds or for assessing the selectivity of a lead candidate in a drug discovery program. We have developed a VCS protocol and have begun to assess its potential utility. Thus far, we have prepared more than 1,300 proteins from the Protein Data Bank (PDB) for docking. Each protein was virtually pre-screened against a normalizing set of ligand structures. Statistics of the normalization dockings provide a base-line calibration with which to judge the potential significance of VCS results for small molecules of interest. Case studies involving known inhibitors are presented.

P-12. Butch Knudsen and Julie Harmon

“The Functionalization and Dispersion of Nanotubes in Poly (4-methyl-1-pentene)”

Department of Chemistry, University of South Florida

NASA has recently been tasked with the return of astronauts to the moon and planetary missions. People living in space not only need the basics of food and water but something that is often taken for granted, the radiation protection provided by the earth's atmosphere and magnetic field from galactic cosmic radiation. For this purpose a polymer such as poly (4-methyl-1-pentene), PMP, is ideal. The raw material is relatively inexpensive and can be easily obtained and does not cause secondary radiation. However the rigors of space travel may call for even greater strength than posed by the neat polymer. In this research functionalized carbon nanotubes have been dispersed in the neat polymer to study the resulting changes in physical properties. Carbon nanotubes were functionalized using reductive alkylation with the alkyl halide 1-Iodo-2-methylpropane. The resulting nanotubes expressed methyl propane on the surface making them soluble in 4-methyl-1-pentene monomer. Ziegler-Natta polymerization was then used to control the tacticity of the polymer. The resulting product was amorphous when Ziegler-Natta polymerization should have produced a crystalline sample. The experiment was run several times with the same result and the research is ongoing.

P-13. Kurt Van Horn and Roman Manetsch

“Templated Assembly of DNA Fragments via Complimentary Reactive Functionalities”

Department of Chemistry, University of South Florida

DNA is known throughout the scientific community as being the key to a large volume of information. DNA replication has been achieved in vitro via the polymerase chain reaction (PCR). We have begun to study a new technique that may be able to complement the reading and replication processes of existing methods. This technique consists of two DNA fragments with complimentary reactive functionalities that can be recognized and bound by a DNA strand. Upon being bound by the DNA, the reactive functionalities react to form a new covalent bond between the two fragments, yielding a new fragment.

P-14. Sebastian Gutmann¹, Matthaeus A. Wolak², Martin M. Beerbom², and Rudy Schlaf²

“Effect of UV and X-ray Radiation on the Work Function of Nanocrystalline TiO₂ Thin Films”

¹Department of Chemistry, University of South Florida

²Department of Electrical Engineering, University of South Florida

The work function of nanocrystalline anatase (TiO₂) thin films was measured using photoemission spectroscopy (PES). Titanium dioxide nanoparticles were dispersed in an ethanol/water solution and deposited in-vacuum using electrospray deposition. A comparison between ultraviolet photoemission (UPS) and low intensity x-ray photoemission (LIXPS) work function measurements on such films showed a strong work function reduction (>0.5 eV) caused by the UPS measurements. Furthermore, it was found that XPS measurements also reduce the work function over a time period of several seconds. These effects are similar in magnitude to artifacts seen previously on indium tin oxide substrates characterized with UPS, and is probably related to the formation of a surface dipole by means of a photochemical reaction with water molecules present on the surface.

P-15. Shikha Mahajan, David Merkler, and Roman Manetsch

“Synthesis of Biotinylated Azido-Adenine-Ribose Derivatives: Potential Activity-Based Protein Profiling Probes”

Department of Chemistry, University of South Florida

Adenine nucleosides and nucleotides (ADoR's) are key molecules in a large number of metabolic and cell signaling pathways. Thus, ADoR-dependent proteins correlate to many human diseases including cancer, cardiovascular diseases, diabetes, and obesity.

Herein, we report our synthesis of biotinylated azido-adenosine analogues for the study of ADoR's-dependent proteomes and the synthetic strategies and challenges involved in their syntheses. The design of these ADoR probes includes a photolabile azide moiety for covalent attachment of the probe to the target proteins as well as a biotin moiety for the isolation of the probe-protein conjugates using avidin affinity chromatography. 2,6-dichloro-purine has been exploited as an important intermediate from which the synthesis of various nucleobase analogues can be channeled. We aim at the optimization and validation of the use of our ADoR-specific probes against a set of purified ADoR-dependent proteins

P-16. Seongmin Hong and Xiao Li

“SERS Detection of Dopamine”

Department of Chemistry, University of South Florida

Appearance of Surface Enhanced Raman Spectroscopy (SERS) became one of the most promising techniques to study the low concentrations of dopamine. SERS takes advantage of the special characteristics of metal nano particles, such as gold, silver and copper allowing it to amplify Raman shift signals. This enhanced technique allows the detection of chemicals that normally are present at relatively low physiological concentrations. Dopamine, a well known neurotransmitter, has important roles of human brain function. Currently available techniques for probing dopamine suffer from insufficient detection limits. SERS may address issues like lower detection limits as well as biocompatibility since the technique is generally nondestructive. Several parameter need to be investigated regarding SERS imaging of dopamine before in vitro experiments can be explored, which primarily includes the optimal noble metal configuration, particle size, and distribution. Using noble metallic nano particles has already experimentally shown enhancement of detection limits for a variety of organic chemicals.

P-17. Arun Babu Kumar and Roman Manetsch

“Development of a Labeling Probe for the Discovery and Identification of Saccharide-Binding Proteins”

Department of Chemistry, University of South Florida

Proteins that interact with carbohydrates in a non-covalent fashion occur widely in nature. Such proteins, which have come into the forefront of biological research in recent years, belong to the class of lectins. Herein we introduce a novel class of multifunctional photoaffinity probes, which guarantee the highest possible affinity combined with a straight forward purification procedure by a fluoruous tag. We discuss the design, the synthesis and the development of a versatile chemical probe for the selective labeling of carbohydrate-binding proteins. We speculate that our proposed labeling and enrichment protocol has potential to accelerate the discovery and identification of unknwn saccharide binding proteins.

P-18. Ranjani Muralidharan and Xiao Li

“Study of the Electrooxidation of Formic Acid and Methanol”

Department of Chemistry, University of South Florida

Anode catalysts have been widely studied for their effects on formic acid and methanol fuel cells. Platinum plays an essential role in these electrocatalytic reactions. The spontaneous deposition of platinum on polycrystalline gold enhances the activity of the catalyst for electrooxidation of formic acid and methanol without having to devote high material costs to solid platinum electrodes. Preliminary studies show increased currents due to Pt deposit on gold. Electrochemical information derived from Cyclic Voltammetry (CV) will be augmented by spectroscopic information to elucidate the mechanism of Platinum catalysis on the oxidation of these emerging fuels.

Undergraduate Posters – Organic Chemistry (NES 103)

S-1. **John Markantonis, Ruizhi Wu, and Kirpal Bisht**

“Stereo-controlled Synthesis of Organic Molecules”

Department of Chemistry, University of South Florida

In our lab we produce organic compounds that do not form naturally or easily. These products are usually a stereo unfavorable form, i.e. a mono substituted product instead of a disubstituted product. These products are then used as biological pre-cursors by addition of functional groups like a thiol group. Once formed the products are isolated by column chromatography.

S-2. **Hiondy Polanco, Yuxue Liang, Gajendra Ingle, and Jon C. Antilla**

“Organocatalytic Asymmetric Addition of Diphenylphosphine Oxide to Imines”

Department of Chemistry, University of South Florida

Chiral phosphine ligands are widely used catalysts in asymmetric synthesis. These phosphorus containing compounds are biologically important. We have developed a new enantioselective method to synthesize α -amino phosphine derivatives. Nucleophilic addition of diphenyl phosphine oxide to N-benzhydryl imines is catalyzed by chiral phosphoric acids. Different chiral phosphoric acid catalysts and solvents were screened. 9-phenanthryl BINOL phosphoric acid (catalyst) and acetonitrile (solvent) at ambient temperature produced the highest yields and enantioselectivity. A wide variety of functional groups are tolerated. Aliphatic imines produced good yields and enantioselectivity

S-3. **Beata Kaminski and Ted Gauthier**

“Synthesis and Characterization of 1400W and 1400W-azide”

Department of Chemistry, University of South Florida

Nitric oxide synthase (NOS) is an enzyme that produces nitric oxide, an important signaling molecule. Many conditions and diseases are related to excess production of NO. Therefore, inhibition of NOS is very significant. 1400W (N-(3-(Aminomethyl)benzyl)acetamidine) has been shown to be a slow, highly-selective, and tight-binding inhibitor of inducible nitric oxide synthase. iNOS is a form of NOS that functions in immune defense. Our studies involve the synthesis and characterization of 1400W. We will also investigate the synthesis of an azido form of 1400W using various methods. Once the best synthesis method has been identified we will synthesize 1400W-azido and perform “click” chemistry to attach biotin or a fluorescent tag for biological studies of iNOS.

S-4. Mario Martinez and Roman Manetsch

“LC/MS–Based Drug Discovery: Fragment Screening for the Development of Potential Bcl-XL Protein-Protein Interaction Modulators”

Department of Chemistry, University of South Florida

A fragment-based drug discovery methodology has been employed for screening fragment libraries for activity against an important cancer target, anti-apoptotic protein Bcl-XL. The methodology uses gel permeation chromatography (GPC) coupled to a liquid chromatography-mass spectrometry system (LC-MS) to assess non-covalent binding complexes between small molecular fragments and Bcl-XL. The fragment libraries are composed of sulfonyl azides and thio acids, fragments which react with one another in an amidation reaction to form N-acylsulfonamides. Additionally, large compound libraries of sulfonamides and carboxylic acids are also to be exploited as isosteres of sulfonyl azides and thio acids, respectively. Screening of sulfonyl azides against Bcl-XL demonstrated the strength of this drug screening methodology, with promising results for four fragments as well as a previously-discovered Bcl-XL-protein interaction modulator.

S-5. Kristopher Hahn, Matt Lebar, and Bill J. Baker

“Synthesis of the C16 – C25 Portion of Palmerolide A”

Department of Chemistry, University of South Florida

Extractions of *Synoicum adareanum*, a tunicate indigenous to Antarctica and commonly found in the shallow waters near Palmer Station, have yielded polyketide macrolides known as the palmerolides. Palmerolide A is of particular interest due to its potent cytotoxicity and selectivity against melanoma cells which in turn makes it a viable candidate for use as an anti-cancer drug. In anticipation of laboratory preparation of palmerolide A, a retrosynthetic scheme has been devised to yield three subunits that when combined will result in the total synthesis of the macrolide portion of the compound. The synthesis of the first fragment, the C3-C14 portion, has been completed with desired functional groups attached which will allow for the coupling of the subsequent fragments. The second fragment will have to incorporate complementary functional groups to the first fragment to successfully duplicate palmerolide A as well as exact stereochemistry around all stereocenters. This synthesis will utilize chiral pool starting material which ensures a quick, reliable route to an enantiopure product. This paper reports on efforts toward the synthesis of the C16-C25 portion which will later be joined with the other two subunits to generate palmerolide A.

S-6. Petoria Gayle¹, Sameer Kulkarni¹, Xiangdong Hu¹, Hong-Gang Wang², and Roman Manetsch¹

“Protein-Protein Interaction Modulators & Role of Target Guided Synthesis”

¹Department of Chemistry, University of South Florida

²Department of Pharmacology, Penn State College of Medicine, 500 University Drive, Hershey, PA 17033

Protein-protein interactions are necessary for basic biological functions. However, modulators to certain protein-protein interactions can have therapeutic effects. In particular, we are focusing on the disruption of the interactions between anti-apoptotic proteins, such as Bcl-xL and pro-apoptotic proteins. Bcl-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 Bcl-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 Bcl-xL, using this approach. We believe that this approach will be utilized for targeting various protein-protein interactions in the future.

S-7. Joseph Gill, Chungsik Kim, and X. Peter Zhang

“Design and Synthesis of Chiral Corroles”

Department of Chemistry, University of South Florida

Early in corrole research the prevailing methods of corrole synthesis were often impractical because of their lengthy synthesis and overall low yields. We use a newer methodology that breaks the overall synthesis into smaller, more manageable reactions which result in higher, more desirable, yields. This design involves palladium-based cross-coupling of bromo-corroles with a variety of different amides. These chiral corroles have been successful in a variety of stereoselective catalytic cyclopropanation reactions.

S-8. Corey Garvin, Michelle Cortes-Salva, and Jon C. Antilla

“Copper Catalyzed Reactions of Amidines”

Department of Chemistry, University of South Florida

Because of the similarity between amidines and guanidines there is currently speculation that amidines can be used for medical applications like guanidines. Currently work is being done to optimize the production of amidines. Our goal is to make innovative and cost effective ways to create these compounds. Inexpensive and commercially available benzamidine salt is reacted with aryl iodides to form the desired amidines analog. After solvent screening was performed, DMF was selected because of its ease of use and its superior yield: as well there is no need for a ligand to make the catalytic reaction successful. The conditions needed for the system are: 1mmol Benzamidine HCl, 1 mmol aryl iodide, 10 mol % CuI, 2mL DMF, and 2 eq. Cs₂CO₃ at 90°C for 24 hours. Wide varieties of aryl iodides were tested giving yields from 2% to 84%.

S-9. Erin Coke, John Struss, Eleanor Clements, and Martha Bromfield

“A Green Bromination/Oxidation Reaction – The Conversion of Simple Non-Aromatic Heterocycles to Lactones, Lactams and Thiophenones”

The University of Tampa Department: Chemistry & Physics

Polymeric DABCO-bromine complex (PDB), a stable, shelf-ready source of electrophilic/free-radical bromine, shows a wide variety of reactivity: a) oxidation of secondary and primary alcohols to the corresponding ketone or aldehyde, b) conversion of amines to imines, c) free-radical bromination of simple aromatic hydrocarbons, and d) electrophilic aromatic bromination in the presence of strong pi-donors. Recently, a new reaction was discovered in which PDB converts tetrahydrofuran (THF) to gamma-lactone using water as the solvent. The byproducts of this reaction are easily removed by separatory funnel extraction. Subsequent removal of the extraction solvent in vacuo reveals a product that requires no additional purification. We hope to expand this process to include other heterocycles such as tetrahydropyran, pyrrolidine, piperidine, and tetrahydrothiophene.

S-10. Charles Myers, Meghanath Gali, and Kirpal S. Bisht

“Synthesis of A Prochiral Diol, 2-(3'-cyclopentyloxy-4'-methoxy phenyl)propyl-1,3-diol, for Enzymatic Desymmetrization”

Department of Chemistry, University of South Florida

2-Aryl propyl-1,3-diol (7) is an intermediate for the synthesis of 2-aryl-β-lactam such as rolipram. The synthetic scheme begins with desymmetrization of the prochiral diol 7 using in vitro enzyme catalysis, specifically the symmetric 2-aryl propyl-1,3-diol is acetylated enantioselectively to receive monoacetate. In the presentation, a practical synthesis of the compound 7 starting with guaiacol (2-methoxy phenol) through several typical reactions involving the unique chemistry of the phenyl ring, including para bromination, palladium catalyzed cross coupling and reduction will be discussed.

S-11. Sahir Quraeshi, Sridhar Kaulagari, Priyesh Jain, and Mark Mclaughlin

“PNAs: Structure, Synthesis, and Application”

Department of Chemistry, University of South Florida

Peptide Nucleic Acids (PNAs) are achiral, uncharged structural mimics of DNA which utilize a pseudopeptide backbone comprised of repeating N-(2-aminoethyl)-glycine units linked by amide bonds. The PNA oligomers are able to form very stable bonds with Watson-Crick complementary DNA and RNA. Due to the PNAs neutral characteristics, the PNA/DNA binding is actually stronger than that of DNA/DNA at low to medium ionic strength. Because of PNA's neutral backbone, however, PNAs show problems such as poor aqueous solubility and poor cell permeability. Many attempts have been targeted towards modifying the backbones of PNA in order to solve this problem. For example, aminoethylprolyl PNA has been synthesized which allows PNAs to form highly stable triplexes. I will present our research of synthesizing PNA monomers and our developments of modified PNA backbones.

S-12. Kirk McDoneld, Pasha M. Khan, and Kirpal S. Bisht

“Pd catalyzed Allylic Alkylation- Application Towards Synthesis of New Anti-HIV and Anti-viral Carbocyclic Nucleosides”

Department of Chemistry, University of South Florida

Pd catalyzed alkylation is one of the most synthetically useful reactions and has been extensively used in organic synthesis. Hence, in quest of synthesizing new bioactive compounds, organopalladium chemistry was utilized in conjunction with enzyme catalyzed reactions. New optically pure carbocyclic nucleosides can be synthesized starting from a meso-diol via Pd(0) catalysis. These compounds are analogs of nucleosides such as neplanocin, aristeromycin, abacavir which have been used as anti-HIV and anti-viral drugs. Some of these carbocyclic nucleosides can also act as adenylyl cyclase inhibitor which is an enzyme required during conversion of ATP to cAMP.

S-13. Cynthia Lichorowic and Edward Turos

“Water Soluble N-Thiolated β -lactam Antibacterials”

Department of Chemistry, University of South Florida

Antibiotic-resistant bacteria are an exponentially growing problem. As bacteria inevitably become resistant to each antibiotic, new and more effective antibiotics must be developed. This project deals with one such family of antibacterial agents, N-thiolated β -lactams, by modifying the structure to allow better solubility in water.

N-thiolated β -lactams function differently than previously known β -lactams. They do not bind to the penicillin-binding proteins of bacterial cells and are not destroyed by β -lactamase proteins that cleave penicillin in drug-resistant bacteria. Unfortunately, the N-thiolated β -lactam is hydrophobic and in order to be used in vivo, must be made more water-soluble. Previous work in Dr. Turos' laboratory has found that the activity of the antibiotic is not significantly affected by changes in the ring's substituents and so it is my hypothesis that these side chains can be modified to achieve a water soluble molecule that is still effective as an antibiotic.

Undergraduate Posters – Analytical Chemistry (NES South Hallway)

A-1. Lieu Huynh, Fang Li, and Abdul Malik

“Pre-concentration and Analysis of Haloacetic Acids in Drinking Water”

Department of Chemistry, University of South Florida

Haloacetic acids (HAAs) are disinfection byproducts of drinking water. Chlorination of water generally forms monochloroacetic acid (MCAA), dichloroacetic acid (DCAA), and trichloroacetic acid (TCAA). The human consumption of water containing these HAAs is linked to bladder, kidney, and rectal cancers. According to the US EPA dichloroacetic acid and trichloroacetic acid are known to be carcinogenic to human. The maximum allowable amount of HAAs in drinking water is 60µg/L. This concentration includes various forms of chloro- and bromoacetic acids. Sol-gel capillary microextraction provides an excellent solvent-free technique for preconcentration of these trace analytes. In this work, sol-gel germania capillary microextraction was used to extract MCAA, DCAA, and TCAA in different types of drinking water for subsequent analysis by gas chromatography. Poly(dimethylsiloxane) (PDMS) and poly(propylene glycol)-block-poly(ethylene glycol)-block-poly(propylene glycol) (PPG-PEG-PPG) were used as polymers for the creation of organic-inorganic hybrid coating to extract HAAs.

A-2. Nicole Rubin and Dean Martin

“A Study of Copper Complexes Associated with Cuprilig Synthesis”

Department of Chemistry, University of South Florida

Cuprilig is a metallolig, i.e, a metal derivative of a commercially available immobilized ligand, Octolig®, that consists of polyethylenediamine moieties covalently bound to a high-surface area silica gel. Cuprilig has been proven to remove aqueous arsenic (as arsenite or arsenate) from 300 ppb to < 2 ppb (99% removal) and has achieved quantitative removal other nuisance anions found in water. An up scaling of Cuprilig has already been performed by Dean F. Martin and previous students. The calculation result indicated that a synthesis of Cuprilig that required an input greater than 6 ppm of Cu(II) ion with Octolig®, would result in a pH so low that the tendency to chelate would be 100-fold worse than at pH 7. It was also thought that it would be too diluted for commercial application. However, D. F. Martin used 4,256 ppm of Cu(II) ion, and the synthesis of Cuprilig was successful. This indicates that something is affecting the pH in a favorable way that would permit commercial preparation. By performing spectroscopy on the eluants of the column as well as measurements of pH and total dissolved solids (TDS), one can better understand the success of the synthesis of Cuprilig.

A-3. Maria Parra, Fang Li, and Abdul Malik

“Sol-Gel Capillary Macroextraction”

Department of Chemistry, University of South Florida

The purpose of this research is to use sol-gel coated capillaries. Specifically, sol-gel Germania based materials for capillary microextraction of various polar an analytes such as aldehydes and ketones, and nonpolar analytes such as alcohols, and amines using gas chromatography and high performance liquid chromatography as the methods for extraction.

A-4. Farzana Shaik, Mike McIntosh, and Xiao Li

“Establishing Quantitative Parameters for the Electrochemical Detection of Curcumin using Platinum Ultramicroelectrodes”

Department of Chemistry, University of South Florida

Curcumin is a polyphenol that illustrates an extensive range of benefits due to its inherent antioxidant behavior. We aim to study the oxidation and reduction patterns of Curcumin in a basic phosphate buffer. The electrochemical technique used was cyclic voltammetry (CV), where a working electrode potential is ramped linearly versus time, similar to linear sweep voltammetry. We hope to establish a quantitative Curcumin detection limit of the CV method using ultra platinum microelectrodes which were made in our own lab. Based on ongoing cyclic voltage results we noticed that certain PH levels maintain conditions for unsaturated Curcumin without excessive amounts of self-oxidization over time. We found that Curcumin capitulates distinct quantitative results; however our research is still ongoing.

A-5. Jessica Hoffman, Scott Segro, and Abdul Malik

“Quantitative Analysis of Oligonucleotide Class Compounds via Sol-Gel CME-HPLC”

Department of Chemistry, University of South Florida

Sol-gel capillary microextraction (CME) is on the forefront of research and method development in analytical separations and sample preparation, but its advantages over conventional methods in the analysis of biological macromolecules have not yet been studied extensively. This work presents a comprehensive sol-gel CME-HPLC approach for the quantitative analysis of oligonucleotide class compounds, which is of critical importance in evaluating pharmacokinetics and pharmacodynamics during the clinical development of new drugs. This method also offers the sensitivity required to quantify nucleotides, such as GMP and GTP that are known biomarkers for disease and genetic disorders.

A-6. Frederick Stull and Dean Martin

“A Comparison of the Ease of Separation of Sulfate, Phosphate, Nitrate, and Nitrite from Aqueous Solutions using Octolig®”

Department of Chemistry, University of South Florida

One proposed method of storing liquid radioactive waste is vitrification. The vitrification process, however, suffers from several problems derived from the presence of sulfate, phosphate, nitrate, and nitrite in the liquid radioactive waste. We have previously discovered that an inexpensive commercially available immobilized ligand, Octolig®, is effective at removing large proportions of the problematic species individually from an aqueous environment. In the current study, we are determining the effectiveness of Octolig at removing the problematic species combined in an aqueous solution that is similar in proportion to that found at the Hanford site, a location containing liquid radioactive waste. A solution containing the aforementioned ions was made and passed through Octolig®. The effluent solution was tested for the presence of the ions and compared to the initial solution. The results showed that over 98% of the problematic species were removed from the aqueous solution by Octolig®.

A-7. Ronelle Bailey, Minhphuong Tran, and Abdul Malik

“Microextraction of Biomolecules Using Silica-based Sol-gel Coated Fused Silica Capillaries”

Department of Chemistry, University of South Florida

A positively charged sol-gel coating was developed using a solution containing two precursors: tetraethoxysilane (TEOS) and N-tetradecyldimethyl[(3-trimethoxysilyl)propyl] ammonium chloride (C14-TMS). The charged sol-gel coating was developed for microextraction of biomolecules. Silica-fused capillaries with a surface-bonded tetradecylsilane (TDS) stationary phase coating were successfully fabricated. The positively charged sol-gel coating allows for microextraction of negatively charged analytes from a solution sample via electrostatic interactions. Subsequent analysis by high-performance liquid chromatography (HPLC) allows for separation of the bioanalyte. HPLC will, therefore, be used to analyze the microextraction efficiency of the sol-gel coating method and further analyze the biomolecule.

A-8. Karin Thatcher and Dean Martin

“Effect of Octolig® Treatment on the Growth of Lyngbya Majuscula”

Department of Chemistry, University of South Florida

The increasing occurrence of nuisance algal blooms worldwide has compelled the development of more effective treatments to control their rapid growth. *Lyngbya majuscula* (a.k.a. *wollei*) is a nitrogen-fixing blue-green alga that has been observed blooming in Crystal River, Florida. These blooms are detrimental to local aquatic environments and release toxic compounds that cause skin irritations like “swimmer’s itch” in humans. The present study utilized Octolig®, a granular immobilized ligand (IMLIG) consisting of polyethylenediamine moieties bound to high-surface area silica gel, to remove essential nutrient metals and anions from river water. Dissolved oxygen measurements monitored the growth of this alga in both treated and untreated river water for 11- to 15-day periods. Octolig® treatment was found to significantly reduce photosynthetic activity and growth ($p < 0.05$), leading to algal decomposition. These results were strongly supported by pH and fresh weight measurements as well as observational data.

A-9. Judy Triplett, Scott Segro, and Abdul Malik

“Tri-block Copolymer/Germania Sol-gel Coating for HPLC-CME”

Department of Chemistry, University of South Florida

A germania based sol-gel coating using a tri-block copolymer was developed for capillary microextraction (CME) hyphenated on-line with high-performance liquid chromatography (HPLC). The precursor, tetra-n-butoxygermane, was used in conjunction with the polymer, poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethylene glycol), to create a sol-gel matrix via hydrolytic polycondensation reactions which were carried out inside a fused-silica capillary. To the best of our knowledge, this is the first time a block polymer has been used as a sorbent in chromatographic separations. Using this amphiphilic polymer, the sol-gel coated capillary demonstrated exceptional performance, extracting trace concentrations of alcohols, amines, ketones, phenols, and polycyclic aromatic hydrocarbons. Additionally, this sol-gel coating demonstrated an excellent stability for extreme pH values. Possessing these outstanding attributes, this sol-gel coating is a highly effective performer as a stationary phase for the microextraction of a wide variety of molecules ranging from highly-polar to non-polar.

A-10. Agnes Prospere, Seongmin Hong, and Xiao Li

“Synthesis of silver and gold colloidal solutions for use in Surface Enhanced Raman Spectroscopy (SERS)”

Department of Chemistry, University of South Florida

Colloidal solutions of metals, specifically those of gold and silver have useful applications in surface enhanced Raman scattering (SERS). These nanoparticles serve as substrates that permit the adsorption of a target analyte onto the surface. Various methods have been developed to synthesize Au and Ag particles, however, in this study, the Lee-Meisel method, the Creighton method and the Leopold and Lendl methods of synthesis were key. Each of these techniques utilized reducing agents. The synthesized particles from each preparation method were examined by scanning electron microscopy to determine and compare size. Size of the nanoparticles can affect the SERS outcome. Results show that most Ag particles are between 90-110nm. Gold particles are much smaller, mainly between 25-30 nm. Further characterization was done using UV-VIS spectroscopy.

A-11. Darius Wynn and Dean F. Martin

“Separation of Aqueous Borates with Octolig and Selected Metalloids”

Department of Chemistry, University of South Florida

Trace elements in any circumstance affect any system, both positively and negatively. However, since the positive effects are generally more welcomed, we shall concern ourselves with the negatives. The species under study are trace amounts of boron and aqueous borates. Our aim is to effectively elute these borates by way of the commercially immobilized ligand, Octolig.

A-12. Tarik Elmohd, Carey Boudreau, Erica Turner, and Abdul Malik

“Sol-gel Germania Sorbents for Capillary Microextraction On-line Coupled to Gas Chromatography”

Department of Chemistry, University of South Florida

A sol-gel method was developed to create germania BMPO-based hybrid organic-inorganic materials for use in capillary microextraction. Capillaries (320 μm i.d.) were pre-treated before fabrication of the monolithic capillaries via sequential rinsing of methylene chloride, methanol, and water to form silanol groups on the capillary surface upon conditioning within a gas chromatograph (GC). Monoliths have inherent advantages over conventional coatings in the preconcentration of analytes, but problems arise due to their tendency to crack under pressure and shrink. Crack free sol-gel germania BMPO 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 gas-phase operations involving elevated temperatures. Detection varies with capillary microextraction sol-gel germania BMPO monolithic capillaries coupled to gas chromatography with flame ionization detector (FID).

A-13. Christopher Lee Lizardi and Dean F. Martin

“Selenium Removal Through the Use of Octolig and its Copper (II) Derivative Cuprilig”

Department of Chemistry, University of South Florida

This study was designed to test the ability of Octolig® in removing nuisance anions of interest. Nuisance anions of selenium (selenites, selenates) are currently causing problems in the contaminated surface waters of the Kesterson Reservoir in California and in West Virginia’s Mud River. High levels of selenium in surface waters which are used for wildlife habitat or drinking water supplies may lead to selenosis, where one may suffer from dermatitis, hair loss, or other symptoms. In the lab selenium in the form of selenious acid was passed through columns containing 22 cm in height commercially available Octolig® as well as a synthesized derivative of Octolig®, Cuprilig. Octolig® is a compound of silica gel that is covalently attached to the immobilized ligand polyethylenediamine. This compound is well known for its removal of transition metal ions, and recently has been found by our group to remove nuisance anions as well. The copper (II) derivative of Octolig®, Cuprilig, was used as well for a comparison of effectiveness. After Cuprilig column chromatography of the selenious acid solution total dissolved solid levels have been lowered from 179.4 from the stock solution, to 48 for the effluent. We have also found Octolig® to lower TDS from 60.8 in the stock solution to 9.3, and 6.2 for two respective trials. Further analytical investigation will allow for the determination of specific anion removal as well as the comparative efficiencies of the Octolig® and Cuprilig compounds.

A-14. Christopher Cook, Fang Li, and Abdul Malik

“Sol-Gel Column Technology”

Department of Chemistry, University of South Florida

A method for using sol-gel chemistry to prepare fused silica columns for high resolution gas chromatography is described. Traditionally, column fabrication was a multifaceted and time consuming procedure. The old way prescribed a four step process that included surface treatment, deactivation, coating, and stationary phase immobilization. The new sol-gel approach condenses this fragmented process into a one step procedure. A sol solution fills a capillary and is allowed to react for a fixed amount of time. The result is the evolution of a sol-gel network that is physically bonded to the capillary. The wall bonded coating provides enhanced thermal stability and lacks the need for free radical crosslinking procedures. Sol-gel coatings also provide the additional benefit of increased surface area, evident by scanning electron microscopic studies. Note that no original research will be presented only theory and reproduced experiments with minimal results.

A-15. Bryan Vo and Dean Martin

“Removal of Fluoride from Drinking Water using Octilig®”

Department of Chemistry, University of South Florida

The goal was to determine how effective the compound Octilig® was at removing aqueous fluoride from drinking water.

The electrode potentials of standardized concentrations of the NaF solution was determined using a Orion 290A Fluoride electrode with a calomel electrode. Those data were used to create a calibration equation, emf as a function of log F⁻). A 0.01 M NaF solution in DI water was passed over a 1.9 ID Chemglass chromatography column packed with 22 cm of Octilig® at a rate of 10 mL/min, and collected 50-mL fractions. For each fraction, total dissolved solids (TDS) was measured as well as the fluoride ion activity. Using the latter data, and the calibration equation, the percent of fluoride removed was calculated. Preliminary results indicate quantitative removal.

Undergraduate Posters – Biochemistry, Polymer, Physical, and Computational Chemistry (NES 104)

B-1. Arjun Rammohandas, Peguy Gaboton, and My Lien Dao

“Biochemical Detection of Microsporidemia”

Cell Biology, Microbiology, and Molecular Biology, University of South Florida

Microsporidia are ubiquitous opportunistic parasitic unicellular eukaryotic pathogens that can infect a variety of species, including humans. Distinctive features of microsporidia include a pore wall composed of chitin and the presence of an internal polar filament which is protruded and used by the organism to pierce and inject a host cell with its sporoplasm in the infection process. A protocol was developed to isolate by dilution and differential centrifugation a 12,000 x g pellet from 0.5 ml samples of frozen blood obtained from healthy blood donors previously obtained from Dr. Chamizo (ACH, St. Petersburg, FL). Analysis of the pellet obtained by using a chitin stain and observation on the light microscope showed the presence of microsporidia in a number of samples. These results were further confirmed by binding of the spores onto a chitin-binding matrix, followed by in-situ immunochemical staining using a pan-specific antibody to *Encephalitozoon* species. Of the 28 samples tested so far 13 (46 %) were tested positive, denoting a high incidence of asymptomatic microsporidia carriers. Confirmation by polymerase chain reaction analysis is underway. The present report is the first to show that microsporidemia is prevalent in the asymptomatic population, and hence raised our concern for the use of blood harboring microsporidia in transfusion to immunodeficient or immunosuppressed children.

B-2. John Rodriguez, Dean F. Martin, and Ted Gauthier

“Mathematical Treatment to the Production of TAGs by A Green Alga, Chlorella Vulgaris”

Department of Chemistry, University of South Florida

The interest in biofuels has led to a concomitant interest in the production of triacylglycerides (TAGs) from which methyl esters of long-chain fatty acids are produced for diesel fuels. A previous study by G.M Padilla (Padilla 1970) found that adding glycerol to a toxin, *Prymnesium parvum*, in natural seawater lowered the doubling time by 50%, and increased the yield of the toxin by 200% within 24 hours of adding the neutral lipids to the sample. These results along with others, (Paster et al., 1966) and (Pratt, 1940) have indicated that the first order rate constants for log-growth phase of algal growth can be used to calculate not only growth characteristics (growth constants, k , and doubling times or mean generation times), but the rates of production of significant constituents as well. Examples of the utility of the approach and prospects for current efforts will be considered.

B-3. Revika Matuknauth, Gabriela Wright, Haikou Bian, Steve Enkemann, Bernadette Sosa, Pedro Santiago and Doug Cress

“Transcriptional Repression of the Ret Oncogene by RB”

Department of Chemistry, University of South Florida

Rb is a tumor suppressor gene that regulates many biological pathways. We examined mice in which Rb was excised in osteoprogenitor cells. We find that these osteoblasts are deficient in cell to cell adhesion. We examine the hypothesis that Rb directly regulates the expression of genes involved in cell adhesion. The expression pattern of many genes involved in cell adhesion was significantly affected in Rb (-/-) osteoblasts relative to Rb (+/+) counterparts. PCR was used to quantify the regulation of selected adhesion-related genes by Rb. The proto-oncogene Ret was among the Rb-repressed genes. Ret is a tyrosine kinase that has been shown to phosphorylate beta-catenin, which then initiates gene expression triggering cell cycle. Our findings suggest that Ret may integrate the roles of Rb in both cell cycle control and in control of cell adhesion. Preliminary analysis of the Ret promoter indicates that Rb can indeed repress Ret expression.

B-4. Mary Falatek, Courtney Duboulay and Wayne C. Guida

“Computational Studies of MDM2 Interactions”

Department of Chemistry, University of South Florida

The p53 protein acts as a tumor suppressor and is an important molecule in human cancer. The p53 protein is activated in response to physiological stress, such as cell damage, resulting in apoptosis or cell arrest. Human MDM2, when activated, negatively regulates the p53 gene product by binding to it and restricting its transcriptional activation. Over expression of MDM2 is seen in many human tumors, resulting in suppressed p53 function. Because of its importance in cancer development, the p53–Mdm2 complex is a target for anticancer drug design. The difficulty in developing a suitable inhibitor of MDM2 lies within the uncertainties of the actual MDM2 protein structure. Using the computational molecular modeling program, Maestro™, the 1t4f, 2axi, and 1rv1 crystal structures from the RCSB PDB, as well as an unpublished Moffitt crystal structure of the MDM2 protein were investigated to determine the best model. This was done by creating a correlation curve from the Glide docking scores of known inhibitors of MDM2 and their IC50 values. The results of this project suggest that the Glide scoring is inadequate for measuring findings that are predominately lipophilic.

B-5. Felipe O. Cameroamortegui, Muna H. Barazanji, Emma K. Farrell and David J. Merkler

“GC-MS of Primary Fatty Acid Amide Metabolites from Mammalian Cell”

Department of Chemistry, University of South Florida

The focus of the research being performed revolves around primary fatty acid amides (PFAMs), which are signaling lipids in the central nervous system that have been generating attention in the scientific community. PFAMs being studied include oleamide, linoleamide, and elaidamide. Functions of oleamides include regulation of the sleep/wake cycle and hibernation, modulation of memory processes, and stimulation of Ca²⁺ release, among others. Linoleamide has also been known to increase Ca²⁺ as well as inhibit the erg current in the pituitary cells. Finally elaidamide is an endogenous epoxide hydrolase inhibitor. Other PFAMs include palmitamide and palmitoleamide, as well as tridecanamide from exogenously added tridecanoic acid.

These PFAMs are collected from mouse neuroblastoma and sheep choroid plexus (SCP) cells through cell and media extraction methods described in Sultana and Johnson (2006), derivitized through the use of BSTFA (N,O-bis(trimethylsilyl)trifluoroacetamide) and measured quantitatively by GC-MS. Results are measured after incubation with the corresponding fatty acid over time.

B-6. Emma Kathleen Carter, Carissa Vetromile, and Randy W. Larsen

“Towards the Formation of Novel Hybrid Biological Metal Organic Materials”

Department of Chemistry, University of South Florida

The purpose of this research is to form a hybrid, co-crystallized material comprised of Cytochrome C (Cty C) and [Cu₂(5-OH-bdc)₂L₂]₁₂ [where (5-OH-bdc)₂ = 5-hydroxybenzene-1,3-dicarboxylate and L is a dimethyl sulfoxide, methanol, or water ligand] hydroxylated nanoballs. This hybrid material could possibly stabilize Cty C in other environments and increase its catalytic activity. The OH-nanoball is stable in ~.8 mol fraction of H₂O in methanol. The optical absorption of the OH-nanoball shows a characteristic absorbance at 695 nm that correlates to the MLCT. The intact nanoball itself is not fluorescent, however, when it degenerates, the fluorescence due to Benzene Dicarboxylate is observed at 350nm. The stability of Cty C in methanol is under investigation using specific spectroscopic markers that correlate to a tryptophan. The optical absorption and steady-state emission of the protein in different water methanol solutions is being observed and compared to that of the OH-nanoball.

B-7. Sibel Demirel, Ruben Durand, Daniel Leyva, Mrunal Tailor, Vasiliki Lykourinou, and Li-June Ming

“Cu(II)-Bound Copolymers as Catalysts in Oxidation of Catechols and Oxidative DNA”

Department of Chemistry, University of South Florida

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 (from vinylpyridine). The 1:1 Cu(II) complexes of these copolymers exhibit a significant catalytic activity toward catechol derivatives in the air with or without H₂O₂ and toward DNA cleavage with H₂O₂. Reactive oxygen species such as H₂O₂ occur naturally in the body and can be further activated by redox-active metal ions. The interaction of these Cu(II)-copolymer complexes with H₂O₂ can generate substantially more active intermediates responsible for the significant oxidative activities we observed.

B-8. Timothy Backus, William A. Maza, and Randy W. Larsen

“Synthesis, Structure, and Characterization of A New Crystal Involving a 4,4'-bipyridine Dimer and p-aminobenzoic Acid”

Department of Chemistry, University of South Florida

The interactions underlying the assembly of functionalized small molecules can shed light on those pertaining to higher order supramolecular complexes such as those between protein and ligand as well as pharmaceutical co-crystals. In the present study, a new coordination complex between 4,4'-bipyridine (bpy) dimers and para-amino benzoic acid (*p*-aba) is characterized by single crystal X-ray crystallography and steady-state UV-visual absorption, and theoretical calculations. The resulting non-covalent complex displays interesting charge transfer characteristics which are further described based on experimental results and computational modeling.

B-9. Isaac Dodd, Jason Cuce and Bill J. Baker

“Systematic Management of Research Data Using a Relational DBMS”

Department of Chemistry, University of South Florida

The Medical Malaria Ventures (MMV) project for drug discovery involves testing over 70,000 specimen, demanding an electronic means for data management. A relational DBMS facilitates sorting, tracking, storing, and reporting on a repository of numerical data associated with large volumes of single-copy specimens being tested, fostering systematic procedures for data entry, conveying infrastructure to collected data, providing a management system for directing research electronically, and controlling data manipulation to further benefit research. Extraction and bioassay data could be obtained while recording procedures performed and numerical amounts of each specimen remaining for further testing. The extraction and testing process of each specimen could be streamlined and batch experimentation expedited without concern for individual specimen specifics due to variable data. This process could reduce costs and delivery time on eminent research such as drug discovery, providing an easier framework for performing calculations and statistics on data gathered at any point of time during research and reduces possibilities of error or missing data in results and findings.

B-10. Amanda Preece, Parul Jain, and Julie Harmon

“Conductive Polymer Films”

Department of Chemistry, University of South Florida

Conductive films made of polymers have many different uses to covering computer screens or formed into military weaponry due to the excellent surface resistivity and the ability of the polymer to be electronically conductive. Polymer films were synthesized and characterized by utilizing the various methods of doping, Induction Based Fluid analysis, Differential Scanning Calorimeter, and polarized microscope viewing. Serial dilutions were made to aid in the creation of the polymer films. Doping assisted in the characterization of the film's conductivity. The Induction Based Fluid machine made precise deposit of the polymers. The Differential Scanning Calorimeter helped characterize the polymers by examining the phase transitions of different polymer combinations. The polarized microscope helped characterize the polymer films. The research resulted in the fabrication of polymer films.

B-11. Christian Cioce, Jon Belof, Brian Space, and X. Peter Zhang

“Determination of the Reaction Mechanism of Cobalt-Catalyzed Asymmetric Z-Cyclopropanation of Alkenes via Quantum Computation”

Department of Chemistry, University of South Florida

The use of [Co(3,5-DitBu-ChenPhyrin)], [Co(P1)], as a catalyst for the asymmetric Z-cyclopropanation of alkenes is currently being implemented by Dr. Zhang at the University of South Florida. The reaction of styrene with ethyl α -nitrodiazoacetate, catalyzed by [Co(P1)] in dichloromethane, yielded 99% product with a Z/E isomer ratio of 91:09. Though this cobaltoporphyrin proves to be effective in catalyzing asymmetric Z-cyclopropanation reactions, the mechanism of catalysis is unknown. To better understand this mechanism, we seek to describe the reactants in terms of their physical characteristics via computational methods. For this investigation, Hartree-Fock (HF) and Density Functional Theory (DFT) ab initio methods are implemented, with all calculations computed using GAMESS (General Atomic and Molecular Electronic Structure System). Geometry optimization, orbital analysis, as well as molecular dynamics are a few of the physical parameters used to determine the catalytic mechanism.

B-12. George Rhoden, Christi Young, and Alfredo Cardenas

“A study of the Influenza A Virus Non-structural Protein 1 (NS1) RNA Binding Domain in A Water Box using the NAMD Program for Molecular Dynamics”

Department of Chemistry, University of South Florida

In 1918 a deadly strain of the influenza A virus killed over 40 million worldwide and today kills hundreds of thousands. The influenza A virus mutates rapidly year to year, and after a strain of the virus mutates vaccines are drastically less effective. The non-structural protein 1 (NS1) RNA binding domain changes little after mutation so attacking this domain would be a more effective way to combat this virus. By examining the RNA binding cavity and a solvent-exposed salt bridge of the NS1 RNA binding domain using with Nano-scale Molecular Dynamics (NAMD), we hope to find any flexibilities or instabilities in the binding cavity that could possibly be exploited for drug application. Simulations of the NS1 RNA binding domain were performed with 0.1M KCl and with no salt in a water box over a 50ns period.

B-13. Pamela Castro, Brent Hilker, and Julie Harmon

“Characterization of Polymers”

Department of Chemistry, University of South Florida

Polymers are large molecules made up of repeating units connected by covalent chemical bonds. Currently, several methods are known and used to identify them. The focus of this research is the determination of the average viscosity molar mass (M_v) of poly(methyl methacrylate) (PMMA) through viscometry and the Mark-Houwink Sakurada equation. Using chloroform as a solvent, a capillary viscometer apparatus was used to measure a PMMA standard obtaining intrinsic and relative viscosity along with the viscosity ratio. These values were then plotted utilizing Huggins-Kraemer equations. The molar mass characterization of the PMMA standard was confirmed against its reported value.

Undergraduate Posters – Inorganic and Natural Products Chemistry (NES 108)

I-1. Rosemary Persaud¹, Jaime H. Noguez¹, Tina S. Mutka², Dennis E. Kyle^{2,3}, and Bill J. Baker^{1,3}

“The Chemical Investigation of Antarctic Marine Organisms for Anti-Malarial and Anti-Leishmanial Compounds”

¹Department of Chemistry, ²Department of Public Health and ³Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida

Malaria and Leishmaniasis are two of the thirteen neglected tropical diseases and are responsible for over 500 million severe infections each year. The growing resistance of the parasites responsible for these diseases to current treatments is of worldwide concern, making the search for new drugs of utmost importance. In an effort to combat this resistance, a number of Antarctic specimens were extracted and screened against these parasites. Organisms that showed any activity against either parasite were further separated via chromatography and the compounds responsible for the activity were targeted using bioassay guided fractionation. This paper reports on our efforts to identify active compounds from extracts displaying bioactivity

I-2. Jennifer Drozd, Catherine Geiser, and Mike Zaworotko

“Melatonin Co-crystals”

Department of Chemistry, University of South Florida

Melatonin, a naturally occurring hormone in the body, is appraised as a successful dietary aid for sleeping disorders, a preventative treatment for Alzheimer’s disease, and a protector against certain hemolytic conditions. Melatonin exhibits an extremely quick half-life, low bioavailability and low solubility. With the knowledge of co-crystal engineering, the object is to create a co-crystal with melatonin in which the physical properties lead to better pharmacokinetics. Using the known methods of co-crystal development, melatonin will be experimentally combined with biologically propitious co-crystal formers. Modern techniques, such as the single crystal and powder x-ray diffraction, infrared spectroscopy, and differential scanning calorimetry, prove necessary when analyzing newly formed crystals. With these modern proficiencies readily available, the determination and classification of melatonin co-crystals can be done efficiently.

I-3. Lisha Luttenton, Matt D. Lebar and Bill J. Baker

“Accumulation of Vanadium, Manganese, and Nickel in Antarctic Tunicates”

Department of Chemistry, University of South Florida

Tunicates, marine organisms also known as sea squirts, often sequester rare metals such as vanadium, manganese, and nickel. These rare metals are thought to be utilized by tunicates as a means of defense. Tunicates have been known to accumulate metals by exploiting organic chelators. Tunicate-derived chelators are being tested as possible therapeutic agents for those who have diabetes. Our library of Antarctic tunicates was screened to identify organisms with high concentrations of rare metals. The freeze dried tunicates were digested in hot concentrated acid and then analyzed via atomic absorbance spectrometry. Tunicates containing an exceptional amount of vanadium, manganese, and/or nickel will be further studied to identify any organic chelator present

I-4. Kevin Dubois, Jason A. Perman, and Michael J. Zaworotko

“Synthesis and Characterization of a Series of Isostructural Metal-Organic Frameworks”

Department of Chemistry, University of South Florida

Porous 3-dimensional metal-organic materials (MOMs) are useful in gas sorption applications due to their high surface area to mass ratios and thermal stability. The properties of MOMs can be tuned based on the functionalities of the ligands and metals. TriNA, a novel molecule analogous to nicotinate, is constructed using cocrystal controlled solid state synthesis (C_3S_3) for use as a ligand in metal-organic materials. Single crystal and powder X-ray diffraction confirms that isostructural body-centered cubic frameworks are produced after TriNA is reacted with either cadmium, copper, nickel, or cobalt. The thermal stability and porosity of each framework has been quantified by thermal gravimetric analysis and BET surface area analysis, respectively. Comparative studies of the isostructural frameworks quantify the effect the metal has on material properties.

I-5. **Ryan Baker¹, Jackie Salm¹, Samantha Landolfa¹, Roberto Lopez¹, Tiffany Lanham¹, Minh Cong Nguyen¹, Anangamanjari Pedapudi¹, Michele Summerville¹, Hoangmy Chau¹, Elisa Herrera¹, Matt Lebar¹, Charles Harter¹, Tina S. Mutka², Dennis E. Kyle², and Bill J. Baker¹**

“New Malarial Drugs; Screening Microbes to Treat Malaria”

¹Chemistry Department, University of South Florida

²Department of Global Health, University of South Florida

Malaria, a vector-borne infectious disease, is caused by protozoan parasites of the Plasmodium genus. According to the World Health Organization, in 2006 an estimated 247,000,000 individuals were infected, accounting for 891,000 deaths. Unfortunately, malaria is becoming increasingly more resistant to current drug therapies, therefore there is a need for new anti-malarial drugs. A collection of 70,000 fungi and bacteria are being screened for biological activity towards malaria. Organisms are lysed, their organic compounds extracted and then diluted in DMSO for bio-assay. These samples are being screened for any anti-malarial properties. The hits will be further investigated in an attempt to isolate specific biomolecules that can potentially be used as drug candidates.

I-6. **Mary-Ellen Edmiston, Hiren Shah, Mohamed Alkordi, and Mohamed Eddaoudi**
“A Zeolite-like Metal-Organic Framework as a Platform for the Oxidation and Epoxidation of Alkenes”

Department of Chemistry, University of South Florida

The use of $[\text{In}_{48}(\text{HImDC})_{96}]_{48-}$ encapsulating 5, 10, 15, 20-tetrakis(1-methyl-4-pyridinio)porphyrin tetra(*p*-toluenesulfonate), as a successful catalyst, has been shown with the oxidation of cyclohexane by tert-butyl hydroperoxide. The (In-HImDC)-based rho-ZMOF meets the criteria for a satisfactory host matrix. 1) It possesses large cavities, capable of housing one guest porphyrin per each cavity. 2) Has mild synthesis conditions, incorporating framework construction and porphyrin encapsulation in one step. 3) Maintains its framework integrity in aqueous media. And, 4) has a low affinity for the oxidation products that are attained in the catalysis reactions. The previously successful demonstration of a rho-ZMOF encapsulated metalloporphyrin in enhanced hydrocarbon catalysis was the basis for this experiment. Specifically, it was intended to demonstrate that the presence of the (In-HImDC)-based rho-ZMOF host encapsulating the Mn-porphyrin catalyst in the reaction of tert-butyl hydroperoxide and cyclohexene would bring about the oxidation of cyclohexene in high yield.

I-7. Garrett Craft¹, Wai Sheung Ma¹, Bill J. Baker^{1,3}, Tina S. Mutka², Dennis E. Kyle², and Lilian L. P. Vrijmoed⁴

“Anti-Malarial Bioassay Guided Fractionation of Hong Kong Endophytic Fungal Extracts”
Departments of ¹Chemistry and ²Global Health and ³Center for Molecular Diversity in Drug Design, Discovery and Delivery, University of South Florida, Tampa, FL 33620 and ⁴Department of Biology and Chemistry, City University of Hong Kong, Hong Kong SAR

Endophytic fungi are characteristically found growing within the intercellular tissue of living plants so as to exploit a continual source of carbohydrate. Such relationships are often symbiotic for these fungi produce powerful mycotoxins that reduce host predation. Lipophilic (1:1 DCM: MeOH v/v) extractions performed on 84 strains of endophytes collected from Hong Kong mangroves were screened for anti-malarial activity, with 7 extracts demonstrating activity of interest. Upon normal phase fractionation via MPLC, 19 of the resulting fractions maintained the former activity with 10 that exhibited >67% malarial inhabitation across all four replicate trials of both low and high concentrations. ¹H NMR spectra were obtained from most fractions with further bioassay-guided fractionation of these extracts planned. This poster summarizes both experimental procedure and results of such research to date.

I-8. Alyssa Kennedy, Heather Clarke, and Michael J. Zaworotko

“Designing Cocrystals using the Carboxylate-phenol Supramolecular Heterosynthon”
Department of Chemistry, University of South Florida

Crystal Engineering, the rational design of functional molecular solids, has emerged as one of the most appealing areas of chemical research. Crystal Engineering provides a means for understanding and specifically manipulating the physical properties of existing crystalline solids. A primary means of designing new crystalline solids is cocrystallization. One of the fundamental principles behind the formation of cocrystals is to understand the intermolecular interactions within the crystals. A direct application of this technique was applied by the use of complementary hydrogen-bonding between carboxylates and phenols. This is relevant as there are numerous examples of pharmaceuticals and important biologically relevant compounds which are zwitterionic. There is currently no crystal engineering strategy pertaining to zwitterions and there is limited information in the literature pertaining to co-crystals of zwitterions. The model compound betaine was used to analyze this supramolecular heterosynthon.

I-9. **Emily E. Mevers¹, Rebecca J. Gridley¹, John A. Maschek¹, Nerida G. Wilson², Sydney K. Pierce³, James B. McClintock⁴, Charles D. Amsler⁴, and Bill J. Baker¹**

“A Chemical Investigation into Austrodoris Kerguelenensis, an Antarctic Nudibranch and Elysia Clarki, A Saccoglossan from the Florida Keys”

¹Department of Chemistry; University of South Florida

²Scripps Institute of Oceanography, University of California San Diego, La Jolla, CA

³Division of Integrative Biology, University of South Florida

⁴Department of Biology, University of Alabama at Birmingham, Birmingham, AL

Opisthobranchs are slow-moving and shell-less molluscs found all over the globe. As easy targets for predators, they often possess chemical defenses in the form of either taste-deterrent or toxic compounds. In collaboration with biologists, our lab is investigating nudibranchs and sacoglossans from the Antarctic Peninsula as well as the Florida Keys. *Austrodoris kerguelenensis* is known to contain a family of diterpenoids known as palmadorins. Previous studies have elucidated six palmadorins from a prior collection season; new collections have revealed several novel compounds of the same class displaying the diversity within the species. Accordingly, genetic studies on individuals have shown a high diversity of genetic lineages represented by our sampled animals. Our research will answer questions about how the diversity of the palmadorins varies from year to year, as well as the effect of genetics, size, color, location and depth of the individual organism has on their metabolite profile. The kleptoplastic sacoglossan *Elysia clarki* is a new species of sacoglossan closely related to *E. crispata*. These organisms are known to contain the propionate-derived tridachiapyrones, however no chemical investigation has been done on *E. clarki* collected from the Florida Keys. We have isolated the known compounds crispatone and tridachiapyrone A, as well as other known and novel metabolites.

I-10. **Hiren Shah, Mary-Ellen Edmiston, Mohamed Alkordi, and Mohamed Eddaoudi**

“Zeolite-like Metal-Organic Frameworks: Platforms Encapsulating Lewis Acid Catalysts”

Department of Chemistry, University of South Florida

Zeolite-like metal organic frameworks (ZMOFs) have recently been brought to the forefront of research due to the many applications of their extra large pores, one of which is catalysis. The anionic framework of the Indium-imidazoledicarboxylate based rho-ZMOF can accommodate many different cationic species of Lewis Acid catalysts, such as Pd²⁺, Zn²⁺, and Al³⁺. These three Lewis Acid catalysts show activity towards Diels-Alder reactions. The use of rho-ZMOF has the potential to facilitate the purification process simply through filtration in the use of these catalysts in heterogeneous mixtures. Heterogeneous catalysis systems, in general, offer the advantage of catalyst recyclability and thus improved turn over number (TON). The porosity of rho-ZMOF also offers a size limitation that could potentially prove useful imparting regioselectivity to the catalytic reaction.

I-11. Franka Co, Uma Hannubal, Jackie Wood, Natalie Wright, Jeremy Beau, and Bill J. Baker

“Drug Discovery from Floridian Mangrove Endophytes”

Department of Chemistry, University of South Florida

With the increasing cases of cancer and drug-resistant infectious diseases, scientists in the pharmaceutical industry are diligently working to stay ahead. In an effort to help in this global health situation, our group is seeking new drugs from natural products. Recent studies show that mangrove endophytic microbes produce potent metabolites that may be active against those illnesses. We are building a collection of mangrove endophytes from Florida. Collected in the field and cultured in the laboratory, all are chemically extracted and then screened against cancer, malaria, leishmaniasis, and influenza as well as common microbes such as *E. coli*, *S. aureus*, *P. aeruginosa*. This paper reports the initial screening results.

I-12. Nicholas Zoumberos, Ryan Luebke, and Mohamed Eddaoudi

“Targeted Synthesis of Metal Organic Frameworks Featuring Single-Ion Molecular Building Blocks”

Department of Chemistry, University of South Florida

Metal-Organic Frameworks (MOFs) featuring single-ion molecular building blocks (MBBs) are currently of great interest due their ability to form highly porous crystalline structures. MOFs offer tunable platforms for gas separation, gas sequestration, catalysis, drug delivery, and many other applications. An important strategy for design and rational synthesis of new MOFs is targeting specific coordination configurations around the metal centers to generate a variety of structures with different topologies. The strategy presented in this poster features multi-dentate heterochelated ligands (2,5-pyridinedicarboxylic acid) to impart rigidity and varying reaction conditions to direct the coordination configuration.