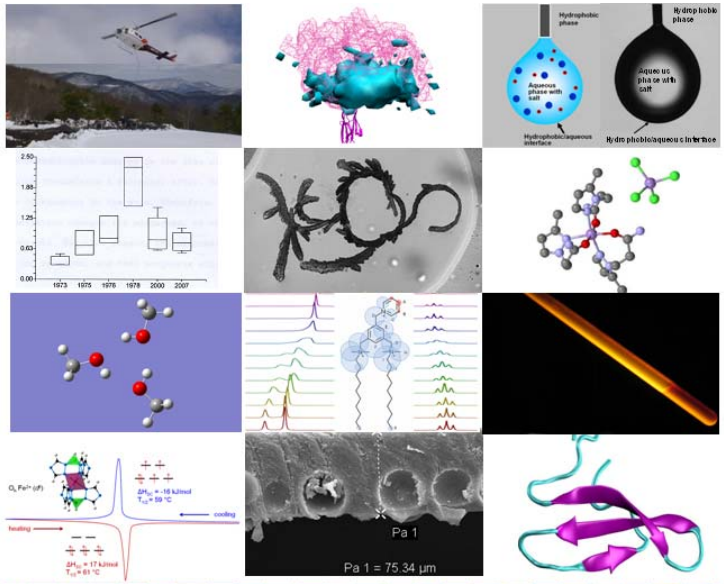
JAMES MADISON UNIVERSITY®

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

38th Annual



Spring Undergraduate Research Symposium

THURSDAY MARCH 21, 2013

ORAL SESSION I: 2:30 – 4:00 PM (ISAT 259)

POSTER SESSION: 4:15 – 5:15 PM (PHYS/CHEM LOBBY)

FRIDAY MARCH 22, 2013

ORAL SESSION II: 1:30 – 3:15 PM (ISAT 259)

KEYNOTE ADDRESS: 3:30 – 4:30 PM (ISAT 159)

See back cover for image description.

Past Keynote Speakers

Each year we feature a keynote speaker for the Department's annual Spring Undergraduate Research Symposium. We are honored to have had speakers who are alumni of the department and are willing to come back and share with our students their experiences of "life after JMU". We thank each of these speakers and look forward to future alumni participation in the Department of Chemistry Spring Undergraduate Research Symposium.

YEAR	JMU CLASS	SPEAKER	AFFILIATION
2013	1999	**Dr. Christy Vestal Martin**	*Vorbeck Materials*
2012	1994 N/A	**Dr. Melissa C. Rhoten** **Dr. Orde Q. Monro**	*Longwood University* *University of KwaZulu-Natal*
2011	1992	**Dr. Morgan S. Sibbald**	*The Sherwin-Williams Company*
2010	1988	**Dr. Kevin Morris**	*Carthage College*
2009	1988	**Dr. Chris E. Holmes**	*The University of Vermont College of Medicine*
2008	1995	**Dr. Jonathan Dattlebaum**	*University of Richmond*
2007	1987	**Dr. Elizabeth Perry (M.D.)**	*Signature Healthcare, Inc.*
2006	1967	**Dr. Carolyn Abitbol (M.D.)**	*University of Miami (FL) School of Medicine*
2005	1975 1976	**Dr. Daniel Downey** **Dr. Gary Rice**	*James Madison University* *College of William and Mary*
2004	1987	**Dr. James (Dusty) Baber**	*National Institutes of Health*
2003	1984	**Dr. Fred King**	*West Virginia University*
2002	1977	**Dr. Roger Bertholf**	*University of Florida School of Medicine*
2001	1979	**Mrs. Katheryn Lam**	*International Business Machines*
1999	1987	**Dr. Jose Madalengoitia**	*University of Vermont*
1997	1986	**Dr. Fred R. Kinder**	*Novartis Research Institute*
1996	1976	**Dr. Terry O. Trask**	*DuPont Chemicals*
1995	1973	**Dr. Carl Lentz**	*Eastman Fine Chemicals*
1994	1990	**Dr. Michele A. Kelly**	*University of Maryland Baltimore County*
1993	1985	**Dr. Cynthia K. Fallon**	*DuPont Chemicals*
1992	1983	**Dr. Laurie Locascio**	*National Institute of Standards and Technology*
1991	1983	**Dr. Noreen Naiman**	*North Carolina School of Science and Mathematics*
1990	1982	**Dr. Matthew T. Stershic**	*Atomchem North Amercia*
1989	1982	**Dr. Michael Kinter**	*Cleveland Clinic Lerner Research Institure*
1988	N/A	**Dr. Thomas J. Meyer**	*Los Alamos National Laboratory*
1987	1980	**Dr. Steven Davis**	*Naval Research Laboratory*
1986	1980	**Dr. Steven A. Hackney**	*Michigan Technological University*
1983	1978	**Dr. Richard B. Lam**	
1982	1975	**Dr. Daniel Downey**	*West Virginia University*
1981	1959	**Mr. Ronald E. Ney**	*Environmental Protection Agency*
1980	N/A	**Dr. Stanley G. Sunderwirth**	*Metropolitan State College (Denver, CO)*
1979	1973	**Dr. Carl Lentz**	*Eastman Fine Chemicals*

38th Annual Department of Chemistry and Biochemistry

Spring Undergraduate Research Symposium Keynote Address

Friday, March 22, 2013 at 3:30pm
ISAT Room 159

"Graphene: Perspectives on Moving a New Nanomaterial from Laboratory Curiosity to Commercial Products"

Christy Vestal Martin (JMU Class of 1999), Ph.D.
Vorbeck Materials
Jessup, MD

Christy Vestal Martin received her B.S. in chemistry from James Madison University in 1999. Her undergraduate work investigating chemical reactions during chemical vapor deposition (CVD) of copper, iron, and chromium films, completed under the direction of Dr. Thomas DeVore, was awarded JMU's Phi Kappa Phi Best Honors Thesis. In 2004, Christy received her Ph.D. in Inorganic Chemistry from Georgia Tech where she was a Molecular Design Institute fellow. Her thesis work focused on the synthesis and property evaluation of magnetic nanoparticles. After graduation, Dr. Martin worked as a Research Scientist for Universal Technology Corporation (UTC) at the Air Force Research Laboratory (AFRL). At AFRL she was responsible for the preparation and characterization of the electromagnetic properties of novel nanocomposites containing dispersed inorganic nanoparticles, core/shell magnetic particles, and carbon nanotubes. Dr. Martin has also worked as a Research Scientist at Luna Innovations focusing on the development of conductive coatings, corrosion resistant coatings, low observable materials, antennas, and energy storage/capacitors. She joined Vorbeck Materials in 2009 where she is currently responsible for product development and commercialization of graphene-based products in electronics, energy, and composites technology sectors and manages Vorbeck's Energy division. In 2012, Dr. Martin was part of a team recognized with a prestigious *R&D Magazine* R&D 100 award for "Graphene Nanostructures for Lithium Batteries".

Oral Session I: Thursday March 21st *(ISAT 259)*		
2:30 - 2:45	Michael Poltash, Brian Huffman, and Dr. Christine Hughey	Effect of polar protic and polar aprotic solvents on negative ion electrospray ionization and chromatographic separation of small acidic molecules.
2:45 - 3:00	Caroline Campbell, Matthew Dent and Dr. Barbara A. Reisner	New Polymorphs in the Zero-Dimensional Transition Metal Hydrotris(triazolyl)borates: M[BH(trz)3]2 (M= Fe, Co, Ni, Zn)
3:00 - 3:15	Jhosdyn Barragan, Gabriel Fitzgerald, Jul Kim, Daniel Moon, Jade LaDow, Kyle Bonifer, Nicholas Minahan, Jason Floyd, Dr. Kevin P. C. Minbiole, Dr. Kyle Seifert and Dr. Kevin L. Caran	The Synthesis and Study of Novel Polycephalic and Gemini Amphiphilic Derivitives of Mesitylene
3:15 - 3:30	Brian J. Reeves and Dr. Brycelyn M. Boardman	The Synthesis of Thienyl Phosphine Ligands for Polymerizable Cobalt Chalcogenide Clusters.
3:30 - 3:45	Rima Janusziewicz, Ryann Diehl and Dr. Christine Hughey	Thermal Stability of Monomeric and Oligomeric Proanthocyanidins in Almonds
3:45 - 4:00	Gabriel Fitzgerald, Jhosdyn Barragan, Jul Kim, Daniel Moon, Jade LaDow, Kyle Bonifer, Nicholas Minahan, Jason Floyd, Dr. Kevin P. C. Minbiole, Dr. Kyle Seifert and Dr. Kevin L. Caran	Modifications of Mesitylene and m-Xylylene Based Amphiphilic Architectures and the Effects on Colloidal and Antibacterial Activity.

Poster Session: Thursday March 21st 4:15 – 5:15 pm *(Ph/Ch lobby)*	
Zachary S. Bartley, Nikita Alexevich and Dr. Brycelyn M. Boardman	Design and Synthesis of Conjugated Polymers for Photovoltaic Applications
Tracy Caldwell and Dr. Nathan Wright	Methods to purify the Ig2 domain and the ZIg9-10 duel domain system of the muscle protein obscurin
Karen Corbett, Dr. Vince LiCata, Renata Esquillo, and Dr. Gina MacDonald	Monitoring the Effect of Salts on the Structure, Unfolding, and Aggregation of the DNA Repair Protein, RecA, Utilizing Attenuated Total Reflectance Infrared Spectroscopy
David D'Amico, Dr. Donna S. Amenta, and Dr. John W. Gilje	Metal complexes with substituted n-pyrazolylpropanamide ligands
Mitchell Delusa, Caroline Livick, Emily Todd, and Dr. Christopher Berndsen	Multi-Enzyme Spectrophotometric Assay for Ubiquitin Conjugation
Matt Dent, Caroline Campbell, Austin Muetterties and Dr. Barbara Reisner	Metal organic frameworks derived from the hydrotris(1,2,4-triazolyl)borate ligand: M[BH($C_2H_2N_3$)$_3$] (M = Li, Na, K)
Kelsey DeWitt, Justin Hagerman and Dr. Yanjie Zhang	Cation-Π Interactions at the Air/Water Interface
Steven Dirks, Dr. Donna S. Amenta and Dr. John Gilje	Synthesis and Spectroscopic Characterization of a Novel Ruthenium Complex with the Acrylamide-based ligand N-pyrazolylpropanamide
Kelly Du Pont, Ashton Knighton and Dr. Christopher Berndsen	Purification and Structural Analysis of the anti HIV-1 protein, BST-2
Sammy Herold, Dr. Donna S. Amenta and Dr. John W. Gilje	Synthesis and Characterization of RuClNO(dppmO)$_2^+$BF$_4^-$ from Ruthenium Based Compounds and Ligands
Chelsey M. McMinn and Dr. Christine A. Hughey	Beer-omics: Molecular fingerprinting of craft beers by positive and negative ion ESI q-TOF MS
Neil Mehta, Rafael Snell-Feikema and Dr. Thomas DeVore	Absorption of Acetic Acid on Copper Minerals
Matthew Oehler and Dr. Nathan Wright	The Purification and Characterization of Ig1-2 Domain of Giant Muscle Protein Obscurin
Katie Olsonowski, Dr. Donna S. Amenta and Dr. John Gilje	Synthesis and Characterization of Ruthenium Complexes Containing the Bis-diphenylphosphinopropane monoxide (dpppO) Ligand
Reid Putney, Dr. Chris Berndsen and Dr. Nathan Wright	Structural and mechanistic investigation of ubiquitination
Rebecca Patterson and Dr. Debbie Mohler	The synthesis of tripod molecules for ultrafast photolysis studies
Michael Rudloff, Alec Woosley and Dr. Nathan Wright	Toward Structural Analysis of the M10 Domain of Titin
Emigdio Turner, Anthony DiDomenico, Alexa DeLuca, Justin Hagerman and Dr. Yanjie Zhang	Two-Component Low Molecular Weight Organogels Formed by Amino Acid Surfactants Amines
Courtney Wardwell, Alan Mo, Dr. Brian Augustine, Dr. Chris Hughes, Dr. Thomas DeVore	Improving the Adhesion of Au Thin Films to PMMA

Oral Session II: Friday March 22nd *(ISAT 259)*		
1:30 - 1:45	Natalie Trinh, Diana Al Husseini, Branden Deyerle and Dr. Yanjie Zhang	Effects of Anions on the Interfacial Tension at the Hydrophobic/Aqueous Interface
1:45 - 2:00	Logan Meyer and Dr. Nathan Wright	Low Resolution Studies of Ig 58 and 59 of Obscurin Using Small Angle X-Ray Scattering
2:00 - 2:15	Michael Metrick and Dr. Gina MacDonald	Spectroscopic Studies on the Influence of Buffer Structure and pH on the Thermal Stability of RecA Reveal Distinct Aggregation States
2:15 - 2:30	Caroline Livick, Emily Todd and Dr. Chris Berndsen	Investigations of the Structure and Stability of Thermotoga maritima Lactate Dehydrogenase
2:30 - 2:45	Arlie Bagley and Dr. Thomas DeVore	Investigation of the Effects of Methanol on Hydrogen Bonding in Various Solvents using NMR
2:45 - 3:00	Alec N. Woosley and Dr. Nathan T. Wright	Characterization and Structural Analysis of Obscurin, a Giant Intracellular Protein Involved in Muscle Integrity and Maintenance
3:00 - 3:15	Skylar White, Dr. Brian Augustine and Dr. Chris Hughes	Real-Time Micro-Phase Separation Kinetic Analysis of POSS-MA Thin Films Using Atomic Force Microscopy
3:15 - 3:30	-- break --	
Keynote Address: Friday March 22nd *(ISAT 159)*		
3:30 – 4:30	Dr. Christy Vestal Martin	Graphene: Perspectives on Moving a New Nanomaterial from Laboratory Curiosity to Commercial Products

Keynote Address

Friday, March 22, 2012 at 3:30pm
ISAT Room 159

"Graphene: Perspectives on Moving a New Nanomaterial from Laboratory Curiosity to Commercial Products"

Christy Vestal Martin (JMU Class of 1999), Ph.D.
Vorbeck Materials
Jessup, MD

A challenge in the commercialization of new nanomaterials is how to translate the significant physical property advantages afforded by the new materials into practical applications. Graphene is two-dimensional (2D) nanomaterial that has generated significant interest (most recently with the 2010 Nobel Prize in Physics awarded to Geim and Novoselov for their work isolating individual graphene sheets) due its unique mechanical, thermal, and electronic properties. This presentation will focus on translating the basic research on graphene's breakthrough materials properties into real-world products. Examples will be given for development of graphene-based conductive inks that harness the exceptional conductivity and mechanical properties of graphene into ultra-flexible and robust inks and coatings for the printed electronics applications. Graphene also offers unique advantages as an electrode material in lithium ion batteries because it is strong, thin and highly conductive. Examples will be given how the unique performance properties of graphene combined with specifically designed chemical modification of the graphene and a novel porous structure has advanced the limit on in what is feasible for lithium battery energy storage.

STUDENT ABSTRACTS

(Student presenters underlined)

Investigating hydrogen bonding between methanol and various solvents using NMR

Arlie Bagley and Dr. Thomas DeVore
Department of Chemistry and Biochemistry, James Madison University

The activity coefficients at infinite dilution resulting from the hydrogen bonding between methanol and various different solvents were determined using NMR By adding microliters of methanol to the solvents and taking ^{1}H NMR, the OH shift could be tracked as a function of concentration. Once the relationship between the observed chemical shifts and the composition are established, the interaction coefficients can be determined by relating the observed chemical shifts to those of the pure solvent and infinitely dilute solutions. NMR was done in a double tube to establish a neat value for methanol. The chemical shift of the infinitely dilute solution was established by extrapolating the chemical shift versus concentration curve to zero concentration. The interaction coefficients can then be used to determine the activity coefficient at infinite dilution and to estimate the strength of the methanol solvent interaction.

The Synthesis and Study of Novel Polycephalic and Gemini Amphiphilic Derivitives of Mesitylene

Jhosdyn Barragan,[1] Gabriel Fitzgerald,[1] Jul Kim,[1] Daniel Moon,[1] Jade LaDow,[2] Kyle Bonifer,[2] Nicholas Minahan,[2] Jason Floyd,[2] Dr. Kevin P. C. Minbiole,[3] Dr. Kyle Seifert[2] and Dr. Kevin L. Caran[1]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Biology, James Madison University
[3]Department of Chemistry, Villanova University

Derivatives of mesitylene were synthesized in order to prepare a series of amphiphiles with *n* benzylic quaternary ammonium headgroups and 3 - *n* benzylic pyridinium headgroups, where *n* = 0 - 3. Reaction temperature, water content, and solvent polarity were found to be key factors in controlling the synthesis of various derivatives. The series includes compounds with tail lengths from 8 – 16 carbons, including derivatives where *n* = 0, 2 and 3. Critical micelle concentration values of final compounds taken through both conductivity and ^{1}H NMR measurements suggest an inverse relationship between amphiphile "tail" length and CMC value. Antibacterial studies also suggest an inverse relationship between "tail" length and antibacterial activity, with the 12 carbon length derivative showing the most promise for compounds where *n* = 2.

Design and Synthesis of Conjugated Polymers for Photovoltaic Applications

Zachary S. Bartley, Nikita Alexevich and Dr. Brycelyn M. Boardman
Department of Chemistry and Biochemistry, James Madison University

Poly(3-hexylthiophene) (P3HT) and poly[2,1,3-benzothiadiazole-4,7-diyl[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl]] (PCPDTBT) are commonly used donor materials in bulk heterojunction solar cells. P3HT forms ordered domains producing efficient cells but are plagued by a small range of absorption; PCPDTBT however suffers from the reverse. The synthesis of the model monomer 3-(6-thienylhexyl)thiophene (1) was used to determine the most efficient reaction pathway. The synthesis of 1 was performed in a one-pot reaction by sequential addition of 3-bromothiophene to an in-situ generated alkyl bisgrignard. GC-MS was used to monitor the progress and to identify the side products of the reaction. Compound 1 was purified using column chromatography and characterized by 1H and 13C NMR, UV-Visible spectroscopy. Compound 1 was then converted into the dibromo species to obtain a monomer capable of polymerization. Various molecular weights of polymer have been obtained and were characterized by NMR and gel permeations chromatography (GPC). UV-visible spectroscopy and fluorescence measurements were used to probe the optical and electronic properties of the polymers in solution and in the solid state.

Methods to purify the Ig2 domain and the Zlg9-10 duel domain system of the muscle protein obscurin

Tracy Caldwell and Dr. Nathan Wright
Department of Chemistry and Biochemistry, James Madison University

Obscurin (800-900 kD) is a giant muscle protein vital to muscle cell organization and maintenance. Mutations to obscurin and surrounding proteins are linked to cardiomyopathies and muscular dystrophies. Here, we describe initial steps to purify one of the domains of obscurin (Ig2) via affinity and size exlcusion chromatrography. These raw materials will be used to collect heteronuclear multidimensional NMR spectra, with the eventual goal of solving the high resolution solution structure of this domain. We are also using these same techniques to purify a dual-domain system, titin Zlg9-10.

New Polymorphs in the Zero-Dimensional Transition Metal Hydrotris(triazolyl)borates: $M[BH(trz)_3]_2$ (M= Fe, Co, Ni, Zn)

Caroline Campbell, Matthew Dent and Dr. Barbara A. Reisner
Department of Chemistry and Biochemistry, James Madison University

Four new coordination complexes have been synthesized using the hydrotris(triazolyl)borate anion, $[BH(trz)_3]^-$ (trz=1,2,4-trizolate). $K[BH(trz)_3]$ (**1**) was synthesized from the reaction between potassium borohydride (KBH_4) and excess triazole (Htrz). DMF solutions of $FeCl_2{\cdot}4H_2O$, $Co(NO_3)_2{\cdot}6H_2O$, $Ni(NO_3)_2{\cdot}6H_2O$, and $Zn(NO_3)_2{\cdot}6H_2O$ were mixed with $K[BH(trz)_3]$ to produce $M[BH(trz)_3]_2$ M= Fe (**2**), Co (**3**), Ni (**4**), Zn (**5**)). Violet (**2**), yellow-orange (**3**), lavender (**4**), and colorless (**5**) prisms were isolated from the reaction mixture after five hours to three days. The IR stretch at 2495 cm^{-1} indicates the presence of the $[BH(trz)_3]^-$ ligand. Powder X-ray diffraction data (PXRD) confirm that FeL_2, CoL_2, NiL_2, and ZnL_2 are isostructural. Compounds **2**, **3**, **4,** and **5** crystallize in the orthorhombic space group *P*bca (Fe^{2+} *a* = 13.2789(13) Å, *b* = 8.7219(9) Å, *c* = 17.6376(18) Å; Co^{2+} *a* = 12.9445(6) Å, *b* = 8.7650(4) Å, *c* = 18.6843(8) Å; Ni^{2+} *a* = 13.0574(5) Å, *b* = 8.7675(3) Å, *c* = 18.3889(7) Å; Zn^{2+} *a* = 12.8688(6) Å, *b* = 8.7795(4) Å, *c* = 18.8388(9) Å). The metal center is chelated by two tridentate $[BH(trz)_3]^-$ ligands. The complexes are packed in face-centered fashion. The structures and magnetic properties of these materials will be discussed.

Monitoring the Effect of Salts on the Structure, Unfolding, and Aggregation of the DNA Repair Protein, RecA, Utilizing Attenuated Total Reflectance Infrared Spectroscopy

Karen Corbett,[1] Dr. Vince LiCata,[2] Renata Esquillo,[1] and Dr. Gina MacDonald[1]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Biological Sciences, Louisiana State University

RecA is an Escherichia coli protein that performs the DNA strand-exchange reaction used in DNA repair. Previous Cirular Dichroism (CD) studies in our lab have shown that the secondary structure, stability, and aggregation behavior of RecA are affected differently by various Hofmeister salts. RecA followed the reverse anionic Hofmeister series in these CD studies. Upon the addition of chloride salts RecA did not completely denature even at 105°C. Sulfate salts completely unfolded RecA at temperatures lower than the control. Here we used attenuated total reflectance infrared (ATR-IR) spectroscopy to further monitor observed changes in the secondary structure, stability, and aggregation behavior of RecA upon the addition of Hofmeister salts. Additional salts beyond those used in the previous CD study were used in our study to further elucidate the effects of chaotropes vs. kosmotropes on RecA. Second derivatives of the infrared spectra were utilized to help isolate and identify structural changes.

Metal complexes with substituted n-pyrazolylpropanamide ligands

David D'Amico, Dr. Donna S. Amenta, and Dr. John W. Gilje
Department of Chemistry and Biochemistry, James Madison University

The reactions of substituted N-pyrazolylpropanamide ligands to various metal ions were carried out to study the coordination chemistry of these ligands. These new ligands, N-3-methylpyrazolylpropanamide (L1), N-pyrazolyl-N,N-dimethylpropanamide (L2), N-pyrazolyl-2-methylpropanamide (L3), and N-pyrazolyl-N-isopropylpropanamide (L4), were synthesized and allowed to react with $MnCl_2{\cdot}4H_2O$, $NiCl_2{\cdot}H_2O$, and $Ce(NO_3)_3{\cdot}6H_2O$. The structure of the compound formed from the reaction L1 with $MnCl_2{\cdot}4H_2O$ was determined by x-ray crystallography and shown to be the $[Mn(L1)_3][MnCl_4]$. Further, the x-ray data implies that two isomers of L1 have formed. This is consistent with spectroscopic data on L1. In other cases crystals were formed and are being characterized.

Multi-Enzyme Spectrophotometric Assay for Ubiquitin Conjugation

Mitchell Delusa,[1] Caroline Livick,[2] Emily Todd,[2] and Dr. Christopher Berndsen[2]
[1]Department of Biology, James Madison University
[2]Department of Chemistry and Biochemistry, James Madison University

Ubiquitin is a 76-residue protein, found in all eukaryotic cells, that plays a crucial role in protein degradation and various other life processes. Despite the major role Ubiquitin plays in many cell processes, the current assays of Ubiquitin conjugation are time intensive and qualitative. We are developing an assay for measuring Ubiquitin activation using the enzymes pyruvate phosphate dikinase (PPDK) and lactate dehydrogenase (LDH) from thermophilic organisms. PPDK catalyzes the conversion of AMP into ATP, pyrophosphate into phosphate, and phosphoenolpyruvate to pyruvate. LDH catalyzes the conversion of pyruvate to lactate and NADH to NAD+. When Ubiquitin is activated by a Ubiquitin conjugating enzyme the products of the reaction act as the substrates for PPDK and the products of the PPDK reaction act as the substrates for LDH. The third step of the assay catalyzed by LDH converts NADH to NAD+ which can be monitored using UV-Vis spectroscopy at 340 nm. We have successfully purified both PPDK and LDH. Preliminary assay data on the PPDK/LDH coupled reaction has been obtained, as well as, data showing the effects of activators and inhibitors on LDH. The temperature range and ideal buffers for both enzymes have been demonstrated using circular dichroism. The future experiments in the lab will feature more testing of the two-enzyme cascade at different temperatures, adding ubiquitin to the assay, crystallization of the thermophilic enzymes, and research and development of potential ubiquitin inhibitors.

Metal organic frameworks derived from the hydrotris(1,2,4-triazolyl)borate ligand: $M[BH(C_2H_2N_3)_3]$ (M = Li, Na, K)

Matt Dent, Caroline Campbell, Austin Muetterties and Dr. Barbara Reisner
Department of Chemistry and Biochemistry, James Madison University

Metal-organic frameworks with zeolitic topologies are a class of porous materials that have applications in gas separation and storage due to their ability to selectively adsorb certain gases. In order to expand this class of materials, $M[BH(trz)_3]$ (M=Li, Na, K; trz = 1,2,4-triazolate) compounds were synthesized from MBH_4 in a triazole flux. By varying the size of the cation, different framework topologies and ligand coordination modes were observed. $K[BH(trz)_3]$ crystallizes from acetonitrile as a non-porous 3-D framework with the hex topology. The framework contains 7-coordinate, face-capped trigonal prismatic K^+ ions that form dimers. $Na[BH(trz)_3]$•DMF crystallizes from DMF as a potentially porous 3-D framework with a dia topology. Na^+ ions are octahedrally coordinated and solvent molecules occupy the pores of the framework in a 1:1 ratio. Two isostructural compounds form as 2-D corrugated sheets with the metal ion in tetrahedral coordination. $Li[BH(trz)_3]$ crystallized directly from acetonitrile and $Cu[BH(trz)_3]$ crystallized from isopropanol in a metathesis reaction between $K[BH(trz)_3]$ and CuI. The structures and characterization of these materials will be presented.

Cation-Π Interactions at the Air/Water Interface

Kelsey DeWitt, Justin Hagerman and Dr. Yanjie Zhang
Department of Chemistry and Biochemistry, James Madison University

A cation-Π interaction is known as a strong, non-covalent binding force formed from electrostatic interactions. These interactions have been found to contribute to protein secondary structures and protein-ligand interactions. Surface pressure-molecular area (Π-A) isotherms were used to study these interactions at the air/water interface. A surfactant, of either L-phenylalanine or L-tryptophan, was spread as a monolayer over a subphase, which contained varying concentrations of L-arginine at pH 7. It was found that the binding of L-arginine to L-tryptophan is stronger than that to L-phenylalanine at the air/water interface. Current experiments are being performed to determine how changing the subphase to L-Lysine will affect the interactions the aromatic ring and the cations on phenylalanine and tryptophan.

Ruthenium Complex Compounds with the Acrylamide-based Ligand N-pyrazolylpropanamide and Spectroscopic Analysis

Steven Dirks, Dr. John Gilje and Dr. Donna Amenta
Department of Chemistry and Biochemistry, James Madison University

The reactions between two ruthenium complexes, mer- $RuHCl(CO)[PPh_3]_3$ and $Ru(NO)Cl_3$, with the ligand N-pyrazolylpropanamide were performed and analyzed using NMR and IR spectroscopy. These data indicate that a bulk of the PPh_3 is displaced, presumably by N-pyrazolylpropanamide but that a portion of the $RuHCl(CO)[PPh_3]_3$ isomerizes to the previously unknown facial isomer. Infrared spectra of the product of the reaction between $Ru(NO)Cl_3$ and N-pyrazolylpropanamide suggest the formation of a new complex. The characterization of the complex is continuing.

Purification and Structural Analysis of the anti HIV-1 protein, BST-2

Kelly Du Pont,[1] Ashton Knighton[2] and Dr. Christopher Berndsen[1]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Biology, James Madison University

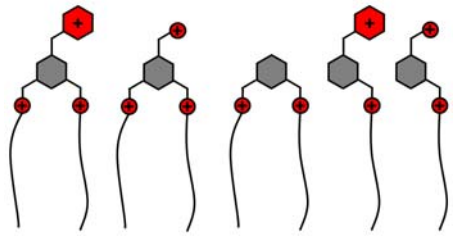
BST-2/tetherin is an extracellular transmembrane protein that inhibits the release of the HIV-1 and other viruses from the cell surface. BST-2 is a homo-dimer that forms a coiled-coil motif, and contains three disulfide bonds, which connects the two subunits. Recent work has suggested that the BST-2 ectodomain is structurally dynamic. Substitution of a heterologous coiled-coil motif resulted in a functional protein while extension of the ectodomain with non-coiled-coil sequences, the ectodomain showed a loss of function. This study focuses on the structure and function of BST-2 with the goal of connecting protein structure to cellular function. We have purified the ectodomain of BST-2 to determine whether BST-2 forms a complete coiled-coil, as suggested by the crystal structures, or whether there are flexible sections, as suggested by the recent literature. We used circular dichroism, limited proteolysis and native polyacrylamide gel electrophoresis (PAGE) to analyze several structural aspects of the BST-2 ectodomain. Reduction of the disulfide bonds does not alter the secondary structure of BST-2. Future work will look at the membrane bound protein of BST-2.

Modifications of Mesitylene and *m*-Xylylene Based Amphiphilic Architectures and the Effects on Colloidal and Antibacterial Activity

Gabriel Fitzgerald,[1] Jhosdyn Barragan,[1] Jul Kim,[1] Daniel Moon,[1] Jade LaDow,[2] Kyle Bonifer,[2] Nicholas Minahan,[2] Jason Floyd,[2] Dr. Kevin P. C. Minbiole,[3] Dr. Kyle Seifert[2] and Dr. Kevin L. Caran[1]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Biology, James Madison University
[3]Department of Chemistry, Villanova University

Department of Chemistry and Biochemistry, James Madison University

In recent years drug resistant bacterial strains have become increasingly more common, leading to a decrease in the effectiveness of traditional antibiotics. It is therefore necessary to develop new antimicrobial compounds that function by diverse mechanisms in order to circumvent resistance. Surface active antimicrobial compounds, acting by either disruption of membrane stability or some more specific mechanism, are promising candidates for new antimicrobials. Changes in membrane composition, a very costly adaptation, are necessary in order to circumvent the activity of these compounds making resistance far less likely. Surface active compounds are most commonly amphiphilic in nature, allowing for interaction with polar and nonpolar regions of lipid membranes. Charged, polar head groups added to amphiphilic motifs allow for columbic interaction between amphiphilie and membrane, and increased solubility due to increased polar nature. Mesitylene and meta-xylene based amphiphiles were synthesized that contained two or three head groups and one or two tails. Pyridine or trimethylamine head groups were initially installed and were separated by the differing polarity of charged products and neutral starting materials. Dimethylamine substituents containing hydrocarbon tails were subsequently installed. This synthetic approach was used to make various amphiphilic architectures that can be used to determine the effect of different head groups on antimicrobial and colloidal activity.



Synthesis and Characterization of $RuClNO(dppmO)_2^+BF_4^-$ from Ruthenium Based Compounds and Ligands

Sammy Herold, Dr. Donna S. Amenta and Dr. John W. Gilje
Department of Chemistry and Biochemistry, James Madison University

Ruthenium based compounds are useful as catalysts for organic synthesis. This study concentrates on the chemistry of $RuCl_3NO(dppmO)_2$. Often ruthenium complexes become catalytically more active if they can be converted into cations. To achieve this, $RuCl_3NO(dppmO)_2$ was allowed to react with two equivalents of $AgBF_4$. A complex can be isolated whose NMR spectra indicate two chelating $Ph_2PCH_2P(O)Ph_2$ (dppmO) ligands and whose IR spectrum shows the presence of a nitroso group. The ^{19}F NMR indicates the presence of BF_4^-. We postulate that two chlorines have been removed and that the complex is $[RuClNO(dppmO)_2](BF)_2$.

Thermal Stability of Monomeric and Oligomeric Proanthocyanidins in Almonds

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The thermal stability of monomeric and polymeric flavan-3-ols, or proanthocyanidins, was measured in blanching experiments as a function of time. The monomeric standards catechin and epicatechin were blanched in 100ºC (HW) for 20 min and aliquots of blanch water were collected in triplicate. The initial and final concentrations of catechin were determined to be 4.84±0.23 and 4.73±0.6 ppm respectively indicating the thermal stability of catechin. Epicatechin was determined to be thermally instable with initial and final concentrations of 2.54±0.08 and 0.29±0.01 ppm respectively correlating to an increase in catechin concentration, indicative of isomerization. Almonds were subjected to the same treatment as a function of time and temperature and were submerged in 25ºC (RT, the control) and 100ºC (HW) water for 2 min. and then removed. Aliquots of blanch water were collected in triplicate over 20 min. Therefore, changes in proanthocyanidins, and their monomers, in the first two minutes were attributed to blanching; changes from 2-20 min. were attributed to thermal instability in the hot blanch water. Proanthocyanidins indentified in both blanching conditions were determined to have a constant concentration within experimental error and therefore determined to be thermally stable. Proanthocyanidins identified only under HW conditions had variable concentrations indicative of thermally instability.

Investigations of the Structure and Stability of Thermotoga maritima Lactate Dehydrogenase

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Lactate dehydrogenase is enzymatically responsible for converting pyruvate and NADH into lactate and NAD^+. Thermotoga maritima is a hyperthermophilic bacterium that contains the most thermostable lactate dehydrogenase (TmLDH) that has been isolated. Very thermostable proteins, either hot or cold, provide a good basis for studying protein adaptations to temperature. Differences between mesophilic and thermophilic proteins can reveal structural adaptations to high temperatures. TmLDH is currently being studied enzymatically and structurally, in order to better understand the stability and enzymatic nature of all LDH proteins. Previous structural work suggested key areas within the TmLDH structure that support catalysis at high temperatures and the role of cadmium in catalysis. In contrast to previous literature, we find cadmium has a negative effect on catalysis and induces protein precipitation. We are further studying the roles of metals on catalysis and attempting to enhance TmLDH catalysis activity at mesophilic temperatures. By understanding a complete enzymatic and structural picture of TmLDH, a better understanding can be made of mesophilic LDHs.

Beer-omics: Molecular fingerprinting of craft beers by positive and negative ion ESI q-TOF MS

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Metabolomic techniques were utilized to fingerprint 27 single-hop India pale ales (IPAs) produced by the Mikkeller brewery in Denmark in 2010 and 2011. The brewer kept all parameters the same and only varied the hop used in each beer. A quality control beer, Green Flash's West Coast India pale ale, was used to monitor sample stability and instrument response over the course of the study. Targeted flavonoids were quantified and their intraday and interday RSDs evaluated. All samples, which were run in triplicate on a UHPLC q-TOF MS, were also spiked with an internal standard. Approximately 5000 molecular features were found in each beer. Differential analysis (e.g., PCA and hierarchical clustering) revealed significant compositional differences between the 2010 and 2011 batches. The "fingerprint" of each hop, was then used in a class prediction model to identify the beers. The model, which is still under development, correctly identified hops in the Mikkeller beers but did not work well on beers made from a mixture of hops (e.g., the West Coast IPA).

Absorption of Acetic Acid on Copper Minerals

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Some industrial and agricultural processes produce Volatile Organic Compounds, which are hazardous to human health and produce air pollution. These VOCs are absorbed by certain rocks and minerals, including the copper based compounds of the study. In this investigation, the absorption of acetic acid on malachite, azurite, copper hydroxide, and copper oxide was investifagated using mass gain and ATR-FTIR. EGA-FTIR was used to investigate the temperature programmed absorption of the acetic acid from these materials.

Spectroscopic Studies on the Influence of Buffer Structure and pH on the Thermal Stability of RecA Reveal Distinct Aggregation States

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RecA is a DNA repair protein found in Escherichia coli, with homologues found in mammalian species. RecA is a DNA dependent ATPase that hydrolyzes ATP in the presence of single or double-stranded DNA. RecA has pH dependent affinities for ssDNA and dsDNA binding and ATP hydrolysis. Previous studies in our laboratory have shown that a variety of salts, substrates and pH conditions alter RecA structure and stability. In this study, three buffers were used to study the thermal unfolding and ATPase activity of RecA. RecA unfolding in HEPES, MES, and potassium phosphate buffers is compared to unfolding in Tris buffer at a variety of pH levels (6.5, 7.0, 7.5, 8.0, 8.5). Circular Dichroism (CD) was used to follow the unfolding transitions and to determine the melting temperature of RecA at each given pH and in each of the various buffers. Activity assays were conducted for each of the solution conditions used for the CD studies in order to study how buffer composition and pH influences RecA activity. Fluorescence data and ethidium bromide exclusion assays support alternate aggregation states influenced by the different buffers suggested by CD and ATPase activity data.

Low Resolution Studies of Ig 58 and 59 of Obscurin Using Small Angle X-Ray Scattering

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Obscurin is a giant muscle protein that is critical for muscle cell maintenance and organization. Mutations in obscurin and obscurin binding proteins have been linked to cardiomyopathies and muscular dystrophy in humans. Due in part to its large size (~900kda) and recent discovery, its structure and function has not been fully characterized; therefore the mutations and resulting diseases are poorly understood. As a first step to biophysically characterizing obscurin, we used small angle x-ray scattering to solve the low resolution structure of a simplified system of two domains (Ig 58 and 59). These data give insight to not only this two domain system but also the ~60 repeating Ig domains at the N-terminus. Interpretation and computer modeling of SAXS data show a dynamic two domain system with a 100° orientation to the other domain. These results suggest that an individual obscurin Ig domain cannot bind to adjacent obscurin domains or even regions that are 5 Ig domains away in primary structure. These data provide insight into how the entire obscurin molecule behaves in solution, and suggests a mechanism that prevents obscurin from forming unwanted self Ig-Ig interactions in vivo.

The Purification and Characterization of Ig1-2 Domain of Giant Muscle Protein Obscurin

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Obscurin (800-900 kD) is a giant sarcomeric signaling protein that is an integral component to muscle cell assembly and conservation. Mutations to obscurin and to obscurin binding proteins are thought to correspond with deformities of the sarcomeric cytoskeleton such as cardiomyopathies and muscular dystrophy in humans. Due to its large size and highly modular nature, obscurin is most easily studied by breaking up the whole protein into independently-folded domains. The first two Ig domains of obscurin (Ig1-2) are connected by a medium-length linker region. How this linker influences the flexibility of Ig1 relative to Ig2 is unknown. Here, we describe the initial steps of Ig1-2 purification and characterization. Purified Ig1-2 will then be used for other experiments including SAXS analysis to more fully probe the conformation of this dynamic system in solution.

Synthesis and Characterization of Ruthenium Complexes Containing the Bis-diphenylphosphinopropane monoxide (dpppO) Ligand

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Ruthenium has a number of uses in both the chemical and medical world. In this study the reactions between $RuCl_3(NO)(PPh_3)_2$ and $RuCl_3{\cdot}H_2O$ with $Ph_2P(CH_2)_3P(O)Ph_2$ (dpppO), were characterized using infrared and nuclear magnetic resonance spectroscopy and elemental analysis. Both ruthenium starting materials produce the same product, $RuCl_3(NO)(dpppO)_2$, but in different yields and purities. The reaction of $RuCl_3(NO)(PPh_3)_2$ produced a 42% yield of an impure product while the reaction of $RuCl_3{\cdot}H_2O$, produced an 86% yield of an analytically pure product. The reaction of $RuCl_3(NO)(dpppO)_2$ with $AgBF_4$ produced a complex which appears to contain a chelated $Ph_2P(CH_2)_3P(O)Ph_2$ ligand. Further characterization of this product is underway.

The synthesis of tripod molecules for ultrafast photolysis studies

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To better understand the role of molecular anchoring groups in electron transfer, a 1,3,5,7-tetraphenyladamantane tripod with carboxymethyl anchoring groups and a perylene complex was synthesized. In order to study the effects of distance on solar cell efficiency, the photoactive perylene “dye” will be placed perpendicular to a semiconductor surface. By varying the distance between the perylene complex and anchoring groups, electron transfer rates will hopefully be better understood while improving solar cell technology. These anchoring complexes will be later studied by femtosecond IR spectroscopy.

Effect of polar protic and polar aprotic solvents on negative ion electrospray ionization and chromatographic separation of small acidic molecules

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A comprehensive study investigated the effect of polar protic (methanol and water) solvents, polar aprotic (acetonitrile and acetone) solvents and a commonly used mobile phase modifier (formic acid) on negative ion electrospray (ESI) response of 49 diverse small, acidic molecules. Flow injection experiments on a triple quadrupole were used to measure the response in neat solvents after optimization of source conditions and implementation of a rigorous quality control program (the later ensured that changes in analyte response were due to the analyte/solvent measured and not changes in instrument performance over time). In all solvents, compounds with electron withdrawing groups and extended conjugation ionized best due to resonance and inductive effects. Ionization was greatest in methanol or water for all compounds that elicited a response, thus revealing that enhanced sensitivity and lower limits of detection are achieved with polar protic solvents. Response in acetone was equal to or slightly lower than acetonitrile in flow injection experiments. Subsequent experiments, investigated the effect of 0.1% v/v formic acid on negative ion response. Results suggest that the effect of mobile phase modifiers is dependent upon the analyte. For example, the response of n-carboxylic acids increased 16.9%, on average, while the response of steroids decreased by 80.2%. Furthermore, the addition 20% water to methanol with 0.1% formic acid decreased the response for the majority of analytes. Future work will investigate the effect of different mobile phase modifiers (e.g., acetic acid, ammonium acetate, ammonium formate and ammonium fluoride) and different solvents (e.g., acetonitrile, acetone and water) on negative ESI response.

Structural and mechanistic investigation of ubiquitination

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The ubiquitination pathway in eukaryotes is responsible for regulating a variety of functions in the cell including DNA repair, protein degradation, and transcription initiation. In this process, ubiquitin, a highly conserved protein among eukaryotes, is covalently attached to a substrate protein with the assistance of conjugating enzymes and acts as a signal for downstream functions. The specific signal can be altered by changing either the number of ubiquitins and/or which lysine residue they are linked with. Initially, ubiquitination was thought to only be involved in proteasomal degradation; however within the last decade other functions have been demonstrated. Ubc13, an E2 conjugating enzyme, catalyzes the formation of ubiquitin chains linked through lysine 63 of ubiquitin in response to DNA damage on the DNA sliding clamp protein PCNA. Much is known about the structure and biological function of these conjugating enzymes, but the catalytic mechanism of transfer of ubiquitin chains to the target substrates remains unsolved. In this study, the structure of Ubc13 will be determined using NMR and compared to the structure of Ubc13 bound to ubiquitin in order to determine conformational changes in the active site that occur upon binding to ubiquitin. We present initial NMR spectra of Ubc13. Kinetic isotope effects, chemical crosslinking, and mutagenesis will also be employed to give further insight into the transition state of Ubc13.

The Synthesis of Thienyl Phosphine Ligands for Polymerizable Cobalt Chalcogenide Clusters

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The synthesis of thienyl phosphine ligands for polymerizable cobalt chalcogenide clusters was performed. The reaction of 2-bromo-thiophene or (2,5)-dibromo-thiophene with n-butylithium, followed by reaction with chloro-diisopropyl phosphine produced (diisopropyl)(2-thienyl)phosphine (1) and (5-bromo-2-thienyl)(diisopropyl)phosphine (2), respectively. Compounds 1 and 2 were then allowed to react with sulfur as well as selenium, yielding (5-bromo-2-thienyl)(diisopropyl)phosphine sulfide (3), (diisopropyl)(2-thienyl)phosphine sulfide (4), (5-bromo-2-thienyl)(diisopropyl)phosphine selenide (5), and (diisopropyl)(2-thienyl)phosphine selenide (6). Compounds 3, 4, 5, and 6 were subsequently allowed to react with dicobalt octacarbonyl, resulting in cobalt chalcogenide clusters with polymerizable phosphine ligands. The intermediates and final products were characterized using FT-IR, GC-MS, UV-Visible spectroscopy, and ^{1}H and ^{31}P NMR spectroscopy. These results indicated that a cobalt chalcogenide cluster was formed due to a characteristic absorption over a wide range of the visible spectrum.

Toward Structural Analysis of the M10 Domain of Titin

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Titin, the largest monomeric protein in humans (~3000kda), functions in muscle cells as a molecular ruler, setting the length and organizing the overall sarcomeric structure. While titin has many attachment points to other connective proteins, one physiologically important interaction involves the extreme C-terminus of titin (the M10 region) binding to the extreme N-terminus (Ig1) of another giant muscle protein, obscurin, in skeletal muscle. This complex plays a critical role in structure and communication between the contractile apparatus and the surrounding membrane system, and is one of only two known link between these two important cellular structures. Mutations in the M10 domain cause molecular deformities that have been linked to limb-girdle muscular dystrophy 2J, A condition that is characterized by pain and weakening of the extremities, eventually leading to the loss of function of the arms and legs. Understanding the specific molecular structure of the wild type M10 titin domain as well as the structural implications caused by the various mutations is fundamental to learning more about this disease. Currently, we have expressed all four known mutations in the M10 domain. Initial CD analysis indicates that wild type M10 is composed predominantly of beta-pleated sheet and that the mutations are also beta-pleated sheets, though in diminished amounts. Additionally, preliminary binding studies of M10 to obscurin indicate a ΔG of -8.1 kJ/mol, which is in agreement with published (Pernigo et al.). These experiments set the groundwork for increase production and analysis of WT and mutant M10 using circular dichroism, isothermal titration calorimetry, and nuclear magnetic resonance spectroscopy.

Effects of Anions on the Interfacial Tension at the Hydrophobic/Aqueous Interface

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The Hofmeister series is a classification of ions in order of the ability of ions to affect the physical properties of processes in aqueous solutions. Although the Hofmeister effect is a general phenomenon, the underlying mechanisms are still elusive. Herein, the Hofmeister anion effects on the surface tension of water and interfacial tension at the hydrophobic/aqueous interface were investigated using an optical tensiometer by a pendant drop method. Surface tension of water increases linearly with salt concentration for all the anions studied; while at the dodecane/water interface kosmotropic anions increase the interfacial tension but chaotropic anions decrease it. The interfacial entropy and enthalpy were determined by varying the temperature for salt solutions at 1M. These studies will provide us with some fundamental insights into understanding the mechanisms of the Hofmeister effects.

Two-Component Low Molecular Weight Organogels Formed by Amino Acid Surfactants Amines

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In recent years, much emphasis has been placed on research in organogels due to their modifiability and relatively low expense. Research is being done in the applications of organolgels as varied as thickening agents in foods and cosmetics, developing solar cell materials, and oil spill recovery. A series of gels containing phenylalanine surfactants and linear amines in non-polar organic solvents were prepared. The melting point temperature of the gels was measured using a falling ball method. The falling ball method was further optimized by switching the size of the ball used and ensuring consistent placement of the gel within the heat source. The structure of the gel was characterized by scanning electron microscopy. Further characterization will be carried out in order to find a mechanism by which these gels form.

Improving the Adhesion of Au Thin Films to PMMA

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Conventional techniques such as O_2 plasma treatment to improve Au thin film adhesion have resulted in limited success. In this study, the adhesion of 6 nm and 100 nm Au thin films onto 0.8 mm poly(methyl methacrylate) (PMMA) sheets was significantly improved when Au thin film samples were exposed to a saturated chloroform environment after metallization. The shear force required to remove the Au films was calculated by placing samples onto a polisher spinning at 150 rpm and using a spring loaded device to apply the force. Au thin samples were characterized through optical microscopy, atomic force microscopy (AFM) and attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR). AFM and optical images show a roughening of the Au thin films after chloroform exposure. ATR-FTIR spectra indicate that residual chloroform solvent remains on the PMMA. Our research indicates chloroform may improve adhesion by relieving the stresses at the PMMA-Au interface. X-ray photoelectron spectroscopy (XPS) studies on chloroform pre-treated PMMA samples show residual solvent at the surface one-week after exposure. We have attributed this to a Lewis acid-base interaction between chloroform and the PMMA surface. We will report on the XPS data of post treated samples.

Real-Time Micro-Phase Separation Kinetic Analysis of POSS-MA Thin Films Using Atomic Force Microscopy

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Poly(propylmethacryl-heptaisobutyl-polyhedral oligomeric silsequioxane) (POSS-MA) is a nanocomposite co-polymer that has nanoscale POSS cages co-polymerized to a poly(methyl methacrylate) (PMMA) backbone. Thin films of POSS-MA were prepared by spin-casting 2.0, 2.5, 3.0 and 3.5 mg/mL solutions of 30 wt% POSS-MA dissolved in chloroform (CHCl3). These samples were scanned using an atomic force microscope (AFM) which produced a 3D profile of the surface. The 3.0 and 3.5 mg/mL solutions formed dendritic microstructures that could be monitored in-situ with the AFM, whereas the 2.0 and 2.5 mg/mL solutions did not result in dendritic growth that could be effectively monitored in-situ with the AFM. Samples sprayed with only nitrogen gas have been shown to form dendritic growth immediately after deposition. Samples that are carefully cleaned by sonicating in acetone, isopropanol and deionized (DI) water result in dendritic growth that is slower and more inconsistent when compared to samples sprayed only with nitrogen gas. Higher order structures form as a result of the POSS cages stacking on top of one another to form a bilayer.

Characterization and Structural Analysis of Obscurin, a Giant Intracellular Protein Involved in Muscle Integrity and Maintenance

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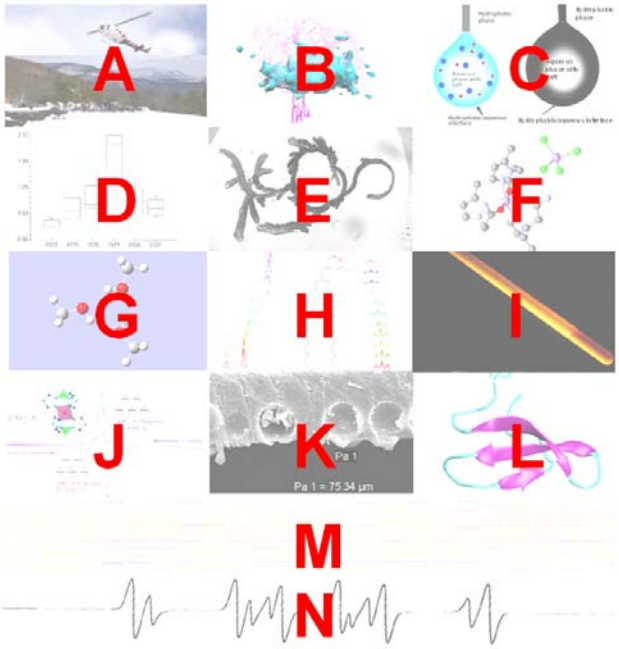
Obscurin (700-800 kD) is a giant modular protein involved in many aspects of muscle cell organization and maintenance. Disregulation of obscurin leads to supermolecular deformities of the sarcomeric cytoskeleton, and mutations of obscurin and its binding targets cause cardiomyopathies and muscular dystrophies. The extreme N-terminal domain of obscurin (Ig1) interacts with the extreme C-terminal domain (M10) of the "molecular ruler" protein Titin, and mutations in M10 lead to LGMD2J. While the structure of M10 has been solved through X-ray crystallographic techniques, the high-resolution structure of obscurin's Ig1 domain remains elusive and unknown. In an attempt to better characterize the biophysical parameters of the M10-Ig1 interaction, here we present partial NMR assignments of Ig1. This work is the first step in solving the high-resolution structure of Ig-1 and eventually the M10-Ig1 complex.



The image on the front cover is a collage of images from the research labs of:

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