Included are the abstracts to be presented during the poster session at Research Day 2014.
Title
Understanding conformational effects on proton affinity of peptides containing lysine and its unnatural homologs

Authors
Batoon, P.; Ren, J.

Introduction
As one of the building blocks of nature, amino acids combine together to form small peptides or large proteins. By using mass spectrometry and and quantum mechanical calculations, it is possible to carry out in-depth investigations on the effects of combining certain amino acids to form small peptides. By studying the fundamental properties of these small peptide, we gain insight and understanding into the catalytic power a large protein of high complexity.

Purpose
Previous studies by our group have shown that polyalanine peptides containing a cysteine placed at N-terminus is more acidic than polyalanine peptides with a cysteine placed at the C-terminus. This greater acidity was found to be a consequence of the favorable interactions between the α-helix conformation of the peptide and the deprotonated cysteine. The same results were also observed in cysteine peptides with two or three residues - for which a helical conformation is not possible. Because the acidic peptides hold a negative charge, this project was aimed to modify the previous study by utilizing a positive charge instead. Similar results are to be expected if the same effect can be observed in polyalanine peptides containing positively charged Lysine (Lys), Ornithine (Orn), 2,4-diaminobutanoic acid (Dab), or 2,3-diaminopropionic acid (Dap).

Methods
Various sequences of acetylated polyalanine peptides were synthesized by solid phase peptide synthesis (SSPS) to contain lysine, ornithine, or unnatural homologs 2,3-diaminopropionic acid (Dap) and 2,4-diamonobutyric acid (Dab). Measurements were carried out using an electrospray tandem-quadrupole mass spectrometer (Varian 320-LC/MS). The proton affinity (PA) was determined qualitatively by the formation and fragmentation of a proton-bound complex of the peptide and a reference of known PA. Conformational search for lowest energy conformers were carried out using Merck molecular force field and AM1 optimization. Geometry optimization and frequency calculations at the B3LYP/6-311+G(d) level were performed on 10 lowest energy conformers to calculate the thermal enthalpy correction at 298 K. Using calculation data, theoretical proton affinity was calculated by an isodesmic reaction scheme with the reference ethylamine. The final results of theoretical calculations would yield most probable conformation of the peptide ion.

Results
Theoretical proton affinities of dipeptides containing a basic residue at the C-terminus, AcDapA, AcDabA, AcOrnA, and AcLysA, have been determined to be 233.6, 240.1, 241.9, and 243.6 kcal mol-1 respectively and agrees well with experimentally determined values of 234.9, 236.6, 242.8, and 240.0 kcal mol-1 respectively. The theoretical proton affinities of dipeptides containing a basic residue at the N-terminus, AcADap, AcADab, AcAOrn, and AcALys, have been determined to be 235.8, 241.5, 242.6, and 245.5 kcal mol-1 and agree well with experimentally determined values of 236.6, 243.5, 245.5, and 249.5 kcal mol-1 respectively. Using collision induced dissociation bracketing (CID bracketing) with reference bases of known proton affinities it has been determined that AcAAADap has a higher proton affinity than AcAADap, and AcAADap has a higher proton affinity than AcADap. It is hypothesized that differences in proton affinities are largely due to a conformational effect. Dipeptides with a C-terminal basic residue form a more compact structure than the N-terminal basic residue isomer. Peptides with longer basic sidechains and longer sequences have more flexibility, allowing the peptide to internally solvate the charge more efficiently.

Significance
By understanding studying the fundamental physical properties of peptides we can gain insight into how proteins operate. By making seemingly small changes to peptide sequence or modification to amino-acids, future researchers may gain further insight into the engineering of useful proteins.
# Title
On the Protonation of Water

# Authors
Bodi, Andras; Csontos, József; Kállay, Mihály; Borkar, Sampada N.; and Sztáray, Bálint*

## Introduction
The proton or, from a chemist’s point of view, the hydrogen ion is omnipresent in chemistry and biochemistry. Proton-transfer reactions, typically coupled with electron transfer, are among the most fundamental processes in biological and chemical systems. Water is singularly important for life, the universe, and everything; its protonation is one of the key chemical processes and the resulting hydronium ion is familiar to everyone who has ever taken a chemistry course. No wonder that the energetics of water protonation, i.e. the proton affinity of water, has been the subject of countless studies.

## Purpose
Most PA measurements nevertheless yield relative rather than absolute values. The proton affinities around and below the PA of water, and especially that of water, have always been problematic to determine. Imaging Photoelectron Photoion Coincidence (iPEPICO) spectroscopy on isolated water molecules and water dimers establishes a new route to determining the water proton affinity (PA) with unprecedented accuracy.

## Methods
Photoelectron photoion coincidence (PEPICO) spectroscopy is a marriage of photoelectron spectroscopy and mass spectrometry. Electron / ion pairs are created by single photon ionization and the two charged species are measured in delayed coincidence with each other. Ions are selected in narrow range of internal energy by collecting only ions created in delayed coincidence with the photoelectrons. In threshold PEPICO, only the initially zero-energy electrons are detected, while in imaging PEPICO (iPEPICO), a whole velocity image is detected in coincidence with the photoions. Recent developments in the experimental technique, including velocity focusing optics for hot electron correction, as well as advances in data analysis that take into account the initial thermal energy distribution of the molecules, has permitted the extraction of dissociation limits and, therefore, bond energies to within 1 meV (0.1 kJ/mol) using the recently commissioned iPEPICO instrument on the VUV beamline at the Swiss Light Source (SLS) synchrotron.

## Results
A floating thermochemical cycle constructed from the OH+ and H3O+ appearance energies and three other spectroscopic values establish the water PA as $683.22 \pm 0.25$ kJ mol$^{-1}$ at 0 K, which converts to $688.81 \pm 0.25$ kJ mol$^{-1}$ at room temperature. The experimental results are corroborated by a hierarchy of coupled-cluster calculations up to septuple excitations and septuple-$\zeta$ basis set. Combined with diagonal Born–Oppenheimer and Dirac–Coulomb–Gaunt relativistic corrections, they provide the best theoretical estimate for both the hydronium ion’s geometry and a water PA of $683.5 \pm 0.4$ kJ mol$^{-1}$ and $689.1 \pm 0.4$ kJ mol$^{-1}$ at 0 K and 298.15 K, respectively.

## Significance
Solely spectroscopic data including new, Imaging Photoelectron Photoion Coincidence measurements on isolated water molecules and dimers, were used in a self-contained, floating thermochemical cycle to determine the absolute proton affinity of water an order of magnitude more accurately than has been possible for the last six decades.
Title
Measuring Drug Dissolution Using a Quartz Crystal Microbalance

Authors
Bonoan, Janpierre; Arucan, Joshua; Gulati, Shelly

Introduction
Dissolution is an important characteristic of drugs that are used to evaluate the properties of the drug, such as rate of release and duration of release. Several current methods exist to measure the dissolution rate of a drug, but many require large amounts of mass, run for several hours, and measure dissolution rate indirectly by taking concentration samples at different time intervals. In an effort to reduce sample size and decrease testing time, a quartz crystal microbalance is being evaluated for use to directly measure mass loss during drug dissolution.

Purpose
The feasibility of measuring drug dissolution on a quartz crystal microbalance is being tested. The QCM vibrates a quartz crystal at its resonant frequency. Any mass that is added or removed from the quartz crystal results in a change in its resonant frequency, which the QCM is able to detect. By applying the drug onto the crystal and flowing a solvent past the drug film, the drug dissolves away and the QCM is able to detect changes in frequency due to the reduction in mass. With the profile of the measured change in mass, the dissolution rate will then be determined.

Methods
The drug is first prepared by dissolving benzoic acid, a sample drug, in isopropyl alcohol. A small drop of the solution is applied onto the quartz crystal and as the isopropyl alcohol evaporates, the benzoic acid then recrystallizes onto the surface of the quartz crystal. The quartz crystal is loaded onto the quartz crystal microbalance with an attached flow cell and, with the help of a syringe pump, deionized water flows into the system, dissolving the benzoic acid. The quartz crystal microbalance is connected to a LabVIEW software which then measures the change in resonant frequency as the mass of the drug sample is being dissolved. The corresponding change in mass (and therefore frequency) is correlated to the dissolution rate of the sample.

Results
Results from the dissolution of benzoic acid using a flow of deionized water on a quartz crystal microbalance exhibit a mass loss trend that is similar to current methods. Additionally, decreasing the flow rate of the solvent decreases the rate of dissolution. This result is also similar to current standardized methods, which exhibit a decrease in dissolution rate with decreased hydrodynamic forces.

Significance
Current methods of measuring drug dissolution require several hundred milligrams of sample per trial. This is becoming more problematic with newer drugs being developed that are more difficult to produce and/or more difficult to extract. On the other hand, with the ability to detect mass changes as low as the nanogram scale, drug dissolution tests using a QCM would only require sample sizes on the order of micrograms. Decreasing sample sizes by several orders of magnitude will help reduce waste, saving researchers time and money.
Title
Finite Element Active Learning Module Assessment of Student Improvements, Learning Styles, Gender Differences and Ethnic Differences

Authors

Introduction
Contemporary engineering education and industry needs bachelor's level engineering graduates with skills in applying finite element methods to essential engineering analysis and design analysis. In response to the need to introduce undergrad engineering students to the finite element method as well as the need for engineering curricula to include more active learning with the design of Active Learning Finite Element Learning Modules (ALM) to undergraduate engineering students. The ALMs are designed to improve student learning of difficult engineering concepts and help students gain essential knowledge of finite element analysis.

Purpose
This is a multi-year research project at a number of engineering campuses where engineering educators provide unique Finite Element Active Learning Modules to their engineering students to improve their student's knowledge of engineering concepts and learn the essentials of using a commercial finite element software package to solving engineering problems. This update on research findings includes statistical results for each ALM which compare student performance before and after the ALM was administered. These results are based upon differences in learning styles of the students as well as a Myers-Briggs Type Indicator of student subgroups by personality. Results are shown for different student learning styles, ethnic groups, and gender groups of students.

Methods
Students were administered specific quizzes on engineering concepts prior to using a specific ALM and shortly after using that ALM. The student gains in knowledge by quiz results were analyzed by student personality types (MBTI), Felder-Solomon ILS for differences by learning styles, gender, and ethnic groups. The quiz data was verified with a statistical T-test to authenticate its accuracy.

Results
The student improvements for academic year 2011-2012 for 12 ALMs reported a % students improvement of 32.33 % from before ALM quiz results to after ALM quiz results. The student improvement for academic year 2012-2013 for 11 ALMs reported a % student improvement of 27.71% from before ALM quiz results to after ALM quiz results. The Gender differences in Delta were insufficient statistical evidence for our small student sample size for academic year 2012-2013. The Ethnicity Differences in Delta was insufficient evidence to support differences in pre-to post-quiz results.

Significance
This paper summarizes the results from two years of a Phase 2 NSF grant (2011-2012 and 2012-2013). Of particular significance is the student improvements in the pre-quiz versus post-quiz scores of 32.3% and 27.7% for each year averaged over the twelve ALMs in 2011-12 and the eleven ALMs in 2012-2013.
Title
BIOMASS ENERGY FOR STABILIZING AGRICULTURAL WASTES AND PRODUCING RENEWABLE ENERGY IN CALIFORNIA

Authors
Camarillo, Mary Kay; Stringfellow, William T.; Domen, Jeremy K.; Hanlon, Jeremy S.; Spier, Chelsea

Introduction
In biomass energy projects, feedstocks consisting of manure, agricultural wastes, and dedicated biomass-energy crops are introduced into anaerobic reactors, where a microbial consortium metabolizes the organic matter and produces a methane-rich biogas that can be used as a renewable energy source. However, start-up of biomass energy facilities represents a significant investment and the economics are highly dependent on factors such as wholesale electricity rates. To make biomass energy more profitable, co-digestion of manures with other agricultural waste products is being explored and that is the focus of this research.

Purpose
In this study, we determined and compared the biomethane potential and biogas production kinetics of egg waste and grape pomace as co-substrates in anaerobic digestion experiments. The objectives were to: 1) characterize the chemical composition of the co-substrates, 2) determine the bio-methane potential of egg waste and grape pomace, and 3) determine biogas production kinetics of egg waste and grape pomace.

Methods
The candidate co-digestates were analyzed for salts, nutrients, organic matter, lipids, protein, lignin, and carbohydrates. Bench-scale testing was done to measure biogas production. In the tests, sealed bottles containing co-substrates, nutrient media, and inoculum were incubated at mesophilic temperatures (39°C) and the biogas production was measured. Three sources of inoculum were used to test the effect of different microbial consortia: a bench-scale reactor operated with a standard loading rate, a bench-scale reactor operated with a low loading rate, and a full-scale reactor.

Results
Egg waste was found to be a good co-digestate, with a BMP of 484 L CH4/g VS, while pomace was found to have a BMP of 99 L CH4/g VS. Egg waste was degraded rapidly, in comparison to pomace, suggesting that shorter reactor residence times could be used, allowing more biogas to be produced from the same size facility. The results indicated that egg waste had lower salt and nutrient content relative to the BMP, which is beneficial for dairy management. Bio-methane yields were not dependent on the inoculum used; however, higher rates of biogas production were observed when the inoculum was derived from a full-scale reactor rather than the laboratory reactors.

Significance
Both feedstocks had high bio-methane yields relative to the salt and nutrient contents. In the bench-scale tests, biomethane potential was not dependent on the age or diversity of the microbial community present in the inoculum; however, biogas production kinetics were significantly different between the reactor cultures, indicating a heterogeneous microbial culture may be superior at adapting to the addition of new co-substrates.
<table>
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<tr>
<th>Title</th>
<th>Growing Neurons from Human Stem Cells</th>
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<tbody>
<tr>
<td>Authors</td>
<td>Cao, William S; Metz, Katy L; Coyne L; Halliwell Robert F.</td>
</tr>
<tr>
<td>Introduction</td>
<td>Induced pluripotent stem cells (iPSCs) are somatic cells that have been reprogrammed to a pluripotent state. Human cell types that are difficult to obtain, such as neurons, can then be derived from iPSCs and provide an alternative to animal tissues in disease modeling, drug discovery screening and toxicity testing.</td>
</tr>
<tr>
<td>Purpose</td>
<td>iCell® Neurons (Cellular Dynamics International) are a new source of human neurons that have been terminally differentiated from human iPSCs. This lab has now begun to explore the physiological and pharmacological properties of these neurons.</td>
</tr>
<tr>
<td>Methods</td>
<td>iCell® Neurons were grown and characterized by immunocytochemical analysis and patch-clamp electrophysiology.</td>
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<td>Results</td>
<td>Morphologically distinct neurons labeled for neuronal specific markers and expressed a range of voltage-gated ion channels. Additionally, they expressed a rich array of ligand-gated ion channels for the major excitatory and inhibitory neurotransmitter receptors. We also determined synapse formation between iCell® Neurons and these cells were able to fire action potentials spontaneously in cell culture.</td>
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<tr>
<td>Significance</td>
<td>Our data provide powerful validity for the use of stem cell derived neurons in biomedical research.</td>
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</tbody>
</table>
Title
Intercultural Willingness to Communicate, Self-Esteem, & Ethnocentrism

Authors
Dong, Qingwen; Harzman, J.; Allen, Megan; Contreras, Michael; Moore, Ki-Shawna; Paderes, Xochitl; Silveira, Sonia; Zepponi, Noah; Zhang, Wei.

Introduction
The human species now utilizes the web for information, orientation, entertainment, and behavioral development. News outlets maximize audience size by replicating information across multiple blogs and Internet platforms. Grass roots groups can now manipulate symbols digitally, allowing for mass-distribution amongst pertinent constituents. The mediums we use to search for information are socially evolving the manner in which the Human brain stores and processes information.

Purpose
The current study examines how willingness to communicate interculturally online and self-esteem may reduce ethnocentrism. In an effort to fill in the body of literature, this study offers the field of intercultural communication a better understanding of how online communication shapes and affects intercultural encounters. As the world is “shrinking”, the influence of cultural diversity on human communication has become greater than ever before. Contact from different cultural backgrounds unavoidably calls for attention to appropriate communicative behaviors. The study provides new insight into willingness to communicate interculturally online in an ever-evolving world.

Methods
Based on a sample of 202 young adults in a university on the West coast of the United States. A group administration data collection method was employed in the study. Three researchers went to seven general education classes to collect the data since these classes tend to be more representative of the university’s population. The six-page questionnaire contained six different measurements. The questionnaire also included a cover letter with an introduction requiring participants to sign consent before participation. Researchers expressed their appreciation to their participants after data was collected. This study used four major indices as key variables. They included ethnocentrism, self-esteem, willingness to communicate interculturally face-to-face, and willingness to communicate interculturally online. The data were analyzed through statistical package for social sciences (SPSS). A set of procedures was followed to provide descriptive analysis and hypothesis testing. Descriptive analysis included frequency and correlation analysis and hypothesis testing included regression analysis.

Results
The study found that a willingness to communicate online, specifically in a context of intercultural communication, had a significant predicting power for a reduction of ethnocentrism. Initially, self-esteem did not maintain any significant effect on ethnocentrism. However, the study also indicated that self-esteem does hold a significant correlation for both a willingness to communicate online interculturally and willingness to communicate face to face interculturally. The study therefore suggests that online intercultural communication has a potential impact on reducing ethnocentrism; limitations and further recommendations were subsequently offered.

Significance
There are several implications to the study. Initially, the study developed a new scale of willingness to communicate interculturally online with very high reliability. Next, the study found that there was a significant negative relationship between willingness to communicate interculturally online and ethnocentrism through correlation analysis. This finding suggests that willingness to communicate interculturally online plays a significant role in reducing ethnocentrism. The Internet makes the world accessible, allowing for intercultural communication without physical boundaries. As Humans engage the Internet for this purpose, they grow more appreciative of alternative cultures. Third, this study revealed the positive correlation between willingness to communicate interculturally face-to-face and willingness to communicate interculturally online. If individuals can recognize and develop online intercultural communication, it will be much easier for them to have an enjoyable face-to-face conversation with others from different cultures. Lastly, this study provides a more complete view of how online communication shapes and affects a person’s intercultural communication activities. Social media can build a more effective strategy of optimizing people’s intercultural communication experience in the online environment.
# Visualizing the Dynamics of Many-electron Wavefunctions

## Authors
Dutoi, A. D.

## Introduction
As experimental techniques begin to probe electronic motions in increasing detail, the need is arising for compact and informative visualizations of simulations of such dynamics. The inherent challenge is that a full many-electron wavefunction is a high-dimensional mathematical object, representing the complicated correlations of strongly repulsive bodies living in a small molecular volume.

## Purpose
The goal is a visualization tool that allows for easy and intuitive interpretation of all this information, while drawing out nontrivial aspects of the many-electron dynamics, such as the complex phase information inherent of a moving quantum-mechanical particle. The procedure should also be defined for any approximation used for the underlying simulation of electronic motions.

## Methods
The scheme proposed and implemented has these properties. A matrix diagonalization (which may be interpreted as an optimization problem) is used to isolate those single-electron states which increase or decrease the most in the extent to which they are used by the many electron state, relative to an unperturbed state of the molecule.

## Results
One of the primary exciting observations from this newly developed tool is that distinction between two paradigms of many-body dynamics is observed, electron transport and energy transport.

## Significance
In the last decade, the field of attophysics has broken into the domain the fastest motions relevant to chemistry, those of the electron. Observing how electrons move even in small molecules will be an intensely interesting field over the next years. This field also has enormous long-term practical importance. Fundamental understanding of how electrons and energy move through heterogeneous materials directly impacts the field of solar energy production, arguably one of the most important technological challenges of the modern age.
**Title**  
Absent voices: Intersectionality and college students with physical disabilities

**Authors**  
Griffen, Jacalyn M.; Tevis, Tenisha L.

**Introduction**  
College students with disabilities stand at a crossroads when transitioning from high school to college and yet are absent from the discussions regarding underserved populations in higher education. This absence is particularly notable in scholarship employing the lens of intersectionality. To address this gap in the current discourse our qualitative case study employs a strengths-based view to examine how typically marginalized college students used the strengths of their socially constructed identities as a dynamic force to find the keys to academic success.

**Purpose**  
The purpose of this study is three-fold: 1) apply intersectionality to an overlooked, unacknowledged sub-group, broadening the theoretical framework’s utility and further expanding the current field-understanding; 2) understand intersectionality from a strengths-based point of view by exploring the experiences of academically successful college students with physical disabilities; and 3) give voice to an omitted compounded sub-group within the greater social and academic communities.

**Methods**  
We utilized a collective case study approach (Baxter and Jack, 2008) with “issue-oriented questions” (Stake, 1995, p. 65) to amass and compare information across three student respondents and two administrators. We used a convenient sample of students who met the following four criteria: (1) have a documented physical disability (for which they may or may not utilize support services); (2) are currently enrolled; (3) in good academic standing with the university; and (4) self-selected to participate in this study. The data collection method for this study was in two phases for both students and administrators; and two separate sets of interview protocols were developed. For students, in the first phase, a demographic survey preceded the face-to-face two-on-one interviews to collect basic background information and inquire about students’ academic support prior to enrolling in college. In the second phase, we conducted three two-on-one interviews with two graduate students, and one undergraduate student. The interview protocol for students was divided into five sections to solicit responses about self, family, high school, college, and social.

**Results**  
We found that the larger themes across all three cases were independence and advocacy. More specifically, independence and the freedom independence can bring to exercise choice and the importance of at least one family member’s support which created the freedom and independence to pursue higher education. Advocacy is in many forms including, exercising their voice as they lobbied for themselves, the choice to advocate on behalf of others, and lastly, the role mentor advocates played in helping them to set, actualize, and take ownership of their academic and life expectations.

**Significance**  
Academic success of students’ with disabilities is typically not part of the narrative when discussing barriers to academic achievement for marginalized groups. The success of these three students surpasses national statistics and expectations for students’ with physical disabilities. All three students perceive themselves as strong, independent, enabled and invested in their own success and the success of others. Again, having a disability goes beyond, race/ethnicity, socioeconomic status, region, or any other socially constructed marginalizing attribute. Therefore, this study concludes that intersectionality is no longer a frame to only understand the plight of the oppressed, since neither the students nor the administrators see having a disability as a deficit. Instead we believe that intersectionality is a lens to also view the strength of those who have been socially constructed as a marginalized other, who chose to re-construct their identity through their academic success.
### Title
Methodologies to evaluate dissolved oxygen impairment in the San Joaquin River for watershed management

### Authors
Gulati, Shelly; Spier, Chelsea; Hanlon, Jeremy; Stubblefield, Ashley.; Jue, Michael; Camarillo, Mary Kay; Stringfellow, William; Weissmann, Gregory; Garcia, Ernesto; Herr, Joel; Sheeder, Scott

### Introduction
To maintain agriculture production and water supplies, large-scale landscape and hydrologic modifications have been made in the Sacramento-San Joaquin Delta, leading to loss of ecosystem function. In the San Joaquin River (SJR) and estuary, discharge of oxygen demanding substances, eutrophication, low flows, and channel deepening have combined to create regional anoxic conditions, negatively impacting critical fish habitat.

### Purpose
The Deep Water Ship Channel (DWSC) located on the SJR adjacent to Stockton, has had intermittent low dissolved oxygen (DO) conditions for decades. As a result of the low DO impairment, the State Water Resource Control Board has implemented a total maximum daily load (TMDL) for oxygen-consuming substances in the SJR at Stockton and defined DO impairment as when DO concentration falls below water quality criteria. As part of the TMDL, studies were conducted to identify sources of oxygen demanding substances to the river and investigate how to better allocate responsibility for DO impairment.

### Methods
In this study, a combination of direct measurements and results from model simulations using the WARMF and Link-Node models were used to examine the causes of DO impairment in the DWSC. Continuous flow and grab samples were used to calculate mass loads of nutrients, total dissolved solids, biochemical oxygen demand, and chlorophyll entering the San Joaquin River (SJR). Loads were simulated using WARMF to determine the impact on oxygen consuming materials by removing a variety of sources and comparing to the baseline scenario. The Link-Node model was also used to examine the DO impairment caused by dredging the river at Stockton to over 30 feet deep (i.e. the DWSC).

### Results
The surface water inputs to the San Joaquin River (SJR) have been well characterized. Major sources of oxygen demand include demand from the SJR upstream of the DWSC, Stockton’s wastewater treatment facility (WWTF), and urban tributaries. By comparison to baseline simulations which include all factors, oxygen impairment attributable to each factor was quantified. Model results suggest that WWTF improvements have reduced the contribution of the WWTF to the DO impairment and that the role of the DWSC in promoting impairment may be underestimated. Import of phytoplankton from the SJR is important, but impacts appear moderated by the lack of flow associated with low DO events.

### Significance
River and Estuary Models have been developed as a tool to inform management decisions. The models can be used to identify sources of low DO to the Deepwater Ship Channel (DWSC), allocate responsibility for the low DO conditions, and to simulate the impacts of management actions on DO, nutrients, and other water quality parameters in both the upstream SJR and in the DWSC.
### Title
Acylation of trans-substituted cyclohexanols: Reversal of diastereoselectivity depends on scaffold substitution and achiral amine catalyst

### Authors
Hackbusch, S.; Watson, A.; Franz. A.H.

### Introduction
Diastereoselectivity in chemical reactions can arise from differences in activation energies associated with the reactants, if the process is kinetically controlled. Such selectivity is influenced by a number of factors, such as solvent polarity or temperature and examples for the complete reversal of diastereoselectivity based on these factors exist in the literature. Additionally, the use of chiral additives, such as chiral ligands in organometallic catalysis, can control enantio- or diastereoselectivity. However, in some cases achiral additives are known to influence the stereochemical course of reactions, as well.

### Purpose
We have previously demonstrated the capability of pyridine and other amine-based catalysts to reverse the diastereoselectivity of an acylation of racemic trans-2-substituted cyclohexanols with racemic acyl chloride. The purpose of this study was to further investigate the effects and causes of these observed amine-induced changes in diastereoselectivity.

### Methods
The acylation reactions of interest were studied in terms of different catalyst-loading and solvent dependence and diastereoselectivity was determined using NMR spectroscopy. Additionally, computational methods were used to aid in explaining the observed reversal of diastereoselectivity.

### Results
Achiral amine catalysts were found to give a linear load-dependence on the observed diastereomeric ratio of the product for cyclohexanols with aromatic trans-substituents. Furthermore, a relatively strong solvent-influence was observed for the uncatalyzed reaction pathway, leading to a reversal in diastereoselectivity in some cases. A potential “induced fit” due to favorable π-π stacking of the aromatic trans-substituent with the pyridine catalyst may explain the observed reversal in diastereoselectivity.

### Significance
Today, there is a large demand for efficient stereospecific and stereoselective synthetic methods in both pharmaceutical research and manufacturing. Understanding the mechanism of the reversal of diastereoselectivity in this particular system will allow for chemical modification on the substrates in a deliberate manner. As a result, improved acylation reagents may lead to a new and efficient separation of racemic acyl chloride mixtures, an underappreciated part of the chemical literature.
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<th>Title</th>
<th>Sexual dimorphism in aortic endothelial function of Zucker diabetic fatty rats: Possible involvement of superoxide production</th>
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<tr>
<td>Authors</td>
<td>Han, X.; Shaligram, S.; Anderson, L.; Rahimian, R.</td>
</tr>
<tr>
<td>Introduction</td>
<td>Premenopausal women have a lower incidence of cardiovascular diseases compared to age-matched men. Premenopausal women with diabetes not only lose this sex-based cardiovascular protection, they also experience a higher risk of cardiovascular diseases compared to diabetic men. However, little is known about the interaction between diabetes and sex in vasculature.</td>
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<tr>
<td>Purpose</td>
<td>This study was designed to investigate whether there were sex differences in rat aortic endothelium-dependent vasodilation (EDV) in Zucker diabetic fatty (ZDF) rats, and the potential role of superoxide.</td>
</tr>
<tr>
<td>Methods</td>
<td>EDV to acetylcholine (ACh) was measured in aortic rings pre-contracted with phenylephrine before and after pretreatment with apocynin (100 μM), a NADPH oxidase (Nox) inhibitor. In addition, the level of Nox (a potent source of superoxide) and PKCβ mRNA expression were determined using real-time RT-PCR.</td>
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<tr>
<td>Results</td>
<td>ACh-induced relaxations were significantly greater in female lean rats compared with male lean rats. Accordingly, male lean rats had higher PKCβI expression level than female lean rats. Diabetes significantly impaired EDV in aortic rings from female ZDF rats, however, potentiated the relaxation in males. Pre-incubation of aortic rings with apocynin increased EDV only in diabetic female group, suggesting impairment of EDV in female ZDF aorta was partly due to an increase in the activity of superoxide. Accordingly, the levels of Nox1, Nox4, and PKCβ mRNA expression were substantially enhanced in aorta of female ZDF rats compared to those in lean animals.</td>
</tr>
<tr>
<td>Significance</td>
<td>These data suggest that an elevation of superoxide may partially contribute to the predisposition of the female aorta to injury in type 2 diabetes.</td>
</tr>
</tbody>
</table>
Title
Tweeting about health care: A social network analysis of Kaiser Permanente’s Twitter handles

Authors
Hether, H.J.

Introduction
As digital media become increasingly important in how Americans obtain information about and access to health care services, understanding how these media are used enables health care organizations to better leverage these media for more effective communication which may yield public health benefits. Social media, in particular, have become essential tools of patient empowerment by facilitating peer-to-peer and organization-public communication; however, little is known about the networks that form on social media properties managed by health care organizations.

Purpose
The purpose of this project is to analyze the social networks formed on Twitter around a health care organization. By analyzing the network structures, we can better understand the connections that are made on these platforms and how information and influence might flow through them. Moreover, by analyzing three networks formed around one health care organization, the study also seeks to identify the value multiple handles may provide to the organization.

Methods
This case study applies two methods, content analysis and social network analysis, to examine the networks formed around one of the nation’s largest health care organizations, Kaiser Permanente (KP). For six weeks during the summer of 2012, all tweets posted by both the organization and members of its publics were analyzed on three of the organization’s Twitter handles. The study identifies characteristics of the actors across the networks, characteristics of the ties between the actors, and overall network centralization measures.

Results
The findings suggest the multiple networks under the Kaiser Permanente umbrella were fairly independent, with minimal duplication in actors. Further, these networks more frequently facilitated ties across organizations, more so than individuals. The networks were more strongly centralized on indegree, suggesting that other actors were more often tweeting to KP than KP was tweeting to specific actors. The low closeness and density values suggest the networks were not well-connected. There were a few critical actors, with many nodes participating minimally. There was low reciprocity, indicating that ties were not mutual in this network.

Significance
The findings suggest that Twitter may not be an effective platform for Kaiser Permanente to build relationships with its members. Instead, Twitter may be a channel that more strongly supports relationship-building among its organizational peers. This suggests that Kaiser Permanente should use other channels to build strong relationships with its members. Furthermore, the data indicate the networks were not well-connected, suggesting that Kaiser Permanente may want to consider how it can support stronger ties across the actors to facilitate a more integrated and cohesive network that would more effectively support communication across the network. These findings also suggest best practices for other health care organizations using Twitter to connect with their key publics.
**Title**  
Peptoid Fragmentation: Where to place the side chain residue?

**Authors**  
Hossain, Ekram; Ren, Jianhua

**Introduction**  
Peptoids (poly-N-substituted glycines) are N-substituted petidomimetics that are completely resistant to proteolysis, have high metabolic resistance and many therapeutic importance such as antibacterial activity, lung surfactant mimetic etc. The rapidly growing number of studies on peptoids and the increasingly diverse structures in peptoid libraries require efficient analytical methods to analyze the sequences and the structural changes of peptoids. Tandem mass spectrometry is a fast technique that is used for peptide sequencing. Our goal is to establish a comprehensive fragment-structure relationship ship and elucidate the fragmentation mechanism using tandem mass spectrometry technique.

**Purpose**  
Direct sequencing of peptoids on the solid support resin by Edman degradation has been a common practice. However, this method is extremely time-consuming, since it requires the synthesis and analysis of standards for each unnatural residue. As a part of our ongoing effort to elucidate fragment - structure relationship for peptoids using tandem mass spectrometry we have studied eight selected peptoids that differ in backbone structure, side chain and their positions as well as the ion generating metal ions.

**Methods**  
Ions were generated by electro spray ionization (ESI) of the analyte solution in methanol/water mixture in a commercial ion trap mass spectrometer in positive ion mode. CID was performed using He buffer gas.

**Results**  
The results indicate: 1) More intensity in metalized ion fragmentation compared to protonated ones. 2) No difference in different mono metalized ion fragmentation 3) Fragmentation is more intense around the basis side chain residue.

**Significance**  
The results show 1) The metal cations has higher affinity towards the basis side chain residue. 2) The position of the basic side chain residue (C or N terminus) can be determined from the fragmentation pattern and intensity of the product ions.
<table>
<thead>
<tr>
<th>Title</th>
<th>Targét versus Targhetto: The Role of Retail Prejudice in Customer Service Delivery</th>
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</thead>
<tbody>
<tr>
<td>Authors</td>
<td>Joseph Mathews, S.</td>
</tr>
</tbody>
</table>

**Introduction**

This study examines a new concept called in-store redlining where standards and upgrades significantly differ between stores in different geographical locations. Retailers practicing in-store redlining base investments in physical upgrades, customer service delivery, merchandise offerings, service environments and in-store maintenance primarily on the location of a store. Specifically, stores located in or close to inner cities, dominated by lower-income, minority populations, have significantly lower investments (Targhettos) as compared to stores located in or close to suburban locations populated mainly with middle to high income Caucasian populations (Targéts). Retailers engaging in this practice essentially offer very different shopping environments and customer service standards within a single retail brand to customers; these varying standards can cause customers to believe that the brand is purposely engaging in practices associated with retail prejudice.

**Purpose**

The purpose of this study is threefold. First, we explore the construct of in-store redlining and examine how perceptions of in-store redlining differ across customers of different ethnic backgrounds. Second, we investigate whether the consumers that do believe in-store retail redlining is currently being practiced, then also consider said practice to be an intentional and prejudicial strategy by the corporate retailer. Finally, the last objective of the research is to examine how perceptions of both in-store retail redlining and active retail prejudice then also influence overall brand perceptions of retailers.

**Methods**

This study was conducted in two phases. Phase 1 involved a quantitative study with a convenience snowball sample of 100 Target store customers. Customers were questioned on issues such as their familiarity with the store, items they purchased at Target and the frequency with which they purchased at Target. Demographic and geographic information was also obtained from these respondents. Finally these respondents were asked to indicate whether or not they perceived Target stores in different locations to be different and were asked to indicate in first, open-ended questions and then, close-ended questions, the specific things they considered to be different between stores. Phase 2 then involved a series of focus groups with middle-income women from different ethnic groups in four cities in the US. Potential respondents were recruited through Parent/Teacher Associations, church groups and teaching staff members at a number of middle schools in each of the three cities. Women and in particular teachers were recruited because of the well-established profile of typical Target shoppers as being female with children attending school. Target also has considerable outreach to schools and focus on teachers as one of their major market segments, making teachers credible populations to recruit potential respondents and focus group members. Eight focus group, with a total of eighty (80) respondents were conducted in these three cities with respondents filling out a paper survey prior to their involvement in a focus group discussion. Respondents in each focus group all self-identified into one ethnic group and multiple ethnicities were not combined in any focus group conducted. There were 3 African American, 3 Caucasian and 2 Latino focus groups conducted. Respondents were briefed before beginning the focus group and after filling out the survey, that the focus group would involve discussion about their shopping experiences at the retail store Target. The lead researcher moderated the various focus groups, utilizing a question script to ensure consistency. Each focus group was monitored for body language and discussion themes by researchers as the focus groups were being conducted, and each session was recorded using both video and audio recorders. The transcripts from the focus group session were then entered into online content analysis software to establish themes and idea nodes for the research. These nodes were then compared to the researcher notes and research trends were established. The quantitative data collected from the paper surveys was also analyzed using SPSS software. The following hypotheses were tested in our analyses: H1: There is a positive relationship between perceptions of differences in the quality of Target stores in different communities and positive perceptions of in-store redlining. H2: There is a positive relationship between perceptions of in-store redlining and perceptions that this practice is prejudicial in nature. H3: Consumers belonging to different ethnic groups will have significantly different perceptions of in-store redlining. H4: There is a positive relationship between perceptions of in-store redlining and a willingness to drive outside of communities to shop at different target stores. H5: There is a negative relationship between perceptions of in-store redlining and overall perceptions of the retailer Target.
Results
A regression analysis was conducted to test hypotheses 1, 2, 4 and 5. The overall regression model was significant (R² = .721, F (5,32) = 16.577, SS= 11.265). H1 was supported (t= 5.068, B= .479, p<.001). This was also supported in all of the focus group discussions. All of the respondents across geographic locations and ethnic groups agreed that there were differences between Target stores in different locations. These findings indicated that there is a positive relationship between perceptions of differences in Target stores in different locations and perceptions of in-store redlining. We also ran another independent t-test to investigate H1. The t-test explored the difference in in-store retail redlining scores of consumers who did perceive a difference versus those who did not. The results indicated that there is a difference (F=2.496; t= 4.142, p<.001) in the in-store redlining perception mean scores of customers who did perceive a difference (Mean= 4.5) versus those who did not (Mean = 3.5). H2 was supported (t=3.817, B= .453, p<.001). Consumers who perceive in-store redlining to be present also consider this practice to be prejudicial in nature. This was again supported by the focus groups. However, African Americans were more likely than both Latinos and Caucasians to suggest that in-store retail redlining was associated with prejudicial practices. Caucasians were the least likely to associate differences across stores with prejudicial practices. An independent t-test was conducted to test H3, which was supported. The mean scores of in-store redlining perceptions for minorities (African Americans and Latinos M=3.58, S.D.=.62) were significantly different from the in-store redlining perceptions scores of Caucasian consumers (M=3.03, S.D.= .552). This was also supported by the focus group discussions. Although all ethnic groups acknowledge the presence of in-store redlining, minority consumers offered stark examples of the differences between stores; indicating differences on almost all categories. Conversely, most of the Caucasian consumers focused on differences associated with only a few characteristics focusing instead on differences in customer types, store cleanliness and customer service delivery. H4 was supported (t= 2.245, B= .266, p<.05). Consumers who perceive in-store redlining to be present are more willing to drive to shop at a different Target store outside of their community. In focus groups, African American and Latino consumers were willing to drive outside of their communities to visit a Target especially if they identified a Targhetto close to their house. Caucasian consumers were typically unwilling to drive long distances to shop at different Target stores; perhaps because many of the Caucasian respondents identified that they lived close to a store they perceived to be of a Target standard. H5 was not supported (t= - 1.276, B= -.126, p= .211). Consumers who perceive in-store redlining to be present, do not necessarily change their overall perceptions of the retailer. Again, this was supported by the focus group discussions. Generally, even with acknowledgement that in-store redlining does exist, consumers in all ethnic groups still were loyal to Target and these perceptions did not change their overall perceptions of the retailer. Interestingly, despite a lack of significance, the relationship was inverse which indicates that as perceptions of in-store retail redlining increases overall perception of Target does decrease.

Significance
Findings indicate that whilst all populations acknowledge differences in Target stores located in urban versus suburban neighborhoods; giving credence to the notion of ‘Target’ versus ‘Targhetto’, there are distinct differences between the groups regarding perceived in-store redlining dimensions and their respective responses to this phenomenon. African Americans and Latinos are far more tolerant of these environments in their neighborhoods than Caucasians and are more likely to drive significant distances outside of their neighborhoods to shop at more desirable retailing environments. When compared to the other two groups in the study, African Americans are more likely to consider the differences a deliberate strategy by Corporate Offices to perpetuate different standards, and Latinos are the least likely ethnic group to complain about the difference in standards and upgrades or to consider the differences in standards a deliberate corporate strategy. In general minority consumers were more likely than Caucasian consumers to associate in-store redlining with retail prejudice. These findings indicate that a majority of Target customers believe the retailer is offering significantly different shopping experiences depending on where you choose to shop. There is the perception that some Target stores are better than others and these “better stores” seem more likely to correspond with affluent, Caucasian neighborhoods than with low income, urban, minority neighborhoods. Additionally, there are significant differences between these groups and Caucasian consumers perceive customer service delivery at these different Target store locations. Caucasians seem less tolerant of varying standards with most white consumers choosing to only interact with stores that meet their standards. Conversely, Latinos and African American consumers, although willing to drive outside of their communities to access better stores, are still considerably more tolerant of stores with lower standards than their Caucasian counterparts. The empirical findings suggest that the Target we see advertised on television and the internet is not the “real” Target and corporate retailers have a lot of work to do to convince consumers that they pay the same attention to all of their consumers
regardless of geographical locations and ethnic background. The question becomes what is this doing to the overall Target brand. Although all ethnic groups seem to still love shopping at Target, in each of the focus groups, consumers of all ethnic backgrounds claimed to either work or live close to a 'Targhetto', but actively avoid said store because of the poor in-store shopping environments. If Target the retailer is suggesting that under performance is one reason behind limited investment in upgrades there may be an argument to use a few 'Targhetto' stores as pilots and evaluate whether upgrades lead to higher shopping revenue as many consumers who currently avoid the store may start shopping there once these changes are implemented. Finally, there are examples of corporations that subscribe to a one store model where regardless of the location the store is consistent and all of the focus group respondents were in favor of such a model. In and Out Burger and Trader Joes both have stores in what could be considered low income urban environments, but the standard is always the same and these standards serve to reconfirm in the minds of the consumer the commitments these establishments have to excellence. Perhaps Target can learn from a little burger company like In and Out Burger.
<table>
<thead>
<tr>
<th>Title</th>
<th>Collective Electronic Coordinates for Efficient Decomposition of Large-scale, High-accuracy Ab Initio Simulations</th>
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<tbody>
<tr>
<td>Authors</td>
<td>Liu, Yuhong; Dutoi, Anthony</td>
</tr>
</tbody>
</table>

**Introduction**
In molecular modeling studies, there are two effective approaches --- ad hoc and ab initio methodologies. The former is efficient and affordable in computation time but only accounts for well-known interactions and proves unable to be used reliably in bond-breaking situations, like in studies of metabolic catalysis. The ab initio method conducts quantum mechanical calculations, and thus it is highly accurate but exceedingly expensive due to its exponential scaling nature. Density Functional Theory (DFT) is the most widely used method in the ab initio approach, which delivers affordable and often acceptable results; however, it suffers from many failure cases, as when breaking bonds.

**Purpose**
To cope with all these problems, we present a new way of applying high-level quantum mechanical theories to large systems. It starts with grouping atoms into subunits. Important interactions within subunit will be computed; then the interactions between groups will be simulated based on the computed eigenstates of subunits.

**Methods**
Our first model, quantum harmonic oscillators, has exact analytical solutions, but real molecules do not. The wavefunctions for harmonic oscillator have intrinsic similarities to the wavefunctions of electrons, so the grouping studies on harmonic oscillator will help to achieve better simulations in molecules.

**Results**
This is a long-term project, and our first model, quantum harmonic oscillators, is devoted to acquiring a better understanding in grouping and recoupling subunits in large systems.

**Significance**
Large-scale simulation is crucial in many research fields, such as drug binding, protein folding and metabolic catalysis. All the treatments in our method are quantum mechanical, which could lead us to highly accurate results, but it is still affordable for large systems. This scheme would also be systemically improvable since it is a wavefunction-based method.
Title
Strategies for Learning Chinese

Authors
Ma, Rui

Introduction
Chinese is a relatively difficult language to learn, however, if equipped with a repertoire of language learning strategies, learners can learn the language much more efficiently. They can also develop into more independent, resourceful, and confident language learners. This project is a small-scale pilot study of learning strategies used by learners of Chinese. This project is also informed by a review of current research on the topic.

Purpose
The topic of language learning strategies has been extensively researched in the field of second language acquisition (Oxford, 2011). Language learning strategies are specific steps, approaches or techniques that learners purposefully take to help them with their language learning and also with use of the second (foreign) language. There is a growing but relatively small research body on strategies specifically for learning Chinese as a second (foreign) language. This presentation will report a brief review of current research studies on strategies for learning Chinese. It will also discuss the results of an original small-scale study of English-speaking college students using different strategies to learn Chinese. The purpose is not only to introduce the concept of language learning strategies to learners of Chinese, but also to provide pedagogical suggestions and guidelines for classroom teachers of Chinese.

Methods
The methods will be designing a language learning strategy questionnaire based on research and then collect questionnaire data, and finally analyze the data to find out significant patterns.

Results
Currently I am still working on the results. I have analyzed data from one class, which revealed that students are not using strategies very often, indicating the necessity of language learning strategy instruction.

Significance
The research body on strategies for learning Chinese is still relatively small. My project will provide more data. Also, more importantly, students and teachers are not generally aware of the importance of using language learning strategies to achieve learning goals. This project aims to advocate the importance and explore potential pedagogical methods.
**Title**  
Knocking out PRAS40 Attenuates Hyperglycemia in STZ-induced Diabetes Mellitus in Mice

**Authors**  
Malla Ritu; Faridi, J.S.

**Introduction**  
Diabetes is a disease in which the body does not respond to the pancreatic hormone insulin properly (insulin resistance). As a result, the cells of the body are not able to take up glucose from the blood. This leads to elevated blood glucose level (hyperglycemia). We hypothesize that there is a key player (called PRAS40) that contributes to higher blood glucose levels leading to diabetes.

**Purpose**  
We propose that the removal of PRAS40 may be a novel treatment for lowering blood glucose. Using a transgenic mouse model, we tested our hypothesis that PRAS40 plays a key role in glucose homeostasis.

**Methods**  
We examined blood glucose levels in diabetic mice in the presence (normal mice) or absence of PRAS40 (PRAS40 knock-out mice). We have both PRAS40 groups of mice available to us already, and we induced diabetes in these mice using a low dose of streptozotocin. We observed reduced serum glucose levels in PRAS40 knock-out (KO) mice. Upon inducing diabetes using STZ, we report that there was lowered blood glucose in PRAS40 KO diabetic mice versus WT mice. Next, to understand the possible mechanism for this reduction in glucose levels, we checked for mRNA expression of glucose transporters (GLUTs) in liver, muscle and adipose tissue.

**Results**  
Both in-vivo and in-vitro studies indicate that PRAS40 knockdown increases GLUT4, p-IRS-1, p-Akt (T308) and p-P70 levels as analyzed by Western blotting analysis and immunohistochemistry.

**Significance**  
This study indicates that PRAS40 could be a novel target for the treatment of DM.
## Title
Development of Fluorescence Assay for Quantification of Transthyretin in Serum

## Authors
Miller, Mark; Chan, W; Alhamadsheh, Mamoun

## Introduction
Transthyretin (TTR or prealbumin) is a protein primarily synthesized by the liver and secreted into the blood, where it acts as the primary carrier of holo-retinol-binding protein and also as a back-up carrier of thyroxine (T4). The level of native TTR in serum is a sensitive and cost-effective indicator of nutritional status. In addition, point mutations in TTR promote TTR amyloidogenesis by decreasing the kinetic barrier for tetramer dissociation, resulting in diseases such as familial amyloid polyneuropathy and familial amyloid cardiomyopathy. Current clinical assays for quantifying TTR tetramers in serum, such as immunoprecipitation-turbidity assays, have significant drawbacks. Therefore, the development of an assay that can accurately measure tetrameric TTR in serum is greatly desired.

## Purpose
We have previously developed a fluorescence probe for TTR in buffer. However, the poor selectivity of this probe has limited its use in serum. Recently, we discovered a number of highly potent and selective TTR ligands. I will be presenting our recent effort to develop these ligands into fluorescence probes that are able to bind selectively to TTR in serum.

## Methods
- Chemical synthesis of the probes
- Evaluation of the probes binding to TTR in buffer
- Evaluation of the probes binding to TTR in serum

## Results
Probes have been synthesized and they bind to TTR in buffer

## Significance
Our probes may potentially be used to quantify TTR as a nutritional marker or in clinical trials to evaluate the efficacy of therapeutic candidates for TTR amyloidosis diseases.
Title
Wireless Power Transfer Research

Authors
Morian, Troy; Basha, Elizabeth

Introduction
Ever wonder how power is delivered to electronic sensors used in remote areas to detect phenomena like earthquakes? Historically, these devices would be powered using on-site generators, but those days will soon be over with the introduction of wireless power transfer technology! Through the usage of electromagnetic induction technology and unmanned aerial vehicles, energy can be delivered wirelessly to remote sensor locations.

Purpose
The purpose of this research is to show how wireless power transfer technology can be harnessed specifically to provide energy to electronic sensors in remote locations using unmanned aerial vehicles (UAVs). The overall goal of this project is to have a UAV fly autonomously to the location of these sensors, hover over them to transfer enough energy to recharge their batteries, and then return to its charging base. The UAV then repeats this procedure for as many times as the sensor's battery runs low.

Methods
A set of copper rings is used on both the unmanned aerial vehicle and the ground sensor to facilitate the wireless energy transfer between the two entities. The rings on the UAV are being driven at a specifically-tuned frequency which allows them to "couple" to the set of rings on the ground sensor.

Results
This research is still very much a work in progress, but the goal is to have a working proof-of-concept that shows the promise of this technology.

Significance
The results of this type of research could potentially change the way power is delivered to electronic devices around the world, eliminating the need for wires to deliver energy.
### Title
pH-Sensitive Cationic Lipid Coated Magnesium Phosphate Nanoparticle for Intracellular Protein Delivery.

### Authors
Naidu, Prathyusha; Fang, Yunzhou; Guo, Xin

### Introduction
Cationic lipid-coated magnesium phosphate nanoparticle (Lip-MgP NP) formulations were developed for efficient intracellular catalase protein delivery. Lip-MgP NP would carry positive charges to allow their adhesion to the negatively charged cell membrane, followed by endocytosis and translocation into endosomes, where the pH will decrease. In response, the magnesium phosphate core of Lip-MgP NP would dissolve to increase the osmotic pressure inside the endosome. The endosome would then swell and destabilize to release the entrapped cargo protein into cytosol.

### Purpose
This project is a novel, expandable nano-system that delivers proteins into cells. Proteins are prone to enzymatic degradation and hepatic/renal elimination while circulating in the blood, and are too large to diffuse into cells. This technique enhances the protein intracellular delivery without losing the stability of the proteins which is a major issue with protein formulations. It also increases the efficacy of the delivery of formulation into cells.

### Methods
The magnesium phosphate (MgP) nanoparticles were prepared by water-in-oil micro emulsion precipitation. The cargo protein catalase was entrapped into cationic liposome by lipid hydration and extrusion. Then Magnesium phosphate (MgP) nanoparticles were mixed with catalase-loaded cationic liposome to form the final Lip-MgP NP formulation.

### Results
The formulated Lip-MgP NPs were of size around 200 d.nm and highly positive zeta potential around 30 mV. UV quantization of hydrogen peroxide degradation by catalase showed faster release of cargo protein from Lip-MgP NPs at pH 5.5 than at pH 7.4. The MTS cell viability assay showed that intracellular delivery of catalase by Lip-MgP NPs successfully protected the cells from exogenous hydrogen peroxide.

### Significance
This project is a novel, expandable nano-system that delivers proteins into cells. It was designed to overcome barriers like intracellular protein delivery including premature deactivation of the cargo protein, insufficient cellular uptake. Liposomes are prepared in such a way that the cargo proteins are neither exposed to elevated temperature or fluctuations in pH. Studies showed that proteins are stable until they are delivered. It is a more effective protein delivery systems. Such a system will greatly facilitate the development of proteins into new medicines.
## Title
An International Study on Shareholder Protection in Minority M&A Transactions

## Authors
Ouyang, Wenjing; Zhu, Pengcheng

## Introduction
We define minority M&A transactions as those initiated by target controlling shareholders to acquire the rest minority shareholders' ownership in the target firm. Minority shareholder protection is the center of corporate governance practices. However, existing studies provide diverse evidence with regard to whether minority shareholders are expropriated by controlling shareholders in minority merger deals.

## Purpose
We use an international minority merger sample covering 55 countries to examine multiple merger outcomes to present a comprehensive analysis of minority shareholder rights protection. Our study provides new evidence of minority shareholder protection in the international scope.

## Methods
Using multivariate regression models, we examine whether the merger premium, the merger payment, and the probability of merger completion is related with the country minority shareholder protection.

## Results
Our results show country-level minority shareholder protection significantly increases merger premium and cash payment probability, but significantly decreases the deal completion rate. These results suggest target minority shareholders get higher payment; they are exposed to less risk of expropriation for being future minority shareholders; and they possess more bargaining power. These results are consistent over all the measures of minority shareholder protection. In robustness tests, we find the results are not driven by observations in a specific set of countries. Furthermore, these results still hold after we control for sample selection bias and endogeneity issues. Overall, these findings suggest minority shareholders in countries with stronger corporate governance mechanisms enjoy higher protection in minority merger deals.

## Significance
This paper provides new evidence of minority shareholder protection in merger transactions. Different from previous studies that are restricted to minority deals in a particular country, our study uses a more comprehensive dataset so that we can more generally examine minority shareholder protection in the international scope. This paper also contributes to the literature of mergers and acquisitions. Compared to vast studies on majority mergers and acquisitions, researches on minority shareholder wealth are limited and the results are mixed. Our design of empirical study allows us to have a more thorough investigation of minority shareholder protection in mergers and acquisitions. Our results indicate existing arguments on minority shareholder protection in different countries can be because of the country-level corporate governance and legal enforcement.
**Title**
Theoretical Elucidation of the Electronic Structure of the [M2X8]n- (n=2-4) Anions

**Authors**
Pastor, Michael B.; Zhao, Qinliang

**Introduction**
A series of complexes with dimeric [M2X8]n- anions (M = Tc, Re, Mo, Os, W; n = 2-4; X = F, Cl, Br, I) have been synthesized and structurally characterized in the literature. Generally, the metal-metal bond distance increases as the bond order in between decreases. However, in the case from [Tc2X8]2- to [Tc2X8]3-, the Tc-Tc bond distance deceased from c.a. 2.15 to c.a. 2.13 Angstrom as the bond order decreased from 4 to 3.5 in the later anion.

**Purpose**
It is important to understand which factors enforce the unexpected decrease of the bond distance in [Tc2X8]n-, and how we can use the factors to tune the metal-metal interactions.

**Methods**
Detail theoretical calculations were conducted on the series of [M2X8]n- anions. Coordinates from the crystal structures in the literature were directly used in geometry optimization for the anions that have been structurally characterized. Models built from analogous compounds were applied for compounds without published structures and hypothetical anions.

**Results**
The study demonstrated that the metals, halides and the charges of the anions cooperatively influence the electronic structure, the bond strength of each type of bond, bond order, and therefore the bond distance between the metal atoms.

**Significance**
This study will help us understand how we can purposefully control metal-metal interactions, and thus fine-tune the reactivities exhibited by bimetallic complexes.
### Title
RATIONAL DESIGN USING AN AMINO ACID CODE FOR PROTEIN STRUCTURE

### Authors
Patel, Shivarni; Joo, Hyun; Su, Dan; Sachdeva, Sameer; Phan, Jamie; Chavan, Archana; Li, Xiaoling; Tsai, Jerry

### Introduction
The goal of protein design is to specify the amino acid sequence that produces a fold with determined functionality. Accomplishing this goal would be greatly aided by knowledge of an amino acid code to protein structure. Such a code must accurately describe the packing interactions of side-chain residues.

### Purpose
The knob-socket model provides such a code by classifying protein structure based on distinct amino acid side-chain preferences which then predicts the knob-socket arrangement of the protein packing. This model was tested in two experimental designs.

### Methods
First, the knob-socket model was used to design a 27 amino acid sequence, KSα1, which has been shown to fold into alpha helix configuration and homodimerizes. By mutating a specific amino acid in the sequence, the knob-socket model predicts strengthened or weakened packing stability. The effects of helix stability and dimerization are characterized with CD spectroscopy and SPR. A second preliminary study has been undertaken that tests the knob-socket model’s ability to design peptides that bind to defined interaction sites on a receptor. The knob-socket model was used to design peptides that fit into the binding sites of the epidermal growth factor receptor (EGFR) and the human epidermal growth factor 2 (HER2), both of which are targets for the treatment of cancer.

### Results
Based on frequency of appearance in known structures, the knob-socket model provides the basis for prediction of stabilizing and destabilizing mutations. The designed peptides demonstrate a 1 to 2 order of magnitude enhancement in binding over naïve approaches that simply connect the variable regions from a binding antibody.

### Significance
The knob-socket model represents a novel and significant advancement in the understanding of protein structure and design based on an innovative characterization of side-chain patterns.
<table>
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<th>Title</th>
<th>Evaluation of AG10 as a Potential Therapy for Transthyretin Cardiac Amyloidosis</th>
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<tr>
<td>Authors</td>
<td>Penchala, Sravan; Wang, Yu; Chan, William; Park, Miki; Graef, Isabella; Alhamadsheh, Mamoun</td>
</tr>
<tr>
<td>Introduction</td>
<td>Cardiac amyloidoses, which are most commonly caused by aggregation of immunoglobulin light chains or transthyretin (TTR) in the cardiac interstitium and conducting system, represent an important and often underdiagnosed cause of heart failure. As no FDA-approved drugs are currently available for treatment of these diseases, the development of therapeutics that prevents TTR-mediated cardiotoxicity are highly desired.</td>
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<tr>
<td>Purpose</td>
<td>Small molecules that kinetically stabilize the TTR tetramer have been shown to inhibit TTR amyloidosis. Previously we reported the first high-throughput screen (HTS) for TTR ligands, which enabled us to identify a variety of potent and structurally diverse TTR kinetic stabilizers. We used these compounds as a starting point for structure-activity relationship (SAR) studies and synthesized a series of analogs of one of best hits from this HTS. Here, we report the development and evaluation of AG10, a potent and selective kinetic stabilizer of TTR that prevents the dissociation of TTR in serum samples obtained from amyloid cardiomyopathy patients and inhibits the toxicity of TTR aggregates towards human cardiomyocytes.</td>
</tr>
<tr>
<td>Methods</td>
<td>The binding affinity of AG10 to TTR was evaluated by Isothermal Calorimetry and fluorescence polarization studies. The selectivity of AG10 to TTR in serum was tested using fluorescence-based competitive assay. Western blot was used to study and measure the effect of AG10 on native TTR stability in serum over a period of 72 hours. Further, preclinical pharmacokinetic studies of AG10 were performed in both rats and mice. The sub-chronic (28 days) toxicity of AG10 was evaluated in rats.</td>
</tr>
<tr>
<td>Results</td>
<td>Western blot studies revealed that the efficacy of AG10 to stabilize TTR in human serum exceeds other TTR stabilizers currently in clinical trials. Biochemical and biophysical studies determined the binding energetics of AG10 to TTR. Crystallographic studies of AG10 bound to TTR gave valuable insights into how AG10 achieves such effective kinetic stabilization of TTR. The preclinical animal studies showed that AG10 was orally bioavailable, and lacked toxicity (during 28 day sub-chronic study in rats).</td>
</tr>
<tr>
<td>Significance</td>
<td>The potency and selectivity of AG10 to TTR in human serum exceeds those of other drugs currently in clinical trials. Further, the oral bioavailability, lack of toxicity in rodents, and additional favorable pharmacokinetic properties make AG10 a very promising candidate compound for treatment of TTR amyloidoses.</td>
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</table>
Title
Design of Dual Chain Antibody Mimics Based on Cetuximab–EGFR Complex

Authors
Sachdeva, Sameer.; Jasti, Bhaskara.; Li, Xiaoling.

Introduction
Antibodies have been widely used as reagents to recognize antigens or proteins in life science research because of their binding specificity. The limitations like high molecular size, high cost of production, long development time have led to the research for antibody alternatives with lower molecular weight, similar binding and affinity properties but without the lengthy and complicate process of generating antibodies. We propose a new rational way of designing antibody mimics utilizing molecular interactions between CDRs of antibody and receptor (antigen) which could be a logical approach to build antibody mimics from ground up.

Purpose
Purpose of the project is to design antibody mimics using the peptides derived from the complementarity determining regions (CDRs) of Cetuximab with different binding regions on EGFR extracellular domain and enhance the affinity and specificity of antibody mimic compared with single chain peptide ligands.

Methods
Antibody mimics were designed based on the interactions between Cetuximab-CDRs and EGFR. Two peptides with sequence of THR-TYR-TYR-ASP-TYR-GLU-PHE (Pep1) and ILE-TRP-SER-GLY-GLY-ASN-THR-ASP-TYR (Pep2) from CDR-H3 and CDR-H2 region were identified from two different regions in the heavy chain according to the interactions analysis between Cetuximab and EGFR. The peptides were conjugated through a disulphide (DS) or a Glycine4Serine (G4S) linker to form an antibody mimic. Docking studies were performed to identify the interactions between single chain peptides and EGFR and to verify binding interactions after the antibody mimics (DS and G4S) were designed using Molecular Operating Environment (MOE) software. Specific binding capability of antibody mimics were evaluated by observing binding/uptake of the FITC labeled antibody mimics in A431, MDA-MB468 cells (overexpressed EGFR) and HEK293 (control) using confocal microscope and flow cytometer.

Results
Docking scores for different confirmations of the antibody mimics were in the range-38.37 to -13.23 and -36.06 to-15.66 for DS and G4S, respectively. Both DS and G4S dual chain antibody mimics retained five interactions with EGFR out of total six interactions in Cetuximab-EGFR complex in docking analysis. Confocal microscopy images display significantly higher cellular binding/uptake of both molecules in EGFR overexpressed cells and negligible binding in control cells. Mean fluorescence intensities (MFI) in flow cytometer analysis using control, Pep1, Pep2, DS, and G4S were 28.15, 87.68, 75.14, 110.49, and 76.29 for A431 cells; 29.35, 71.17, 49.67, 111.94, and 68.03 for MDA-MB 468 cells; and 4.85, 8.65, 6.02, 5.98 and 7.26 for HEK 293 cells, respectively.

Significance
Antibody mimics with dual binding regions can be designed based on Cetuximab-EGFR complex. In vitro cellular uptake studies demonstrated that the designed dual chain antibody mimics can specifically bind to and uptaken by EGFR overexpressed cancers and can be potentially used to target these cancers.
**Title**
Micellar Characterization and Cellular Internalization of RGD based Peptide Amphiphiles for Targeted Delivery to Integrin Overexpressing Tumors

**Authors**
Saraf, Poonam; Li, Xiaoling; Jasti, Bhaskara

**Introduction**
The treatment benefits from current FDA approved drug products for cancer are not optimal and lead to tumor repopulation after treatment. These therapies also suffer from issue of dose related toxicity. Nanotechnology based research is focused on developing drug delivery systems with better tumor cell uptake, specificity and reduced dose related toxicity. The alpha v beta 3 integrin is overexpressed in cancers of the lung, skin and breast and plays a role in the cell motility and migration during angiogenesis. Hence, it is an important target in the treatment of cancer. Peptide based amphiphiles containing RGD motif, which is a known ligand for integrin, can serve as carriers for delivering drugs specifically to integrin over expressing tumors. In the present study a micellar carrier was developed for active targeted delivery of hydrophobic anticancer drugs to alpha v beta 3 integrin overexpressing cancers.

**Purpose**
The objective of this study was to characterize micellar properties, binding, cellular uptake and cytotoxicity of paclitaxel loaded RGD amphiphiles designed as carriers for integrin targeted drug delivery.

**Methods**
Peptide-fatty acid conjugates of fatty acid with cyclic or linear RGD (or GGG as negative control) were synthesized by solid phase peptide synthesis via ADA (8-amino-3,6-dioxo-3-octanoic acid) linkers to form amphiphiles. The amphiphiles were characterized for Critical Micellar Concentrations (CMC) using pyrene fluorescence method. The aggregation number of amphiphiles was determined by steady state fluorescence quenching. The micelles were characterized for antidilution by loading FRET (Forster Resonance Energy Transfer) dyes, namely Dil and DiO and monitoring fluorescence spectra at λex 484 nm and λem 495-600 nm upon dilution with water or methanol. The competitive binding was studied by measuring displacement of fluorescent probe, 5 nM Cyclo[RGDy-K(5-FAM)] bound to 300 nM alpha v beta 3 integrin. The internalization of 200 μg/mL fluorescein isothiocyanate (FITC) loaded micelles and equivalent concentration of free FITC at 37°C in A2058 melanoma cells was determined by confocal laser scanning microscopy and compared with internalization at 4°C. Internalization of amphiphiles was further studied by pretreatment of cells with 0.45M sucrose as clathrin mediated endocytosis inhibitor. Cytotoxicity assays with paclitaxel loaded micelles were performed in melanoma cells.

**Results**
Results: The CMC and aggregation numbers of amphiphiles were reported between 7-30 μM. The high FRET efficiencies upon dilution in water were observed due to entrapment of the hydrophobic dyes in the intact micellar core. Cyclic RGD amphiphile exhibited highest binding with upto 72% displacement of probe. Significantly higher fluorescence upon treatment with FITC loaded ‘RGD’ micelles was observed in cells as compared to treatment of free FITC or FITC loaded in control amphiphile (non targeted ‘GGG’ conjugated micelles). Lower internalization at 4°C and in presence of endocytosis inhibitor confirmed that the uptake was energy dependent process. Lower IC50 value of paclitaxel loaded in micellar carriers was observed compared to free drug in melanoma cells.

**Significance**
RGD peptide amphiphiles formed micelles in aqueous medium, exhibited specific binding to target protein, and showed significantly higher uptake and cytotoxicity in melanoma cells.
**Title**
Flow Fantasy: Soap Bubbles, Sand Box, and More

**Authors**
Shakerin, Said

**Introduction**
Fluid motion is an ever present part of our lives. Examples are: wind in the atmosphere, currents in rivers, and blood flow in our arteries. In addition to gases and liquids, some solids such as granular materials show fluid-like behavior. The world of fluid motion is usually complex but also beautiful. The author is interested in designing science-based devices that exhibit such characteristics.

**Purpose**
The objective is to develop an interactive display that exhibits the beauty and complexity of three materials - liquid dish soap, beach sand, and tiny balls - as they flow in their respective enclosures. The purpose is to provide a device for informal science education for the campus community and its guests/visitors.

**Methods**
The project included three parts: (1) preliminary study to determine the final design, (2) fabricating the final enclosures, and (3) fabricating an attractive frame to house the enclosures for safe installation at the Library. In the preliminary study, geometrical parameters such as shape, size, and enclosure interior details were considered as well as different types of filling materials (fluids). The final design was a circular enclosure that is only 1/16 inch deep and made of acrylic, clear in the front with black in the back to provide contrast with the chosen materials. The enclosures containing soap and sand each have a diameter of 16 inches while the enclosure containing stainless steel balls is only 6 inches in diameter. 3500 precision balls occupy that enclosure.

**Results**
The final display is a large but relatively thin frame that houses the three circular enclosures each of which is attached to a turn table that allows a user to easily rotate the enclosure to initiate the respective flow. Brief text blocks are affixed to the frame to inform users how to use the display, scientific facts demonstrated, and information for further learning. As each enclosure is turned about 180 degrees interesting patterns emerge that show a number of scientific facts such as specific arrangements among soap bubbles and sand mounds and crystalline defects as modeled by the packing of tiny balls. Samples of enclosures made during the preliminary study are available during Research Day presentation for participants to examine.

**Significance**
The display was recently installed on the wall next to the elevator in the Library near Information Commons and is available for public use as shown above. Funding was provided by a 2013 Scholarly/Artistic Activity Grant from the Faculty Research Committee.
**Title**  
Sex-based alteration of relative importance of EDRFs in modulating vascular reactivity in Zucker diabetic fatty (ZDF) rats

**Authors**  
Shaligram, S.; Han, X.; Zhang, R.; Anderson, L.; Rahimian, R.

**Introduction**  
Clinically it has been shown that premenopausal women have a lower incidence of cardiovascular diseases compared with age-matched men. Premenopausal women with diabetes not only lose their sex-based cardiovascular protection but also experience a higher relative risk of cardiovascular diseases compared to diabetic men. Nevertheless, little is known about interaction of sex and diabetes in vasculature.

**Purpose**  
Our study investigates the effects of type 2 diabetes on endothelium-dependent and -independent relaxations. Also, if there are sex-based changes in relative contributions of endothelium derived relaxing factors (EDRFs) in modulating vascular reactivity of mesenteric arteries (MA) from ZDF rats.

**Methods**  
16-18 weeks old male and female ZDF rats (fa/fa) and their lean controls (fa/-) were used. Relaxation responses to acetylcholine (ACh, 10-8 to 10-5M) in MA pre-contracted with phenylephrine (PE) were obtained before and after pretreatment with indomethacin (cyclooxygenase inhibitor), L-NAME (nitric oxide synthase inhibitor) or barium chloride (Kir blocker) plus ouabain (Na+-K+-ATPase inhibitor). Vascular responses to sodium nitroprusside (SNP, 10-9 to 10-5M) were also measured in MA.

**Results**  
ACh-induced relaxations were significantly impaired in MA of ZDF rats compared to their lean controls, regardless of sex. In diabetic females, the relative importance of endothelium derived hyperpolarizing factor (EDHF) in relaxation to ACh was reduced, while in diabetic males, role of nitric oxide (NO) in relaxation to ACh was reduced. Interestingly, relaxation to SNP was enhanced in ZDF rats, irrespective of sex.

**Significance**  
The relative importance of NO and EDHF in regulating vascular tone of rat MA is altered in type 2 diabetes with respect to sex. Furthermore, increased smooth muscle sensitivity to NO may be an attempt to compensate for impaired endothelial function in both diabetic male and female rats.
**Title**
A Pharmaceutical Polymer Demonstration Module for STEM High School Laboratories

**Authors**
Smith, Timothy J

**Introduction**
Many polymers are used as drugs or combined with drugs for a variety of medical applications. This laboratory will demonstrate the process of encapsulation using alginate, a carbohydrate polymer (polysaccharide) extracted from brown seaweed as a basis for a high school STEM laboratory illustrating pharmaceutical principles.

**Purpose**
At the conclusion of this exercise the student should be able to:
1. Prepare calcium alginate beads.
2. Understand the process and potential applications of encapsulation.
3. Understand the concept of negative and positive charge interactions in complex formation.
4. Define the term “polymer” and give an example.
5. Observe the processes of diffusion and chromatographic separation.

**Methods**
1. Add the calcium chloride solution to one of the beakers.
2. Use the dropper to slowly draw up the alginate solution into the pipet, taking care not to draw up air bubbles.
3. While swirling the beaker containing the calcium chloride, slowly add the alginate dropwise (about 1 drop per second) from the pipet. The pipet tip should be positioned about a half inch above the surface of the calcium chloride. You will see beads form; continue swirling.
4. Continue preparing beads until you have added approximately 1 ml (about 20-30 drops) of alginate solution. After this amount is added, continue swirling the beads for approximately 1 min (to stabilize the bead formation).
5. After Step 4, place a filter into the other beaker and collect the beads by filtering off the calcium chloride solution.
6. Discard the calcium chloride solution into the sink.
7. After blotting the excess calcium chloride solution from the bottom of the filter, carefully place the beads into the petri dish, allowing the beads to stay in contact with the filter paper. With a gloved hand, gently “smash” a few of them against the filter paper surface. Describe what was observed.

**Results**
Approximately 4 cohorts of 13 high school students/cohort have readily demonstrated calcium alginate complexation through the method above and were able to correctly identify the principles outlined above.

**Significance**
This simple laboratory illustrates important concepts in the pharmaceutical sciences and is easily applied to virtually any high school laboratory environment.
### Title
In Vitro Permeation Mechanism Study of Griseofulvin loaded Nanoemulsion through MDCK Cells and PAMPA

### Authors
Stowell, Yoshiko; Wu, Huiyi; Jasti, Bhaskar; Li, Xiaoling

### Introduction
Oil in water (o/w) nanoemulsion is a two-phase dispersed system in which the oil can incorporate poorly water soluble drugs to form a liquid dosage form. The enhancement of bioavailability and efficacy with a use of nanoemulsion has often been reported empirically and speculated to be a result of the enhanced dissolution due to a larger surface area, however, the mechanism of nanoemulsion permeation is yet to be explored.

### Purpose
The purpose of the project was to study the effect of drug loading in nanoemulsion and the contribution of free drug in aqueous phase of nanoemulsion formulation on the permeation of drugs through the MDCK cells and PAMPA.

### Methods
Nanoemulsion was prepared using MCT oil as oil phase and Span80/Tween80 mixtures as emulsifier. Poorly water soluble griseofulvin was used as a model drug. To study the effect of drug loading, three levels of drug loading were prepared. In vitro permeation study was conducted using MDCK cells and PAMPA. The sink condition and non-sink conditions were used for the MDCK cells and PAMPA, respectively. The free drug in the aqueous phase of nanoemulsion was separated from oil phase by ultrafiltration of nanoemulsion. The concentrations of griseofulvin were determined by HPLC. The degree of saturation in both aqueous and oil phase was calculated using solubility of the drug in corresponding phase. Two mathematical models were developed to describe the drug permeation in sink and non-sink conditions and permeability coefficients were calculated using these models. The free drug concentration in the aqueous phase was assumed to be constant as the oil phase acted as a reservoir.

### Results
In the sink condition permeation studies using MDCK cells, the flux increased linearly as the concentration of the free drug in the aqueous phase (Caq) increased. For the non-sink condition permeation studies using PAMPA, the concentration in the receptor at a fixed time point increased linearly as Caq increased. A linear relationship between the degree of saturation in the aqueous phase and that in the oil phase was observed. This linear relationship was extended to supersaturated condition. Similar permeability coefficients were obtained from both MDCK cells and PAMPA permeation studies. The experimental data fitted the models under the assumption that the oil phase acted as a drug reservoir to maintain the free drug concentration in the aqueous phase while permeation occurred only from free drug in the aqueous phase.

### Significance
For a nanoemulsion system, the permeation of drug across the barriers depends on the free drug in the aqueous phase, while oil phase serves as a reservoir.
**Title**  
Characterization of chemical additives used in hydraulic fracturing fluid

**Authors**  
Stringfellow, William T.; Domen, Jeremy K.; Sandelin, Whitney L.; Camarillo, Mary Kay

**Introduction**  
Hydraulic fracturing is an oil and gas well stimulation technique in which fluid is pumped into wells under high pressure to fracture geological formations, whereby increasing formation permeability and oil/gas yields. Hydraulic fracturing fluid is a complex mixture typically composed of water, sand, and chemical additives. As hydraulic fracturing becomes increasingly common throughout the United States, it is important to understand the properties of these chemical additives being introduced to the environment.

**Purpose**  
In this study, the chemicals used in hydraulic fracturing fluid were characterized in order to evaluate potential impacts on the environment, human health, and flowback/produced water treatment. The objectives were to 1) compile a list of commonly used compounds in hydraulic fracturing, 2) categorize chemicals based on their purpose in hydraulic fracturing fluid, 3) characterize compounds based on physical, chemical, and toxicological properties, and 4) identify deficiencies in the current state of knowledge.

**Methods**  
A list of chemicals commonly used in hydraulic fracturing fluids was compiled from sources including FracFocus Chemical Disclosure Registry, U.S. EPA reports, and published literature. Physical, chemical, and biological data was compiled from multiple publicly available online chemical information databases and reference books. Toxicity data for all chemicals was categorized according to the United Nations’ Globally Harmonized System of Classification and Labelling of Chemicals (GHS) acute toxicity categories.

**Results**  
Eighty-one chemical additives to hydraulic fracturing fluid were identified. Chemical additives primarily function as gelling/foaming agents, friction reducers, crosslinkers, breakers, pH adjusters, biocides, corrosion and scale inhibitors, iron controllers, clay stabilizers, or surfactants. Fifty-four compounds are organic. Of the organic compounds, twenty-seven are considered readily biodegradable. Most chemicals are not of concern toxicologically; however, three GHS category 1 inhalation toxins and three GHS category 2 oral toxins were identified. Twenty-one of the chemicals have high to moderate theoretical chemical oxygen demands, which may impact treatment of the flowback/produced water and should be taken into account for treatment process design.

**Significance**  
While many of the chemicals used in hydraulic fracturing are not toxic, significant unknowns remain concerning the toxicity of the thirty compounds which do not have available data. Biocides, in particular, are of concern as they contain the greatest number of toxic compounds. Although steps toward increased chemical disclosure are being taken, more information needs to be made available concerning proprietary chemical mixtures and derivatives, chemical concentrations, and the mass of chemicals used in hydraulic fracturing operations in order to better understand the potential environmental, human health, and treatment implications associated with hydraulic fracturing.
### Title
Design, Synthesis, and In Vitro Binding Studies of a Novel Peptide HER2-PEP2 for HER2 Targeting

### Authors
Su, Dan; Jasti, Bhaskar R; Li, Xiaoling

### Introduction
Human Epidermal Growth Factor Receptor 2 (HER2) is a cell surface receptor tyrosine kinase and plays a role in the signal pathways leading to cell proliferation and differentiation. HER2 has been considered as a target for receptor-mediated drug delivery system and antibodies for cancer treatment. This work is about design of a novel peptide that specifically binds to HER2 based on the binding interactions between antibody Pertuzumab and HER2.

### Purpose
To design, synthesize and characterize the binding specificity and uptake of a novel peptide that specifically binds to HER2.

### Methods
Interactions between Pertuzumab and HER2 were mapped by using Molecular Operating Environment (MOE) software. Two key interaction sites were utilized (residues 26-35 and 95-102 on heavy chains of Pertuzumab) to design a peptide binds to HER2. A two-chain peptide (HER2-PEP2) with sequences of Gly-Phe-Thr-Phe-Thr-Asp-Tyr-Thr-Met-Asp and Asn-Leu-Gly-Pro-Ser-Phe-Tyr-Phe-Asp-Tyr linked by Gly-Lys was synthesized by solid phase synthesis. HER2-PEP2 was then tagged with FITC through a 6-aminohexanoic acid linker (Ahx). The peptide was purified using HPLC and characterized using mass spectroscopy. In vitro binding of HER2-PEP was studied using HER2 over-expressed MDA-MB-361 and ZR-75-1 cells and non-HER2 expressing HEK293 cells as control. Cells were incubated with HER2-PEP2 and a control peptide with sequence of Gly-Ala-Gly-Ala-Gly-Ala-Ahx-FITC at concentration of 10μM at 37°C for 15min. Cells were then visualized under fluorescent microscopy. The fluorescence intensities were determined using flow cytometry.

### Results
Under fluorescent microscopy, high fluorescence intensity was observed on MDA-MB-361 and ZR-75-1 cells when treating with HER2-PEP2, while only background fluorescence was observed when treating with control peptide. For HEK293 cells, only background fluorescence was observed on cell surface when treating with both HER2-PEP2 and control peptide. Flow cytometric studies showed that the geometric mean fluorescence intensity (MFI) (n=6) of MDA-MB-361 and ZR-75-1 cells after treating with HER2-PEP2 was about 19 and 8 fold higher than control peptide, while no significant difference of MFI in HEK293 cells was observed between the cells treated with HER2-PEP2 and control peptide.

### Significance
This work demonstrated the feasibility of designing peptide that can specifically bind to HER2 by utilizing the interactions in Pertuzumab-HER2 complex. This peptide can be used for targeting delivery of drugs, diagnostic probes or imaging agents.
**Title**
Light on the Horizon: Polypyridyl Metal Complexes for Use as Optically Active Monomers

**Authors**
Tran-Math, Carolyn; Zhao, Qiliang

**Introduction**
Polypyridyl Ruthenium complexes are studied extensively not only for their catalytic ability, but also for their interesting photonic properties. When a metal ion is bound to a polymeric substrate, the photonic properties serve as a means of both locating the metal core and confirming the electronic configurations of the metal core. However, there are few means in controlling the synthesis of the material, and thus fine-tune their functions.

**Purpose**
It is important to understand how the metal installation process will influence the polymer morphology and thus their applications in material development. This project focuses on the metal-containing monomer synthesis followed by polymerization.

**Methods**
A mixed-ligand complex containing Ruthenium was synthesized, and then characterized with the intent of obtaining a redox-active fluorescent monomer to be tethered to an N-isopropylacrilimide (NIPAM) polymers for study as a light-activating mechanical material. Analogs containing a more abundant metal, Nickel, were synthesized and characterized in parallel.

**Results**
The monomer products were confirmed via high resolution mass spectrometry and NMR. Electronic transitions were collected in the UV-Vis range, and corresponding emission spectra were obtained via spectrofluorometry. DFT calculations were conducted to locate molecular orbital energies, which were experimentally confirmed by electrochemical studies on untethered monomers.

**Significance**
With complete analysis of the monomers and the polymerization process that will follow, the project will shed light on how the monomer structure influences the synthesis, morphology and properties of the desired polymeric material.
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<th><strong>Title</strong></th>
<th>pH-Sensitive Conformatinal Switch Lipoplexes for siRNA Delivery</th>
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<tr>
<td><strong>Authors</strong></td>
<td>Zhao, S; Zheng, Y; Liu, X; Samoshin, Vyacheslav V.; Franz, A; Guo, X</td>
</tr>
<tr>
<td><strong>Introduction</strong></td>
<td>siRNA represents a promising category of therapeutic agents for the treatment of viral and genetic diseases. However, successful gene knockdown by siRNA depends on its efficient delivery into target cells. Previously, we have reported pH-sensitive liposomes with conformational switch (Fliposomes) as a potential delivery system for small-molecule drugs and biomacromolecules. In this study, we prepared complexes of cationic Fliposomes and siRNA to transfect T47D-KBluc cells (human breast cancer), which stably express firefly luciferase.</td>
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<tr>
<td><strong>Purpose</strong></td>
<td>To develop and validate lipoplexes with pH-sensitive conformational switch for effective delivery of siRNA into cultured human cancer cells</td>
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<td><strong>Methods</strong></td>
<td>Cationic lipid and conformational switch lipid was mixed at 1:1 ratio before forming a lipid film on rotovap. The film was hydrated in HEPES buffer pH 7.4 to form Fliposome (liposome with conformational switch). Fliposome sizes were controlled by going through a 0.2 uM filter on an extrusion device. poly-L-glutamic acid (PG) was used as a stabilizer to premix with anti-Luciferase siRNA or anti-GFP siRNA at 1:1 ratio before mixing with Fliposome. T47D-kb luc cells which stably express firefly luciferase and Hep3b-eGFP cells which stably express Green Fluorescence were used as target cells for transfection. Luciferase and GFP suppression were measure on a FLUOstar OPTIMA plate reader.</td>
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<td><strong>Results</strong></td>
<td>Homogeneous Fliposome and their complexes with siRNA were successfully prepared with desired sizes and charge ratios. Electrophoresis studies indicated that PG improved the stability of the Fliposome-siRNA complexes. Significantly more efficient knockdown of the luciferase activity was achieved by the Fliposome/siRNA complexes compared to liposome/siRNA complexes containing the common cationic complexes in both cell lines.</td>
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<td><strong>Significance</strong></td>
<td>A validated method of delivering siRNA into two cultured human cancer cells was developed. Fliposome shows its great potential of being a effective vector for drug delivery.</td>
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<td>Assessment of the effect of 5-HT2A receptors on brain serotonin (5-HT) via a mechanism-based pharmacokinetics and pharmacodynamics model</td>
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<td>Zhou, Zhu; Sun, Jingjing; Uchizono, James A</td>
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<td>Although major ethical challenges make it nearly impossible to invasively and directly measure 5-HT brain levels in humans, neuroimaging technologies have shown macroscopic structural and functional abnormalities in the prefrontal cortex (PFC) and dorsal raphe nucleus (DRN) in depressed patients. Characterization of these two key areas can lead to new strategies in the treatment of depression.</td>
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<td>To develop a mechanism-based pharmacokinetics and pharmacodynamics model to predict 5-HT levels in the DRN and PFC in response to different infusion concentrations of DOI (5-HT2A agonist) given into the PFC.</td>
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<th>Methods</th>
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<td>Extracellular 5-HT levels in the PFC and DRN of rats (n=3-5) were measured by intracerebral microdialysis. A modified indirect model was used to capture the effects at the 5-HT2A receptor. Six model parameters were obtained from model estimation and three were fixed from experimental data. Phoenix WinNonlin® and Berkeley MadonnaTM were used for model estimation, external validation with secondary data set, and simulation.</td>
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<td>The time-course profiles of 5-HT in both DRN and PFC was well modeled with different dosing schemes of DOI. Model parameters were estimated with reasonable precision (CV% ranged from 1.37% to 35.03%), AIC was -72.81149 and SBC was -59.61987. The R² values were 0.9475 and 0.913 for the DRN and PFC models, respectively. Simulations from this model suggested the modulation of the 5-HT2A receptor located in PFC was predictably controlling the 5-HT in DRN and PFC.</td>
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<td>A mechanism based model was developed to identify the neurotransmitter mechanisms, and quantitatively estimate various key parameters of the disease related receptor system. Simulations using this model supports a hypothesized mechanism of 5-HT2A effect on 5-HT.</td>
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