

## **Exploration of the Synthesis of Substituted Tetrahydropyrans**

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*Biochemistry, Chemistry*

The Barbier-Prins cyclization is a reaction that results in the production of substituted tetrahydropyran rings (THP). THPs are six membered rings that contain one oxygen atom. THPs are important base molecules for a number of natural biological products, including the natural fish feeding deterrent, Kumepaloxane. The past research on the Barbier-Prins reaction has focused on varying the substituent aldehydes and ketones and using terminal alkenes. The focus of this work has been the synthesis of cis- and trans-homoallylic alcohols for use in the Prins cyclization. Over 2 summers, the research resulted in the synthesis of 2 novel THPs, but new pathways to develop the desired substituents in a stereospecific manner are still being researched and attempted.

## **Photodecomposition of Quetiapine Hemifumarate in Water**

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*Chemistry, Environmental Studies*

Recent studies have shown the presence of human personal care products in streams and rivers which receive water effluent from wastewater treatment plants. Antidepressants are one class of human personal care product which have been identified in waterways receiving treated wastewater effluent. Quetiapine Hemifumarate (trade named Seroquel) is one antidepressant which could be found in these waterways. This study investigates the photodecomposition of quetiapine hemifumarate. This study determined that quetiapine had a half-life ( $T_{1/2}$ ) of approximately 7.9 hours in East Gemini Lake Water, 63.6 hours in pH 9 buffered deionized water, 105.6 hours in pH 5 buffered water, and 153.7 hours in pH 3 buffered deionized water. Indirect photolysis experiments which eliminated hydroxy radicals raised the half-life in East Gemini Lake Water to 16.8 hours and those which eliminated singlet oxygen raised the half-life to 38.5 hours.

## **Interactions of Magnetic Nanoparticles with Common Human Blood Proteins**

Rachel L Seurer

*Chemistry*

Nanoparticles are quickly becoming important in various biomedical fields. Magnetic nanoparticles in particular are easily directed using magnetic forces as well as having additional applications in magnetic resonance imaging, bioseparation, and treatments such as hyperthermia. Despite considerable progress in the synthesis of nanomaterials our understanding of the interactions of these nanoparticles with living matter has not kept pace. This study looks at how human serum albumin and fibrinogen, the two most abundant opsonin proteins, interact with magnetic nanoparticles using various spectroscopic techniques including UV-Visible spectroscopy, infrared spectroscopy, and fluorescence spectroscopy.

### **Determination of carotenoid composition of egg yolks**

Steven K Sour

*Chemistry*

Carotenoids are a group naturally occurring pigments most commonly found in food. They are known to help prevent cancer, protect cells from free radicals, provide a source of vitamin A, enhance the immune system and help the reproductive system in humans. In this study the carotenoid content of chicken egg yolks were determined using spectroscopic methods (UV-Vis). More specifically, the comparison of carotenoid composition was followed through with chicken eggs from commercially raised chickens and chickens whose diets were Omega-3 fatty acid enriched.

### **Photolysis of the Antidepressant Venlafaxine HCl (Effexor XR) in Surface Water**

Timothy R Juba

*Biochemistry, Chemistry, Environmental Studies, Psychology*

The antidepressant Venlafaxine HCl (VenHCl), trade name Effexor XR, has been found in research to be harmful to aquatic life in and present in the highest relative concentrations in natural water systems. Experiments were run with VenHCl solutions in varying pHs, lake water, and in solutions to test indirect photolysis in test tubes to mimic surface water conditions using natural sunlight and a photoreactor. Samples were analyzed through HPLC-MS to determine the photolysis half-life of VenHCl in surface water, direct and indirect photolysis contribution, photolysis reaction products, and possible mechanisms for the photolysis reaction of VenHCl. The indirect photolysis of VenHCl in East Gemine Lake (EGL) water has a half-life of 45.89 hours and the direct photolysis mechanism showed little contribution to the reaction. Experiments did show potential photolysis products that are stable. The long half-life due to indirect photolysis and lack of photolysis through direct photolysis show that VenHCl are present in natural water systems much longer than expected and thus helps explain the harmfulness of the drug to aquatic life.

### **Development of an Enzymatic Resolution Experiment for First Year Chemistry Labs**

Betsy J Hutchinson

*Biochemistry, Chemistry, Education*

Our goal is for students to develop practical skills in the laboratory so that they are prepared to apply their knowledge in a variety of situations. Our first semester Purification and Analysis I laboratory emphasizes the development of separation techniques without the use of column chromatography. In the pharmaceutical industry, there is a constant need for enantiomerically pure chiral compounds and thus a need for the development of more efficient strategies for racemic-mixture separation. Methods for obtaining enantiomerically pure compounds range from asymmetric synthesis, to chiral column chromatography, to enzymatic resolution. The use of enzymes, such as lipases, presents advantages over the other methods as they catalyze reactions under mild conditions with high enantio- or diastereoselectivity with high efficiency with the possibility of using different reaction media, such as

organic solvents. We are presenting the development of laboratory that could be used for first year chemistry students to resolve and separate secondary alcohols using enzymatic resolution.

### **Plastic Polymers in Helmets**

Benjamin B Jagger

*Chemistry, Physical Education*

The plastic polymers used in helmets help prevent concussions due to their properties. By exploring the synthesis, structures, and polymer properties of polycarbonate and polypropylene I will uncover why they are used for helmets. These polymers have specific properties that make them optimal candidates for being used in helmets.

### **Sublimation Experiment**

Abdinasir A Abukar

*Chemistry*

Abstract Many of the basic skills for working with compounds are developed in the Introductory Chemistry laboratory. Sublimation is one common technique that is usually developed at this stage. We have developed an open-ended sublimation experiment in which students must purify an unknown compound by sublimation. The compound is analyzed by  $^1\text{H}$  NMR, infrared spectroscopy and melting point. Students then select the identity of the compound from a list of possibilities of inorganic, organometallic or organic unknowns.

### **Detection of oxidation level in model proteins upon exposure to magnetic nanoparticles**

Mitchell S Larson

*Chemistry*

Due to their unique properties, a wide variety of magnetic nanoparticles have been developed for cellular labeling, targeted drug delivery, magnetic resonance imaging (MRI) and magnetic hyperthermia. Recently, a large number of nanomaterials have been reported to increase the generation of cellular reactive oxygen species (ROS) causing oxidative modifications of DNA, proteins, and lipids. This project is focused on detection of magnetic nanoparticle induced oxidative modifications in model bovine serum albumin using spectroscopic methods.

### **Characterization and Isolation of active antimicrobial and antimalarial compounds from C. papaya leaves**

Malinda M Madery

*Chemistry*

More than 70 percent of bacterial infections are resistant to a common antibiotic used to treat the infection. Malaria has also become more difficult to treat due to Plasmodium falciparum's resistance to a wide variety of drugs. New antibiotics and antimalarial drugs are constantly needed to control and treat these infections because of this increase in resistance. Natural products have played a significant

role in treating diseases for thousands of years and they are still being discovered. Over 20 new drugs from natural products were launched on the market between 2000 and 2005. Among natural product sources is *Carica papaya*. This plant is known to have antimalarial, antibacterial, anticancer, and antifungal properties; however, the therapeutic compounds have not been isolated or characterized. Silica-gel column chromatography along with Sephadex LH-20 gels will be used for isolation of *C. papaya* leaves, and IR and NMR will be used for characterization. Isolation and characterization of these compounds could lead to useful synthetic treatments used for bacterial and/or malarial infections.

### **Computational based modeling as a means of predicting inhibitor binding to low molecular weight protein tyrosine phosphatases**

Dustin T Hansen

*Biochemistry, Chemistry*

It has been shown that the Low Molecular Weight Protein Tyrosine Phosphatases (LMW-PTP) play an integral role in cellular growth regulation. Based on the present understanding of LMW-PTP, there is great reason to pursue inhibition of this enzyme as an anticancer and anti-diabetes agent. One of the best LMW-PTP inhibitors that has been studied so far is pyridoxal-phosphate (PLP). However, this is only a temporary inhibitor, as the phosphate group is eventually cleaved from the molecule. In order to conserve time and resources computer based modeling techniques were employed to design and test potential inhibitors. Using PLP as a basis, potential inhibitors that lack the cleavable phosphorous-oxygen bond were built using ChemDraw software. Once built, these structures were imported into Maestro (Schrodinger, LLC) and docked into the Human A and B isoforms of LMW-PTP using the Glide program. The docking results of each ligand in each isoform were normalized in order to compare them to PLP and determine which may prove most valuable to test in vitro. Some structures proved to be better theoretical inhibitors than PLP, while many had binding scores that were very close to that of PLP. Using these theoretical data, the computer based modeling techniques have given direction toward which potential inhibitors should be studied in vitro. Further testing in the form of laboratory assays will be necessary to confirm what has been computationally predicted.

### **Studies toward the alkynoic acid cyclization of propargyl proline**

Jacob R Petersburg

*Chemistry*

Cyclization of propargyl proline is being investigated to provide insight into the regioselectivity of the alkynoic acid cyclization. This project will also evaluate compatibility of nitrogen containing compounds as well as the stability of stereocenters under reaction conditions. Propargyl proline was synthesized from propargyl bromide and L-proline methyl ester followed by hydrolysis to give the desired acid.

## **The use of 2D gel electrophoresis (2DGE), Western and Far Western blotting techniques to identify specific proteins and their modifications relevant for cellular responses**

Michael D Freeman

*Biochemistry*

Low molecular weight protein tyrosine phosphatase (PTP) is an enzyme that cleaves phosphates from cellular phosphoproteins, modifying the activity in complex signaling pathways in cells. PTP has demonstrated a role in cell cycle regulation and has been found to be over expressed in certain cancer and tumor cells. In order to determine the intracellular phosphoprotein targets of PTP, proteins were extracted from NIH/3T3 cells grown in culture. Following extraction, the proteins were separated by charge using isoelectric focusing and molecular weight by SDS polyacrylamide gel electrophoresis. After this 2D gel electrophoresis, the phosphoproteins were transferred to nitrocellulose and detected by adding p-Tyr (PY99) primary antibody and anti-mouse IgG with horseradish peroxidase as the secondary antibody attached (Western blot) or mutant PTP as the primary antibody and anti-GST with horseradish peroxidase as the secondary antibody (Far Western). In theory, it is possible to use a mutant version of PTP containing an attached glutathione S-transferase (GST) tag to identify the protein targets through Far Western blotting techniques. The mutant PTP should bind to the intracellular targets without cleaving the phosphate allowing the GST tag to be used as a binding site for a chemiluminescent identifier. Results of the 2-D gels on test samples and Western and Far Western blots on phosphoproteins from NIH/3T3 cells will be shown during the presentation.