

WELCOME TO
THE
WELLESLEY COLLEGE
CHEMISTRY
DEPARTMENT

**Summer Research Opportunities in Chemistry,
Physics, and Geosciences**

January 2009

Britt Argow
Coastal Sedimentology and Geomorphology, Geosciences Department

Projects:

The Coastal Lab's research program is built around the question: how will coastlines respond to the predicted acceleration in rates of sea-level rise? In order to address this question we must understand the sources, transport mechanisms and sinks of sediment in the coastal zone, and how these processes ultimately shape the coast. Current research projects focus specifically on field-scale sedimentation processes in coastal environments.

1. Pocket beach processes on a Caribbean island, Vieques, P.R. Understanding and quantifying both natural processes and anthropogenic effects on tropical island shorelines is increasingly important in light of projected increases in the rate of sea-level rise. This on-going project is currently characterizing the pocket beach systems of Vieques and their relationship with wave energy, sediment source, and long-shore transport of sediment. Grain size, mineralogy, beach profiles (steepness), and shoreline aspect are compared to assess the connectivity and stability of these beaches. Understanding the sediment transport processes of these beaches will ultimately help the Viequesians to better manage their most valuable resource: the beach. Students may currently work in the Coastal Lab analyzing sediment samples from key beaches around the island to begin to quantify sediment transport processes; future field work is planned including expanded sampling schemes and wave data collection and analysis.
2. Winter processes on New England salt marshes. New England marshes experience climatic conditions and have morphologies which differ from their southern counterparts, including: wind and waves, vegetation density, suspended sediment influx, deposition of inorganic and organic matter, compaction, and erosion. Winter processes play a significant role in the vertical accretion of northern high marshes through the process of ice-rafting of sediment, and are also impacted by ice loading and dehydration. Should northern marshes fail to keep up with rising sea level, their platform morphology will result in a different mode of inundation compared to southern back-barrier marshes. Students may engage in field and lab work to quantify sediment transport onto the marsh platform by tidal and ice vectors at several New England marshes.
3. Geomorphology of New England estuarine marsh systems: GIS analysis of feature distribution and large-scale process modeling. GIS is used on extremely high-resolution wet/dry aerial photo pairs and LIDAR elevation data to classify and quantify geomorphological features across the Great Marsh, Plum Island, MA. This estuary-wide database is being analyzed to determine controls on feature distribution, to use to develop a model of northern temperate coastal landscape formation and evolution with changing sea level. Students may engage in field work at the Plum Island LTER or GIS analysis in the Geoprocessing Lab at Mount Holyoake, as well as in the lab at Wellesley College.
4. Response of freshwater estuarine marshes to sea-level rise: changes in sedimentation. This project is in the planning stages, but will involve field work in major estuaries such as the Chesapeake Bay, followed by lab work at Wellesley College and Tulane University.

Opportunities for Students: Students interested in working in the GEOS Coastal Lab should contact me directly to talk about opportunities and projects that might be a good fit. Previous science classes, especially Geoscience, or prior experience working outdoors and along the coast are helpful, although not required. Summer research funding preference is to students with greater coursework exposure/interest.

Contact: Office SC260; phone: 781-283-3165; email: bargow@wellesley.edu

Chris Arumainayagam

Projects:

Students working in my laboratory will study the interactions of low-energy electrons with nanoscale thinfilms using post-irradiation temperature programmed desorption (TPD). We have previously demonstrated that the exposure of multilayers of an adsorbate to low-energy (≤ 55 eV) electrons under ultrahigh vacuum (UHV) conditions ($p \sim 1 \times 10^{-10}$ Torr) followed by temperature programmed desorption is an effective method to investigate the effects of high-energy radiation, including ion-molecule and radical-radical reactions. Students will have a choice of four projects:

1. We have recently completed the first direct investigation of the low-energy electron-induced production of molecular species from the chlorofluorocarbon CF_2Cl_2 , commonly known as CFC-12.¹ Our experiments were motivated by a newly proposed hypothesis which suggests that low-energy electrons, produced by cosmic rays and trapped in water ices in polar stratospheric clouds, in addition to UV-VIS photons from the sun, interact with chlorofluorocarbons to produce chlorine atoms that subsequently destroy ozone in the Antarctic. In contrast to previous studies of *photon*-induced dissociation, our studies of *electron*-induced dissociation demonstrate facile C–F bond cleavage in CF_2Cl_2 .^{2,3} Experiments involving the electron irradiation of CF_2Cl_2 adsorbed on ice are currently underway.
2. Understanding the decomposition of halocarbons by low-energy electrons could provide critical new concepts of importance to the emerging cold plasma technology aimed at on-site, cost-efficient destruction of hazardous halogenated organic compounds. Although relatively high-energy (100 - 300 keV) electrons are utilized to produce the cold plasma, it is the low-energy (≤ 15 eV) secondary electrons that are postulated to initiate the decomposition of the halocarbons. Among the objectives of the proposed research are: identifying all of the electron-induced reaction products of several halomethanes, investigating the dependence of the yield on electron fluence (electron flux multiplied by exposure time), and probing the dependence of the reaction cross section on initial electron energy.
3. The goal of third project is to determine the human source of the most potent greenhouse gas ever identified in the atmosphere: trifluoromethylsulfur pentafluoride (SF_5CF_3). SF_5CF_3 has been found to follow similar trends in concentration and stratospheric lifetime as SF_6 . Because both SF_6 and fluoropolymers are frequently used together in high-voltage environments, it has been postulated that SF_5CF_3 is a product of the reaction between SF_5 and CF_3 radicals. Results of recent experiments conducted in my laboratory have demonstrated the formation of CF_3 radicals during electron irradiation of CF_3I .⁴
4. It has been proposed that glycine, the simplest amino acid, may be formed in interstellar medium from reactions of acetic acid and ammonia induced by cosmic radiation. Because the interaction of cosmic radiation and matter produces large amounts of low-energy electrons, the low-energy electron-induced reactions of acetic acid and ammonia coadsorbed in nanoscale thin films will be investigated.

Opportunities for Students: Students should have completed one semester of chemistry and should have had prior exposure to physics.

Contact: Office SC 202 Phone: 781-283-3326, email carumain@wellesley.edu

¹ N. Nakayama,* S.C. Wilson,* L.E. Stadelmann,* H.D. Lee,* C.A. Cable,* and C.R. Arumainayagam; “Low Energy Electron-Induced Chemistry of CF_2Cl_2 : Implications for the Ozone Hole?” *J. Phys. Chem. B* **108** (2004) 7950–4.

² M. Rajappan, L. Zhu,* A.D. Bass, L. Sanche, C.R. Arumainayagam, “Chemical Synthesis Induced by Dissociative Electron Attachment,” *J. Phys. Chem.* **112** (2008) 17319–17323.

³ A. D. Bass, C.R. Arumainayagam, L. Sanche, “Revisiting the electron stimulated desorption of anions from thin films of CF_2Cl_2 .” *International Journal of Mass Spectrometry* **277** (2008) pp. 251–255.

⁴ N. Nakayama,* E.E. Ferrenz,*D.R. Ostling,* A. S. Nichols,* J. F. Faulk,* and C.R. Arumainayagam, “Surface Chemistry and Radiation Chemistry of Trifluoriodomethane (CF_3I) on Mo (110),” *J. Phys. Chem. B* **108** (2004) 4080–5.

Daniel Brabander
Environmental Geochemistry, Geosciences Department

Projects:

Current research focus is environmental geochemistry and the quantification of biogeochemical processes in watersheds, aquifers, and in the urban environment. Applications include bioremediation, environmental biomonitoring, fate and transport of contaminants (toxic metals) in watershed and aquifer systems, isotopic dating and mapping of contaminants within sediments and soils, and sustainable urban agriculture.

5. Sustainable urban agriculture. With funding from the EPA and a partnership with The Food Project we have been examining the issue of lead contamination in urban backyard gardens in Roxbury and Dorchester MA. After analyzing over 700 soil samples we have determined that the neighborhood average soil lead concentrations are over twice the EPA action level. Research is ongoing to isotopically fingerprint the sources of lead and to evaluate what fraction of the lead is bioavailable. In partnership with The Food Project we are also designing and implementing geochemical and culturally appropriate remediation schemes.

Clark H. F. *, Hausladen D. M. *, **Brabander D. J.** (2008) Urban gardens: Lead exposure, recontamination mechanisms, and implications for remediation design. *Environmental Research* 107: (3) 312-319. Clark H. *, **Brabander D.**, Erdil R. * (2006) Sources, sinks and exposure pathways of lead in urban garden soil. *Journal of Environmental Quality* 35: (6) 2075-2083.

6. Legacy pollutants in the Neponset River Watershed. With funding from our research partner, the Neponset River Watershed Association, we have been developing a watershed-wide GIS-based inventory of heavy metals in surface river and millpond sediments with the goal of identifying both ecological risk and mobility potentials. In addition we are linking historical land use patterns with geochemical records preserved in sediment cores. These research efforts on a watershed scale will inform both policy recommendations and shed light on fate and transport mechanisms of legacy pollutants in urban-suburban watersheds.

Estes E. R. *, Shafer T. D. *, **Brabander D. J.** (2008) Comparing spatial and temporal trace metal geochemical signatures in two branches of the Neponset River Watershed. *North Atlantic Chapter of the Society for Environmental Toxicology and Chemistry 14th Annual Meeting*, Bar Harbor, ME.
Brabander D. J., Pighetti E. H. * (2008) Spatial and temporal trace metal geochemical signatures in urban pond sediments: Records of past land use in the Neponset River Watershed. *North Atlantic Chapter of the Society for Environmental Toxicology and Chemistry 13th Annual Meeting*, Bristol, RI.

7. Historical metal pesticides. Using a combination of limonological techniques, dendrochemical records, and archival data on historical orchards, students in my lab and at Boston University have been evaluating the isotopic composition of lead associated with lead arsenate pesticide manufacturing and application. We are examining mobility of lead and arsenic in dendrochemical records and in soil matrices using in situ analytical methods and by sequential extraction techniques.

Burnet A. *, Kurtz A. C., **Brabander D. J.**, Shailer M. (2008) Dendrochemical record of historical lead contamination sources, Wells G&H Superfund site, Woburn, Massachusetts *Journal of Environmental Quality* 36:1488-1494.

Opportunities for Students:

For summer research in my lab, preference will be given to students who have completed two semesters of introductory chemistry (CHEM 205) and at least two semesters of geosciences course work typically including GEOS 201 (Environmental Science), 203 (Earth Materials), and GEOS 315 (Environmental Geochemistry).

Contact: Office SC390; phone: 781-283-3056; email: dbraband@wellesley.edu

Dora Carrico-Moniz

Projects:

My research projects involve the use of organic synthesis to prepare novel compounds of medicinal importance. Two current areas of research in my laboratory are: 1) Design and synthesis of naturally occurring organic molecules and analogues as anticancer agents; 2) Design of therapeutic agents against Hepatitis C Virus and efficient fluorescent probes for screening of antiviral agents. Students working in my laboratory will have the opportunity to learn about and apply techniques used in drug discovery, including organic synthesis, structure-activity relationship (SAR) studies, lead compound optimization, and assay development.

1) Design and Synthesis of the Natural Product Angelmarin and Structural Analogues as Anticancer Agents.

Pancreatic cancer has the highest mortality rate of any human cancer and current treatment options for patients are very limited. The discovery of novel molecules possessing antitumor activity provides an avenue towards the development of new therapeutics for pancreatic cancer. Natural products are privileged structures often possessing important biological activity. As such, they provide scientists with promising lead structures from which analogues with improved biological activities (e.g., potency, selectivity, pharmacokinetics) can be prepared.

Recently, a novel anticancer agent, angelmarin, was isolated from extracts of the medicinal plant *Angelica Pubescens* and found to exhibit toxicity specifically against the pancreatic cancer cell line PANC-1. Based on its promising biological activity, we have selected this natural product to serve as a scaffold to develop novel anticancer agents. Research in my laboratory is currently focused on two major goals: a) the asymmetric total synthesis of angelmarin, and b) lead compound optimization guided by structure-activity relationship (SAR) studies to develop a superior therapeutic agent.

2) Design of Hepatitis C Virus Therapeutic Agents and Efficient Fluorescent Probes to Evaluate their Efficacy.

Hepatitis C affects more than 170 million people worldwide and this chronic disease often leads to liver cirrhosis and hepatocellular carcinoma. Among several important drug targets, the NS3/4A protease of hepatitis C virus (HCV) has emerged as a critical target for HCV therapy. The NS3/4A serine protease of HCV is responsible for the cleavage of viral nonstructural polyprotein and its activity has been shown to be essential for the maturation of the viral proteins.

These research projects focus on two major goals: a) design and synthesis of two families of HCV NS3/4A protease inhibitors as antiviral agents, and b) development of efficient fluorescent protease probes to evaluate the antiviral efficacy of the HCV inhibitors designed in our laboratory.

Opportunities for Students: I will be accepting students into my research group for the Summer and Fall of 2009. For the summer, suitable preparation consists of at least one semester of Organic Chemistry.

Contact: Office: SC 266B; phone: (781) 283-2970; email: dcarrico@wellesley.edu

Web: <http://www.wellesley.edu/Chemistry/Dora/index.html>

Don Elmore

Projects:

Students in my research group use computational molecular modeling and biochemical assays to investigate two areas of biochemical interest: 1) antimicrobial peptides and 2) ion channels.

1) Antimicrobial peptides are produced by an incredibly vast array of organisms—including plants, insects, humans, and even bacteria themselves—and are a potentially valuable alternative to address the increasing problem of bacterial resistance to antibiotics. Some of these peptides act by entering cells and disrupting an essential intracellular process. Since these peptides effectively cross cell membranes, they could also be used for drug delivery or cellular transfection applications. Currently, research in my lab is focused on histone-derived antimicrobial peptides that readily cross membranes. For example, many of our initial studies have involved buforin, a peptide that enters bacteria and binds to DNA. These studies utilize a wide variety of in vitro and in vivo experiments to characterize peptides. As well, we use computer simulations to help us interpret our experiments in terms of intermolecular interactions, such as hydrogen bonding between peptides and the lipid membrane or DNA. Overall, these studies help us understand how histone-derived peptides function and aid in the design of novel antimicrobial peptides.

2) Ion channels are proteins present in the membranes of all cells. These proteins can be either open or closed, and when they are opened by some stimulus they allow ions to pass through the hydrophobic membrane. Channels that open when they bind a small molecule—called ligand-gated ion channels—are critical to a variety of physiological processes, particularly in the nervous system. Thus, many neurological diseases are related to mutations in these ion channels that cause them to function incorrectly. In order to understand these channel-related diseases, it is necessary to understand how channels function on the molecular-level. However, there is little experimental data on the molecular-level structure of ligand-gated ion channels. Research in my group uses a variety of computational methods to produce structural models of a newly discovered family of ligand-gated ion channels. We also use experimental biochemistry to probe the structure of the channels and verify our computational models. In addition to learning about the physiological role of ion channels, we are also interested in using our models of ligand-gated ion channels to design biosensors for small organic compounds, such as environmental pollutants and explosives. This project is an active collaboration with a research group at Washington University with expertise in electrophysiological measurements of ion channels and surface chemistry for sensor design.

Opportunities for students: I will be taking students in my lab for Summer and Fall 2009, and I strongly encourage any interested students to contact me to discuss potential projects. Based on their interests, students working on either antimicrobial peptides or ion channels can focus on a computational or experimental project or a project that combines both types of methods. (No previous programming or computer experience is necessary for computational projects.) Although many students in the lab have completed organic chemistry and a course in either biology or biochemistry, I will also consider students who have completed one year of chemistry.

Contact: Office SC E208; Lab SC E314; x3171; email: delmore@wellesley.edu

Nolan Flynn

Projects:

The group's research lies at the interface of biomaterials chemistry and nanoscience. Projects within the group focus on two main biomedical applications: (1) controlled drug delivery, and (2) improvement in biocompatibility/reduction of biofouling.

(1) Stimuli-Responsive Hydrogels Containing Metal Nanostructures

We have developed methods for creating metal nanostructures within polymer matrices. These polymers, which are called hydrogels, contain large amounts of water under some conditions. However, when an environmental factor such as temperature, pH, or ionic strength is altered, the hydrogels deswell, expelling their contents. Introduction of the nanostructures allows us to tune the conditions under which the hydrogel passes through this phase transition. We are currently investigating the synthesis, characterization and drug delivery potential of a number of different types of hydrogel matrices and metal nanostructure combinations. Factors such as the charge on the polymer backbone, the type of metal nanoparticle, and the size and charge of the drug molecule are important for potential applications.

(2) Surface Modification Using Polymers and Functionalized Gold Nanoparticles

The ability to resist the adhesion of biomolecules such as peptides, proteins, and, ultimately, cells, is vital to the function of many types of biomedical devices. This ability is particularly important for biomicroelectromechanical systems (bioMEMS), which often have features on the micrometer or nanometer length scale. We are working to develop simple methods for coating a variety of material types (gold, titanium, silicon, silicon oxide, silicon nitride, polymers) used in biomedical devices. We are currently investigating two avenues for improving biocompatibility and mitigating biofouling—namely, thin films of either polymers or functionalized gold nanoparticle. Synthesis, coating methods, and characterization are all vital to the advancement of this project.

Opportunities for Students:

For the summer, appropriate preparation involves the completion of at least one semester of organic chemistry or research experience involving synthesis. Preference is given to students who have completed one additional upper-level chemistry course (biochemistry, inorganic, analytical, or physical chemistry).

Contact: Office: SC 266C; phone: 781-283-3097, email: nflynn@wellesley.edu

David Hawkins Geosciences Department

Projects:

This summer, I will focus on two projects designed to provide temporal links between subvolcanic magmatic rocks and associated volcanic rocks. The overall goal is to constrain the time scale of magmatic processes that operate in the shallow crust at the intersection of plutonic and volcanic environments and to link evidence for eruptions in plutons to the volcanic products of those eruptions. The tools I employ include field studies, petrography (polarized light and electron microscopy), the elemental and isotopic geochemistry of rocks and minerals, and U-Pb zircon geochronology. The field areas are on the coast of Maine and lab work will be completed at both Wellesley and MIT. The two projects, listed below, will focus on rocks exposed on the coast of Maine and will provide research opportunities for several students.

1. Temporal Evolution of the Subvolcanic Vinalhaven Intrusion on the Coast of Maine. The Vinalhaven Intrusion was constructed over at least 700 thousand years 419 million years ago, but spatially and genetically related volcanic rocks are about 1 million years older than exposed levels of the intrusion. Zircon U-Pb geochronologic data suggest the lowermost, unexposed portions of the intrusion span the age gap between the pluton and the volcanic rocks. This project is designed to constrain the age of the earliest part of the intrusion by determining precise U-Pb ages on the zircon xenocrysts preserved in a mafic sill/lava flow in the volcanic section that we believe sampled the intrusion before silicic volcanism began. This project, which is funded by a grant from the National Science Foundation, will involve some field work, petrography and U-Pb zircon geochronology.
2. Temporal Evolution of the Cadillac Mountain Intrusive and Cranberry Island Series Volcanic System. The Cadillac Mountain Intrusion preserves geologic evidence for eruptions from a subvolcanic magma system and the products of those eruptions are believed to be the Cranberry Island Series volcanic rocks exposed nearby. This project is designed to link the intrusive history of the system to the volcanic history of the system via detailed field work, petrography and precise U-Pb zircon geochronology. I can accommodate several students on this project.

Opportunities for Students:

For summer research in my lab, preference will be given to students who have completed at least one semester of introductory chemistry and at least two semesters of geosciences course work, preferably GEOS 203 (Earth Materials) and GEOS 206 (Structural Geology). I will also offer students with less experience the opportunity to be field assistants on Mt Desert Island.

Contact: Office SC266D; phone: 781-283-3554; email: dhawkins@wellesley.edu

David Haines

Projects:

My research is synthetic organic chemistry based, but is focused on making molecules that we expect have biological activity. Through our collaborations at Tufts Medical Center and at Duke University, we have ready access to biological testing for the compounds that we design and synthesize.

We currently have two projects related to diabetes on-going in our laboratory:

1. Type II Diabetes results from the failure of the body to produce sufficient insulin to process blood glucose. This failure can arise from several sources, one of which is the process by which insulin production and release is induced by a small peptide (GLP-1) released by the small intestine upon consumption of food. We are studying the mechanism by which GLP-1 turns on the beta-cells of the pancreas, with the hope of being able to replicate this process using small molecule drugs. We are studying this mechanism by modifying some of the amino acids of GLP-1 which are essential to the initiation. Our collaborators then test these molecules in biological systems, allowing us to develop an understanding of the relationship between the structures of the amino acids and their biological activity. We have found some amino acid analogs that activate insulin production as effectively as the natural amino acids. We have several more analogs to synthesize and incorporate into peptides to complete the series.
2. One of the most difficult aspects of developing drugs is finding a molecule that will bind at the site of interest in the biological system. We have found a small molecule that binds selectively to the GLP-1 receptors in the pancreas. Our studies have shown that this molecule binds in a location that is very close to where GLP-1 binds, and, in fact, utilizes some of the same receptor amino acids in its binding as does the activating portion of GLP-1. We have developed an effective synthesis of this molecule, and are modifying this synthesis to make analogs of the molecule to let us further define its interactions with the receptor, and to possibly strengthen its binding. Currently the molecule is an inhibitor of insulin production, but by using the structure-activity relationships that we develop as described in #1 above, we hope to be able to convert it into an activator of insulin production.

During my sabbatical this year, I have begun working on developing an inhibitor of an enzyme found in Chlamydia. Inhibition of this enzyme could result in a long lasting treatment for infection. It is possible that I will be bringing portions of this work back to Wellesley.

Opportunities for students: I will be accepting multiple students into my lab for the summer of 2009 and beyond. A strong background in organic chemistry would be very useful but is not required. (Contact by email: dhaines@wellesley.edu)

Michael Hearn

Projects:

Research in our lab centers on the synthetic organic chemistry involved in the development of new drugs against tuberculosis. We use the traditional methods of experimental organic chemistry to prepare novel compounds and characterize them. Efforts in synthesis are guided by results from iterative biological assays done by our physician collaborators as we seek the compounds with best antimycobacterial activities. Students carry out reactions and use a variety of spectrometric techniques to affirm the structures of the products and correlate the structures with biological activities.

Opportunities for Students: It is likely that we will have space available for new research students in the summer of 2009. Chemistry through Organic II is preferred, through Organic I required.

Contact: Office SC E212, Telephone (781) 283-3127, E-Mail mhearn@wellesley.edu

Yue Hu

Projects:

My research interests fall into the general category of complex fluids. The systems that I have studied are colloids — mixtures of small, undissolved particles suspended in other surrounding substances. We have discovered that mixtures of silica particle in silicone oil, initially a viscous past, became a free-flowing liquid in about 2 weeks of time.^{5,6} Non-aqueous silica gels, similar to the ones we have studied, are used widely as "fillers" for optical-fiber cables. Silica is also the most widely used reinforcement agent for silicone rubbers. The interaction between silicone oil and silica, however, is not well understood on a molecular level. Our work therefore contributes to the understanding the properties of these systems from both a fundamental science and a practical application point of view. My recent research projects are related to the study of silica gels:

1. Quantitative characterization of the silica/silicone oil system. Namely, study how the viscosity of the silica/silicone mixture changes with time (the *aging process*).
2. Investigation of the effects of additives like surfactants. Our preliminary investigation shows that surfactants slow down the aging process. A gel is formed when particles suspended in a fluid form a network due to colloidal interactions, and adding surfactants will change the way particles interact with each other. We need to obtain quantitative information about this process in order to gain insight into the mechanism responsible for the silicone/silicone oil gel-fluid transition.
3. Electrical properties of silica suspensions. We want to measure how the dielectric properties of the mixture change with time. This involves measuring the *dielectric dispersion* (dielectric constant and conductivity as a function of frequency) of the suspensions, and monitoring the changes as the samples age.

Opportunities for Students: I will be taking students for the summer and Fall of 2009. Students who have finished two semesters of introductory physics will be able to join me in this research effort. The experimental work will be conducted at Professor David Weitz's lab at Harvard University.

Contact: Office SC 584 x3325, email: yhu@wellesley.edu

⁵ Seila Selimovic* and Yue Hu, "Aging Effects in Suspensions of Silica Particles", in *Dynamics in Small Confining Systems*, the Materials Research Society Symposium Proceedings Series, ed. by J.T. Fourkas, P. Levitz, M. Urbakh, and Kathryn Wahl, **790**, 233 (2004).

⁶ "Seila Selimovic,* Sarah M. Maynard,* and Yue Hu, "Aging Effects of Precipitated Silica in Poly(dimethylsiloxane)," *Journal of Rheology* (2008), to be published.

Nancy H. Kolodny

Projects:

My research involves the application of multinuclear Nuclear Magnetic Resonance (NMR) spectroscopy and imaging to problems in biology and medicine. The projects range from ^{31}P and ^{23}Na NMR spectroscopic studies of pH homeostasis in cyanobacteria (in collaboration with Professor Mary Allen of the Department of Biological Sciences), to the manganese-enhanced MRI study of neural development in crustaceans and MRI and in vivo MR spectroscopy studies of normal and Rett syndrome mice using our micro-MRI system (in collaboration with Barbara Beltz and Joanne Berger-Sweeney of the Department of Biological Sciences). Students work with living systems such as cyanobacteria, which they grow themselves under a variety of normal and stressful conditions, or mice or crayfish, which are maintained in the Animal Facility in the Science Center. All experiments are done using the Bruker Avance 400 MHz NMR spectrometer and micro-MRI system in the Science Center.

Opportunities for Students:

I will accept students to work with me this summer. **It is preferable that Wellesley students interested in working with me have already begun doing so.** Some study of biology, physics and/or physical chemistry is preferable.

Contact: Office SC 258 x3044, email nkolodny@wellesley.edu

Courtney Lannert

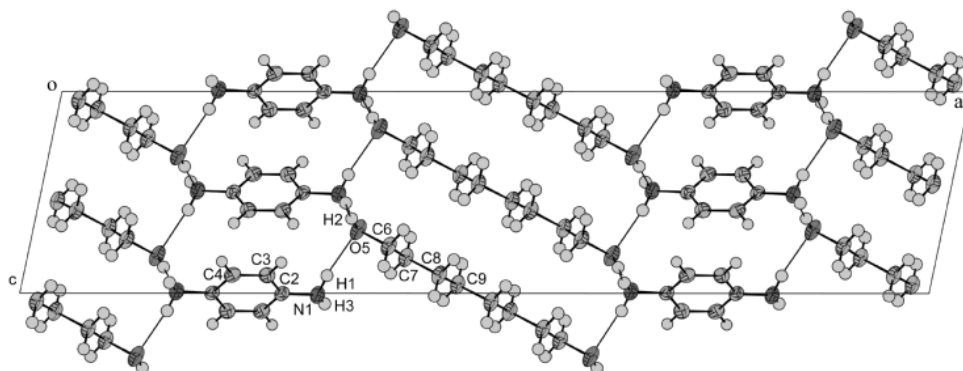
Projects:

My research focuses on collective and quantum properties of condensed matter systems. Recently, advances in dilute atomic systems have allowed researchers to study the nearly zero-temperature quantum properties of matter with newfound control and accuracy. In my research, I use simple simulations to theoretically predict the behavior of these fascinating new systems. The information gleaned leads to new understanding of the quantum world as well as possible applications to quantum computing.

I anticipate working with students who would like to gain experience with the numerical modeling of physical systems. I work mostly with simple code in Matlab that can numerically solve the time-dependent Schrödinger equation. This allows us to predict both the ground state of the system and its evolution in time under various real experimental conditions. Phenomena such as collective modes and quantum interference are two striking consequences of the quantum nature of the system that can be accessed through these methods.

Email: clannert@wellesley.edu

James Loehlin



Projects:

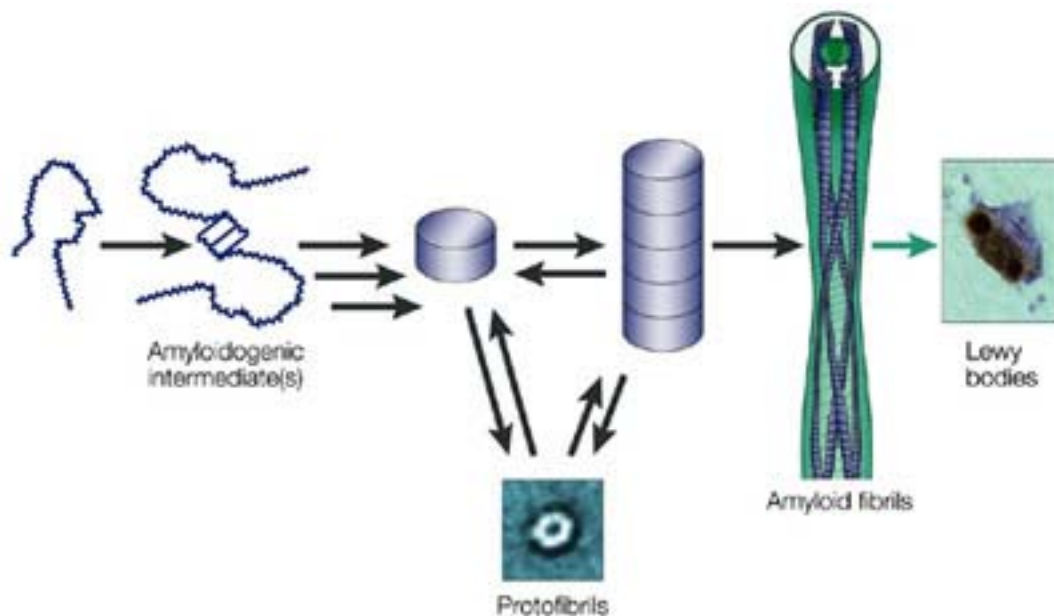
1. Crystal growth and structure determination of new materials with intermolecular hydrogen bonds. These projects involve determining suitable methods to obtain high quality crystals for structure determination, and then the determination of the structure.
2. Participation in the project attempting to grow crystals with programmed structures where diols and diamines are added in layers with changes in the diol and/or diamine from layer to layer. This is an attempt to produce a new category of matter, which does not grow naturally. If successful, the results may lead to a variety of uses in material science. A variety of techniques are involved in the growth experiment and the characterization of the resulting materials.

Opportunities for Students:

Projects 1 and 2 are suitable for 350, 360 projects for students with a couple years of chemistry. Since they involve physical chemistry, a strong background and aptitude in physical chemistry is a plus.

Contact: Office/lab SC 227, phone x-3043 or email: jloehlin@wellesley.edu

Julia Miwa



Projects: My research group is investigating the aggregation of the protein α -synuclein; aggregation of this protein is a key event in Parkinson's Disease. We use solid-phase peptide synthesis to prepare 20-residue fragments of α -synuclein. The fragments are purified by High Performance Liquid Chromatography (HPLC); their behavior is subsequently evaluated using fluorescence, infrared, and circular dichroism spectroscopy. We frequently adjust our strategies and tactics in light of new research that is published regarding α -synuclein. Current areas of interest include the preparation of α -synuclein fragments with covalently-linked fluorescent probes. All students in the laboratory learn solid-phase peptide synthesis and HPLC. There are opportunities for standard organic synthesis as well.

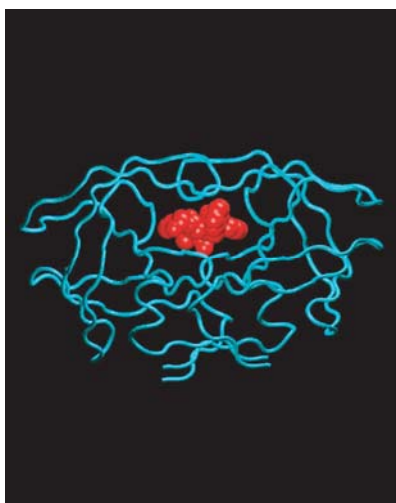
Opportunities for Students: Students should have completed Chem 211 or the equivalent. Preference is given to students who have completed a full year of organic chemistry.

Contact: Office SC 266A x3128, email jmiwa@wellesley.edu

Mala L. Radhakrishnan

Projects:

In my lab, we develop and apply computational techniques to analyze and design drugs and other biologically important molecules. Currently, we are focusing our efforts on two major HIV protein drug targets, HIV protease and HIV reverse transcriptase. Current projects include (1) developing and applying methods to design optimal drug cocktails that collectively bind to major mutant forms of HIV-1 protease, (2) analyzing clinical HIV mutation data to determine the major, “representative” mutant forms of HIV protease, (3) mapping out, through drug design and analysis, the structural and chemical determinants of binding promiscuity in HIV reverse transcriptase (i.e. what makes a drug promiscuous, such that it can still be a good drug even when the target rapidly mutates?), and (4) improving our physics-based modeling of these biological systems, through evaluating how well we model the electrostatic interactions between molecules.



**Crystal structure of the drug amprenavir bound to
HIV-1 protease
Kim *et al.*, *JACS*, 117:1181-1182, 1995**

Opportunities for Students:

Students should meet with me individually if they are interested in joining my group. An interested student should have a willingness to learn computer programming and other aspects of computational science. Coursework in any science – physics, chemistry, biochemistry, or biology, at any level – is definitely helpful, but a willingness to learn some aspects of all these scientific fields in an integrated fashion is most important.

Contact: SC 552, x2981, mradhakr@wellesley.edu

Didem Vardar Ulu

The unifying theme of the research in my laboratory is to combine structural and biochemical studies to investigate the macromolecular structure, function, and stability of proteins. Most of the proteins involved in important biological pathways are large multi-domain proteins, which makes it a challenge to study them at a molecular level. Therefore, in my laboratory we are using the protein dissection methodology, where such a multi-domain protein is studied as an assembly of structurally independent, minimal functional units that can be characterized in isolation.

Student joining my laboratory would have an opportunity to participate in different stages of projects that utilize a wide spectrum of techniques such as chromatography, various spectroscopic methods including Fluorescence Spectroscopy, Nuclear Magnetic Resonance (NMR) Spectroscopy, Circular Dichroism, and Isothermal Calorimetry (ITC) as well as molecular biology to design and clone DNA constructs suitable for bacterial expression systems.

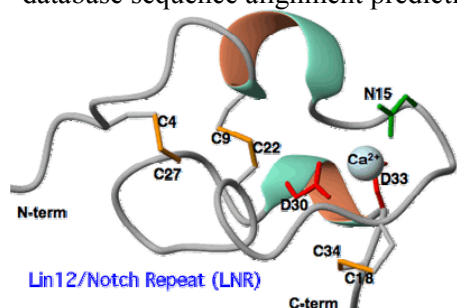
Current Projects:

Despite the significant amount of research conducted in the field, one of the profound mysteries of biochemistry is still how the linear amino acid sequence encodes a fully folded and functional protein. In order to understand this “second half of genetic code”, we need many more detailed studies directed to understanding the forces that stabilize a native protein. The focus of the current projects in my lab is to provide a very detailed study and characterization of a small and independently folded polypeptide motif, called the Lin12/Notch Repeat (LNR).

LNRs were first described as three unique tandem modules crucial for the regulation of ligand induced proteolytic cleavage of the Notch receptor. More recently, they were identified within functionally unrelated multi-domain proteins with different domain organizations, such as pregnancy associated proteins, and stealth proteins. LNRs belong to a subset of small disulphide-rich protein folds (SDFs), which are among the most frequently utilized structural units in all of biology. However, LNRs are functionally different from most other SDFs since they participate in intramolecular regulation rather than intermolecular recognition.

Based on the existing biochemical and structural information of a prototype LNR (Figure 1) and the protein database sequence alignment predictions, each LNR contains ~35-40 residues, has at least two disulphide bonds, and an absolute requirement for a Ca^{2+} ion to fold into its native structure with a very small amount of regular secondary structure.

Figure 1: NMR solution structure of LNRA from human Notch1
Vardar et al. *Biochemistry*, 2003, Vol. 42, 7061-7067



Currently in my lab we are carrying out extensive biochemical and biophysical characterization of the first two LNRs from human Notch1 protein. We routinely introduce the DNA for the various versions of these protein constructs into different bacterial expression systems, optimize growth and expression conditions, purify our proteins using many different chromatography methods including affinity, reverse phase HPLC, ion exchange, size exclusion and refold them into their native structures. Then we use high resolution HPLC, Mass Spectrometry and ITC to characterize them. Based on our findings and the new questions that come up during these initial studies we are also planning projects to extend these characterizations to other LNRs from both the remaining Notch proteins as well as from other proteins such as PAPP-A and Stealth Proteins. The two specific questions we are attempting to answer through this work are:

1. What is the inherent metal ion specificity and selectivity for the different LNRs?
Is it the same for the folding process and the post-folding binding process?
2. How does the number of predicted disulfides affect the folding and stability of the different the LNRs?

Finally we are also very interested in discovering more LNR or LNR-like motifs in other proteins through the use of bioinformatics and also designing mutations on the existing proteins to alter metal ion selectivity, binding affinity as well as the stability of these protein modules.

The overall goal for this research is to fill the existing gaps in our understanding of the sequence-structure-function relationship for these LNRs within the relevant specific biological background and also provide new insights into our global understanding of protein folding and stability.

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Wilton L. Virgo

Project: Catching Molecules in the Act of Fragmentation

Chemical reactions in the atmosphere are initiated and driven by photochemistry. For example, the photodissociation of NO₂ is the initial step in production of ozone (O₃) in the troposphere:



In order to understand how pollutants such as NO₂ and tropospheric O₃ are produced and removed from the global atmosphere, fundamental questions in chemistry must be addressed. How does a photon of light exchange energy with a molecule? How can a photon break a chemical bond? When resonance occurs, energy flow is rapid. Can we observe this energy flow in an experiment?



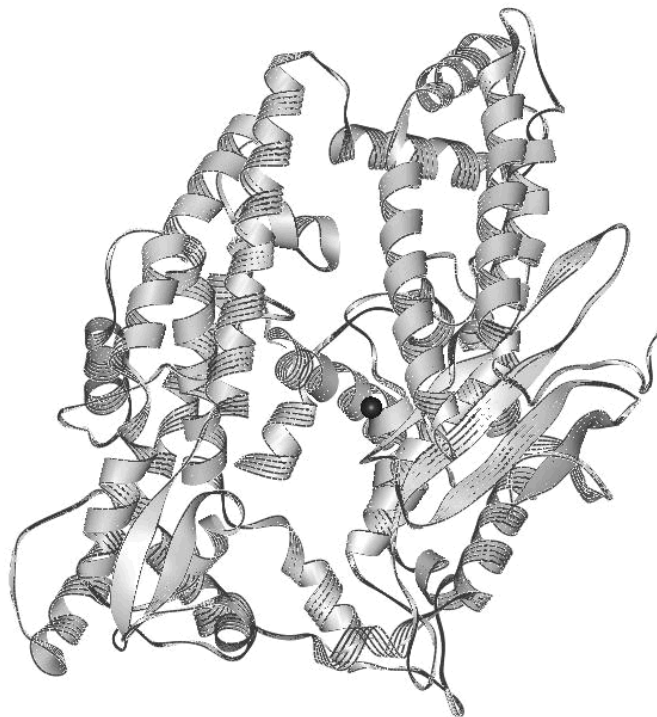
PCCP: 8(24) (2006)

Opportunities for Students:

In Chemistry 105, we learn about the periodic table, and the simple quantum ideas about atomic structure that provide the framework for understanding the diverse properties of matter. In the Virgo Research Group, students will extend these simple ideas and apply them to cutting-edge science using molecular theory, lasers, molecular beams, ion optics and sophisticated camera technology. Lasers can be used to transfer specific amounts of energy to molecules and cause fragmentation, just like the process described in (1). Quite surprisingly, the molecular fragments can be observed in the laboratory using a high-tech camera! Does this sound too good to be true? YOU can be a member of the team building this experimental apparatus.

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Adele Wolfson



The focus of research in my lab is enzyme mechanism and regulation. We study the enzyme thimet oligopeptidase (TOP), the structure of which appears above, as a model of a metalloenzyme with a wide range of distribution and function.

Projects:

1. Structure/function of thimet oligopeptidase (TOP): TOP hydrolyzes small bioactive peptides. It is involved in blood pressure and pain regulation, and is implicated in antigen presentation and neuroendocrine function. My lab is studying how the enzyme can accept such a wide range of substrates. Student projects involve kinetic and denaturation studies of wild type and engineering versions of the enzymes, using fluorimetry, purification involving column chromatography and electrophoresis, physical studies using microcalorimetry and mass spectrometry, and molecular modeling (in collaboration with Prof. Don Elmore's lab).
2. Regulation and localization of TOP: Because it breaks down the pituitary hormone GnRH, TOP is implicated in regulation of reproductive cycles and behavior. We study where TOP is found mouse brain, and how the levels and localization change in response to steroid hormones. These experiments involve fluorimetric enzyme assays, western blots, and immunohistochemistry. This work is done in collaboration with Prof. Marc Tetel of the Neuroscience program at Wellesley College.

Opportunities for Students:

I will accept students for Spring '09, Summer '09 and Fall '10. For Spring and Fall, students should have taken a biochemistry course. For summer, all students with one year of chemistry (preferably also with some biology background) will be considered.

Because of my responsibilities in the Dean's Office, students in my research group should be comfortable working rather independently

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