Sabbatical Report
Spring, 2018
Mark Perri, Chemistry

Introduction: I originally proposed to use the sabbatical time to work on two projects. First, I had been studying volatile organic compounds emissions emitted from grass when it's wounded (better known as mowed). Second, I wanted time to make improvements to a website that I have developed to teach computational chemistry to undergraduates. Sabbatical proposals are due quite a while before the actual work is to be performed and I ended up having the students who were working on the grass project transitioning out of my lab at this time and other students transition in who were more interested in analyzing hops instead of grass. So my work in Spring 2018 was focused on two projects: (1) Analysis of alpha acids and volatiles in hops and (2) Improvements to my computational chemistry teaching website.

Project 1: Analysis of Alpha Acids and Volatiles in Hops:

Hops are used in beer to provide bitterness, a unique taste, and antimicrobial / preservative properties. Sonoma County has several local breweries and Chemistry Students are often interested in the Chemistry of Beer, both out of curiosity and out of a desire for career training. I have had several students ask about studying beer. Based on previous studies of volatile compounds emitted from grass, I decided to take on this hops project where we could study the bitterness (produced by α-acids such as humulone; Fig. 1) and also the volatile components that produce the unique taste of hops.

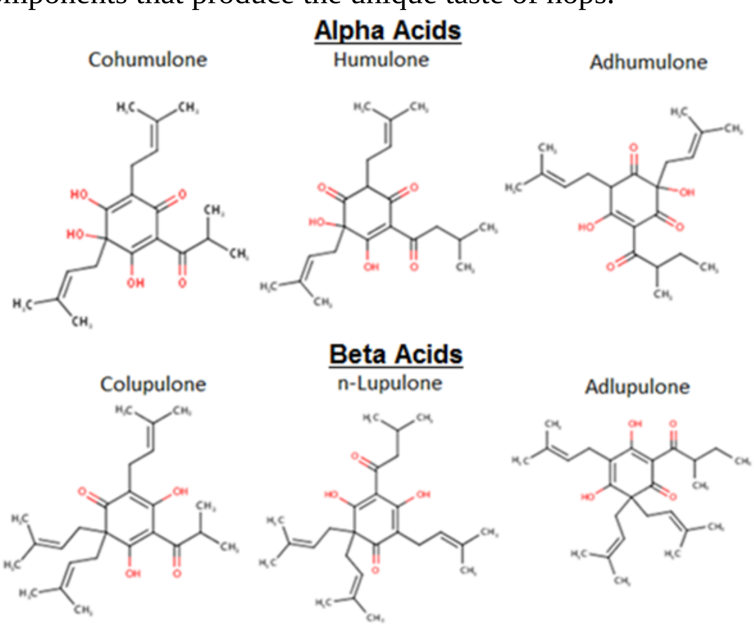

Figure 1: Typical acids found in hops. From: Schindler, R.; Sharrett, Z.; Perri, M. J.; Lares, M., Quantification of A-Acids in Fresh Hops by Reverse-Phase High-Performance Liquid Chromatography. ACS Omega 2019, 4 (2), 3565-3570.

During sabbatical our group was able to prepare a manuscript detailing the results of the first part of the project. In this manuscript we explain a method to separate and quantify α-acids (Cohumulone, Humulone & Adhumulone) and ß-acids (Colupulone, n-Lupulone & Adlupulone) in freshly harvested hops (Fig. 1). In this study we used reverse-phase high-performance liquid chromatography (Fig. 2). Our results showed that these acids could be quantified in fresh hops, giving our method an advantage over previously published methods. Because our method used fresh hops we could analyze hops as it is being grown, with a goal to be able to help farmers know when is the best time to harvest their hops. Currently farmers harvest based on the moisture content of the hop cone and based on its smell. We wanted to create a method that could be used to inform farmers of the quantity of acids (which determine bitterness) of a crop as it grows.

Samples of cascade hops were taken from hops farms around Sonoma County as a function of time. Instead of farmers relying on an approximate literature value of 5 – 7% w/w alpha acid content we were able to show a range of fresh hops alpha acid content from 1.8 – 9.0 % w/w (Table 1). We plan on continuing this project to also determine the volatile components of hops (students have been gathering preliminary data, but we are still working on perfecting a method for this). This work resulted in the following publication: Schindler, R.; Sharrett, Z.; Perri, M. J.; Lares, M., Quantification of A-Acids in Fresh Hops by Reverse-Phase High-Performance Liquid Chromatography. ACS Omega 2019, 4 (2), 3565-3570.

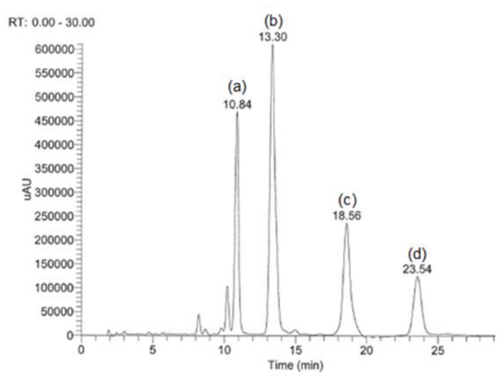

Figure 2: An example chromatogram of a typical 1.0 mg/mL standard injection. From: Schindler, R.; Sharrett, Z.; Perri, M. J.; Lares, M., Quantification of A-Acids in Fresh Hops by Reverse-Phase High-Performance Liquid Chromatography. ACS Omega 2019, 4 (2), 3565-3570.

Table 1: Summary results of Sonoma County Cascade Hop samples. From: Schindler, R.; Sharrett, Z.; Perri, M. J.; Lares, M., Quantification of A-Acids in Fresh Hops by Reverse-Phase High-Performance Liquid Chromatography. ACS Omega 2019, 4 (2), 3565-3570.

Sonoma Country Cascape Hop Samples:						Literature:
Location	Farm	Year	Harvest Date	Moisture Content %	Alpha Acid % w/w @ 10% Moisture	Alpha Acid % w/w @ 10% Moisture
Sonoma	BiRite	2015	8/11/2017	66.08	5.98	5.0 - 7.0
			8/18/2017	60.32	5.87	
			8/25/2017	68.13	7.19	
		2016	8/11/2017	66.97	6.79	
			8/18/2017	62.65	6.09	
			8/25/2017	67.12	7.03	
Sebastapol	Warm Springs	2016	8/11/2017	63.54	7.55	
			8/18/2017	64.16	6.78	
			8/25/2017	70.35	8.97	
	Scott	2016	8/11/2017	41.52	3.49	
			8/18/2017	58.34	5.43	
			8/25/2017	65.01	5.39	
Cloverdale	Eric	2016	8/18/2017	69.84	5.38	
Santa Rosa	Cassius	2017	8/11/2017	64.58	1.76	
	Fogbelt Brewing Co.	2016	8/11/2017	73.81	5.36	
			8/18/2017	61.35	6.22	
			8/18/2017	71.08	6.89	Wild Hop

Project 2: Improvements to the Chem Compute Website

I have developed a website called Chem Compute (chemcompute.org), which provides free access for undergraduate chemistry students to perform computational chemistry exercises. Typically software for this costs thousands of dollars. Many departments (including SSU) cannot afford this software, creating an access gap. Computational chemistry is an important career option for Chemists and using computers in science is a very important skill in general for STEM majors. I also feel that using computational chemistry helps students to learn chemistry because in essence, computational chemistry deals with chemical bonds. This is a fundamental concept for Chemistry majors.

During my sabbatical time I made several improvements and additions to the website. Most improvements are not visible on the website. These improvements are on the back end. The website allows students to submit computational chemistry jobs to super computers around the country. There is a great deal of infrastructure (databases, message passing systems, file transfer, and communications) that goes into making it possible for a student in Idaho to click a button on a website and for a supercomputer in San Diego to perform a calculation and then return the results to the student. In previous years the website has had problems when large Universities have used it. For example, Wake Forest University uses the website for their General Chemistry class with enrollment of 500 students. In order to serve this many students in a week I had to make several optimizations to the back end and enable the use of load balancing and elastic nodes (the ability to bring multiple web and computation servers online based on demand). This programming was tedious and took quite a while, but the servers can now handle the load of large Universities. Wake Forest used the site just recently and had no problems.

Sabbatical also gave me time to present my results. I spoke at the American Chemical Society National Meeting in New Orleans about the infrastructure improvements in the website (Perri, M.J. Chem Compute Educational Gateway. American Chemical Society Workshop on Science Gateways. American Chemical Society National Meeting, New Orleans, LA. March, 2018)

Additions were made to the website as well. I was able to add an experiment for non-Chemistry majors. Usually these computational experiments are used only by upper division Chemistry majors. I thought that the website could help non-majors as well, and so I wanted to use it in Chemistry 102 (Chemistry in Society, a GE non-majors class). I spent time during sabbatical developing and refining a lab for use in Chemistry 102. The lab was written to help students understand concepts that are important, but difficult. For example, naming chemical compounds is extremely important because chemists need a common vocabulary. Recognizing the name of a compound can help students to understand if something is toxic or not. There is a common misconception that you shouldn't eat anything that you can't pronounce. That is not good advice, and by learning chemical nomenclature I hope to teach the students that there are qualities of compounds that are actually important to their toxicity. In Chemistry 102 we discuss global warming and the greenhouse effect. It is important for students to understand the physical basis of the greenhouse effect and one of the sections in the lab helps students to discover that based on the infrared spectrum of molecules. This lab was trialed in Chemistry 102 in the semester after my sabbatical and I learned a great deal from that experience. I plan on making improvements soon. My student, Mary Akinmurele is working with me on this project and she was able to help out in the implementation of the lab and gained valuable experience. She presented with me about our website just recently at the American Chemical Society National Meeting (Perri, M. J.; Akinmurele, M.; Whitnell, R.; Reeves, M. In Chem Compute Science Gateway for Undergraduates, American Chemical Society National Meeting, Orlando, FL, Orlando, FL, 2019)

During this sabbatical time I was able to do some data processing in preparation for a manuscript that I prepared the summer after sabbatical. I was able to show an increase in student evaluation (SETE) responses after I started incorporating the website in classes (table 2). Survey data also showed an increase in confidence in using computers, and that in general, students agreed that the computer assignments provided deeper insight into class material. This was recently accepted for publication (Perri, M. J.; Akinmurele, M.; Haynie, M., Chem Compute Science Gateway: An Online Computational Chemistry Tool. In Using Computational Methods to Teach Chemical Principles, Grushow, A.; Reeves, M., Eds. ACS Press: 2019 (In Press).)

Table 2: Increase in student evaluation responses after using Chem Compute in class. Maximum score is 5.0

Evaluation Question	*Before Chem Compute*		*After Chem Compute*	
In this course, my instructor enables me to participate actively in learning	4.6	4.6	5.0	5.0
My instructor stimulates interest in the course	4.2	4.4	4.9	4.9

Classes (left to right): 2012 Spring P-Chem (N=20), 2013 Spring P-Chem (N=29), 2015 Spring P-Chem (N=14), 2017 Summer Gen-Chem (N=7)

Table 3: Preliminary Survey Results

1 Strongly Disagree … 4 Neither Agree nor Disagree … 7 Strongly Agree

	PRE (N=117)	***POST (N=27)***
I feel confident using computers to solve chemical problems.	4.75	5.41
I am interested in using computers to solve chemical problems.	5.21	5.52
I feel that the computer assignments provided deeper insight into the class material.		5.50

Community Service

My sabbatical gave me an increased ability to volunteer. I volunteered at two local schools in Novato (San Jose Middle School and Novato High School). Normally my work schedule doesn't allow me to volunteer at these schools because of their hours, so it was nice to get a chance to do this if only for a semester. At San Jose Middle School I volunteered with their AVID program and helped students with their schoolwork in small groups. At Novato High School I started out helping students with their Chemistry homework, but quickly I was helping with math and environmental sciences as well.

I also spent some time learning to bake so that I could volunteer for Cake4Kids, which provides birthday cakes to children who wouldn't otherwise get one. As a parent of two small children I feel that this is an important charity and I continue to bake cakes and cupcakes for them when my schedule permits.

Publications Resulting From Work Done During Sabbatical:

1. Perri, M.J., Akinmurele, M., Haynie, M. Chem Compute Science Gateway: An Online Computational Chemistry Tool, in Using Computational Methods to Teach Chemical Principles. ed. Grushow and Reeves. Accepted / In Press

2. Reeves, M., Berghout, H., Perri, M.J., Singleton, S., Whitnell, R. How can you measure a reaction enthalpy without going into the lab? Using computational chemistry data to draw a conclusion, in Using Computational Methods to Teach Chemical Principles. ed. Grushow and Reeves. Accepted / In Press

3. Schindler, R.; Sharrett, Z.; Perri, M. J.; Lares, M., Quantification of A-Acids in Fresh Hops by Reverse-Phase High-Performance Liquid Chromatography. ACS Omega 2019, 4 (2), 3565-3570.

4. Perri, M.J. Chem Compute Educational Gateway. American Chemical Society Workshop on Science Gateways. American Chemical Society National Meeting, New Orleans, LA. March, 2018

5. Perri, M. J.; Akinmurele, M.; Whitnell, R.; Reeves, M. In Chem Compute Science Gateway for Undergraduates, American Chemical Society National Meeting, Orlando, FL, Orlando, FL, 2019.