CHEM MAJOR NEWS

In Conjunction with the American Chemical Society
Student Affiliates at the University of Pittsburgh

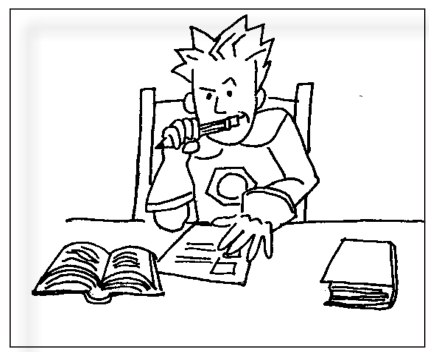
Volume 25, Issue 3 November 6, 2015

Some Incredibly Important Dates to Know...

November 06: Deadline for undergraduates to apply for April 2016 graduation in 140 Thackeray Hall

November 25- November 29: Thanksgiving Recess-No Classes! Have a great Holiday!

Congratulations to our ACS-SA!



Our ACS-SA has been named an Oustanding Chapter for the 2014-2015 academic year. This recognition was given to only 55 Chapters out of the almost 900 Chapters nationwide. This is the 27th year in a row that we have received national ranking and it is only possible because of all the hard work and efforts of our members. We will celebrate this recognition on Friday, November 20, 2015 at 12:00 Noon in 150 Chevron Science Center. All are welcome to join in the festivities.

2015-2016 ACS-SA Officers and Staff

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Stephanie McPhillips-*Senior Affairs Committee*

Visit us at http://www.chem.pitt.edu/acs-sa/

Our November Schedule

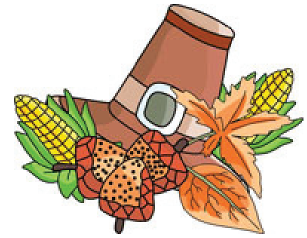
November

06 Preparing for Saturday Science *with Pat and Zach*

13 Green Polymers

20 Celebration of our National Ranking with the ACS!

27 Thanksgiving Break--Enjoy!



Everyone is welcome to attend our weekly ACS-SA meetings. Every Friday at noon we get together in 150 Chevron Science Center to hear interesting talks, learn more about science and enjoy each other's company. Come join us for all of the above mentioned meetings.

Saturday Science Academy

Looking for something fun to do on November 14, 2015? Try Saturday Science! It is an opportunity to help ambitious area high school students learn both general and organic chemistry in the lab. With your help, the students get to make crystal gardens, do a simple thin layer chromatography experiment, witness an acid base reaction with dry ice, measure the pH of some favorite soft drinks, and synthesize slime. Volunteers will play the role of a teacher: demonstrating the experiments, helping the students perform them, and finally, answering their questions. Saturday Science is a fun and rewarding volunteer experience in chemistry. So, are you still looking for something fun to this year? Join us for the ACS-SA meeting on Friday, November 6, 2015 at NOON in 150 CHVRN to plan for this great day. If you cannot be there on Friday, e-mail Zach (zae6@pitt.edu) or Pat (paa29@pitt.edu), our Outreach Coordinators and let them know you're interested in helping out and then join us on Saturday, November 14, 2015 at 9:00 a.m. in the Chevron Lobby.

HAPPY THANKSGIVING

Green Chemistry

by: Viktor Polites

Redesigning the Reaction Vessel: Flow Chemistry

Over the past century, organic chemists have remarkably advanced the scope and selectivity of reactions available for small molecule synthesis. However, while the chemistry in the flask has advanced, the flask has remained largely unchanged.[2] Flow chemistry has become routine in the petrochemical and commodity chemicals industries, but the pharmaceutical industry and academic labs have been slow to follow suit, adhering to traditional batch reactions.[3]

There are several reasons why it is attractive to do certain reactions under flow conditions. Flow conditions allow for highly efficient and even heat transfer. Reactions can be accelerated by rapid heating, and exothermic reactions can be sufficiently chilled to stay isothermal and prevent thermal runaways.[2-3]

In addition, flow reactors are ideal conditions for reactions requiring a gaseous reagent. The gas can be injected directly into the flow-stream, creating a segmented flow in which the gaseous reagent saturates the reaction solution. Ye[3b] and coworkers used a flow reactor to achieve multi-gram scale Pd(II)-catalyzed aerobic alcohol oxidations using dilute oxygen gas (8% O_2 in N_2). Since the flow conditions ensured oxygen saturated the solution, it suppressed the pathway which destroys the catalyst, aggregation of Pd(0) metal. This problem did not manifest in small batch reactions but hindered the scale up of batch reactions. That 8% O_2 in N_2 was a sufficient oxygen supply was important as it was below the explosive threshold.

Furthermore, flow reactors offer a suitable platform for conducting multistep reactions quickly and without purifying intermediates. For instance, McQuade[1] and co-workers reported a rapid 3-step single reactor synthesis of ibuprofen from commercially available starting materials (Fig. 1). The reactor is relatively small and simple (500 cm of tubing and 5 syringe pumps) and was capable of synthesizing 9 mg/min of ibuprofen.

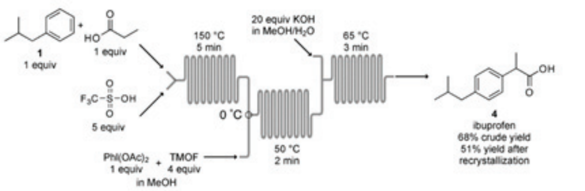


Figure 1. Schematic of McQuade's continuous flow synthesis of ibuprofen. The reactions are a Friedel-Crafts acylation, followed by 1,2-migration, and finally saponification.1

Lastly, photochemical reactions are naturally optimized under flow conditions by providing a far greater photon flux than can possibly be achieved in batch reactions. A notable example was reported by Kopetzki[4] and co-workers. Through singlet oxygen generation with a photosensitizer and visible irradiation, they achieved an efficient semi-synthesis of the anti-malarial drug artemisinin from a related but cheaper natural product, dihydroartemisinic acid.

In spite of these advantages to flow chemistry, academic labs and pharmaceutical manufacturer still largely conduct reactions in batch. Flow reactions may require reaction-specific equipment for proper introduction of reagents. Residence time must be optimized by varying flow rate and/or reactor length. Given the diversity of reactions performed in academic labs and at pharmaceutical plants, it is more convenient to perform reactions in batch. Moreover, particularly sluggish reactions or reaction of slurries can only be conducted in batch.[3a] All factors should be considered when deciding whether to use a flow or batch process.

References:

1. Bogdan, A. R.; Poe, S. L.; Kubis, D. C.; Broadwater, S. J.; McQuade, D. T., Angew. Chem. Int. Ed. 2009, 48, 8547-8550.
2. Wegner, J.; Ceylan, S.; Kirschning, A., Chem. Comm. 2011, 47, 4583-4592.
3. (a) Hartman, R. L.; McMullen, J. P.; Jensen, K. F., Angew. Chem. Int. Ed. 2011, 50, 7502-7519; (b) Ye, X.; Johnson, M. D.; Diao, T.; Yates, M. H.; Stahl, S. S., Green Chem. 2010, 12, 1180-1186.
4. Kopetzki, D.; Levesque, F.; Seeberger, P. H., Chem. Eur. J. 2013, 19, 5450-5456.

The Chemistry Behind that Agave Liquor

by: Nuria Marquez

According to Aztec mythology, Mayahuel, the goddess of fertility with 400 breasts, lived with her evil grandmother, Tzintzimitl in the dark corners of the sky. When Mayahuel and Quetzalcoatl (big-time, head Aztec god) met, they fell in love and started planning Mayahuel's escape. As soon as her grandmother found out, she killed Mayahuel. Quetzalcoatl buried her body in the middle of the desert, mourning her immensely.

His god friends saw how much he was suffering so they made a beautiful plant with 400 leaves sprout from the place where she was buried. This did not help Quetzalcoatl. He visited the plant every day and cried for Mayahuel. In a second attempt at helping their friend, the Aztec gods made the plant produce a powerful elixir to help Quetzalcoatl forget his problems. That plant was an agave plant and that powerful elixir was tequila.

Tequila is thought to have been around since 300 BC, when it was simply a fermented drink from the blue agave plant, originally called Mezcal. Once the Spaniards invaded Mexico, they brought with them distilling technology responsible for what we now know as tequila.

The production of tequila is a process protected and regulated by the Mexican government in the region for the appellation of origin Tequila, Jalisco in central Mexico. There are eight stages of production: jima, hydrolysis, extraction, formulation, fermentation, distillation, aging and bottling.

It all starts with the blue agave plant. The 'jimador' harvests the plant and cuts the agave leaves until the heart or 'piña' is left clean. This core is then cooked in a brick oven or an autoclave to break down the inulin polymers and obtain the glucose and fructose that make this sugary alcohol. About 15 pounds of agave cores are needed to produce one liter of tequila.

At this point, the piña is a fibrous material filled with juice. The cooked piñas are crushed with a 'tahona,' which is basically a giant wheel that moves in circles around a stone basin. The crushed fibers are then washed with water and strained to remove the juices. At this point, the manufacturers have to classify the tequila in one of two categories: Tequila or 100% Agave Tequila.

If it is not 100% Agave Tequila, then the agave musts can be enriched with other sugars accounting for up to 49% of the sugars used. This means that 51% of the drink comes from the fermented blue agave sugars and you will have a horrible hangover the next day. Tequila that is 100% agave will not have the same effect.

After formulation, the juice is fermented for up to 12 days and then distilled. This distillation is done in two phases, the first is destroying or smashing, liquor is obtained with an alcohol level of about 20% per volume. The second is rectification. This phase consists of a pot filled with the liquid and heated. The vapor from the liquid flows upwards and condenses at the top of a column. It condenses in three ways: the heads are usually volatile compounds (aldehydes and other superior alcohols), the body is the desired tequila product and the tails are the less volatile compounds that are recycled, namely methanol.

The tequila is then placed in a barrel, usually oak that previously held bourbon or whiskey, and aged. The type of tequila depends on the length of aging; a silver tequila is not aged at all, a 'reposado' is at least two months old, an 'añejo' is at least one year, an 'extra añejo' is at least 3 years old.

It's then bottled and shipped and mixed by the lovely servers of Mad Mex for us to enjoy. So even though you may not be mourning the death of your many-breasted lover, you can enjoy tequila knowing the chemistry behind this sugary elixir.

Sources:

http://www.tequila.net/tequila-production-and-export-statistics.html
http://izkalitequila.com/blog/the-7-steps-of-tequila-making/

Studying Abroad as a Chemistry Major

by: Gabbi Hill

I am a chemist. I like my chemistry classes. I like working in the lab. I even have a favorite pipette (P200). But, two months ago, I had the incredible opportunity to study abroad in Edinburgh, Scotland to study creative writing, as well as research the September 2014 Referendum. Since then, I have learned that I'm more than what I thought I could be. I am a tea-loving, creative writing, haggis-trying, extroverted-if-necessary, occasionally stubborn, somewhat artistic chemist. I learned more about myself in the span of a five weeks than I had in almost two years since being in college.

When I first began my search for a study abroad program, I had toyed with the idea of going somewhere in South America. I was concurrently studying Spanish at the time, and had taken up to Spanish Conversation through Pitt. When my pre-requisites for both writing and literature were fulfilled by the middle of my sophomore year, however, I realized I couldn't imagine not taking a writing class. Afterward, my decision to study abroad in Edinburgh became slightly more apparent after deciding to cease my minor in Spanish and, alternatively, minor in creative writing.

At the time of my search for a program, I felt inclined to explore health related programs (of which they were far and few), as I had been considering applying to physician assistant school post-graduation. The Pitt in Edinburgh Program, however, was too enthralling to resist.

I studied abroad for a total of five weeks; I took classes for four weeks and then traveled alone for my final week in Scotland. The two classes were Scottish Literature taught by Mark Kemp and Traveler's Journal taught by Jeff Oaks. The Scottish Literature course offered a very bare-bone exemplification of which novels depict Scottish culture, historically and presently. The Traveler's Journal consisted of weekly blog posts (https://pittinedinburgh.wordpress.com/), as well as daily detailed logs in our journals, provided for us at the beginning of the course. The program was small; only a total of ten people were on the trip. We took afternoon trips to castles and museums. Weekends were spent traveling to areas out of Edinburgh, such as the Isle of Skye and Melrose Abbey.

When people talk about their study abroad trip, the most common statement people make (including myself) is, "It was a great experience." But, what we, post-study abroad travelers, can never put into words is that these trips alter the way the brain functions. I do not, of course, have any empirical data, other than my traveler's journal and my memories. The world is not two-dimensional but multi-dimensional.

I am a chemist. I like facts and linear layouts and well-written protocols and duplicate sample sizes and anything pertaining to organized lab notebooks. But I am also a writer. I like sketching and scatterbrained-thinking and jotting down notes on napkins. I like trying to find meaning in a rock splitting the distance between my two feet in large boots and a large loch because I've been traveling alone for a week and the most communication I've had today was a slight smile towards a stranger and her dog.

I am a lot of things (as most of us are). Exploiting the study abroad option as a Pitt student studying a science was one of the best decisions I have ever made because I had the opportunity to figure those things out. And, I hope you do too.

DEPARTMENT OF CHEMISTRY

Undergraduate 2016 Summer Research Fellowships in Organic & Biological Chemistry

- We are pleased to offer Undergraduate Summer Research Fellowships for Pitt students sponsored by *the UPitt Organic and Biological Chemistry Divisions*.
- These Fellowships are intended to support a full-time organic or biological chemistry research project, including stipend & supplies, in the summer of 2016 at the Department of Chemistry in Pittsburgh.

Please submit applications consisting of a current resume, course records, and a letter of recommendation by a suitable Faculty Sponsor with details of the planned research project (not exceeding 1 page) by

FEBRUARY 20, 2016 to Prof. **PETER WIPF,** CHVRN 757.

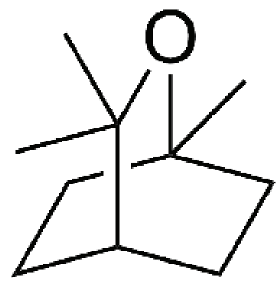
- The Award will be presented at the Undergraduate Award Ceremony in April 2015.
- The Awardee and Faculty Sponsor(s) are strongly encouraged to present a poster on their research at Science 2016 in Pittsburgh in the fall of 2016, and/or actively participate in an equivalent departmental, regional or national scientific conference.

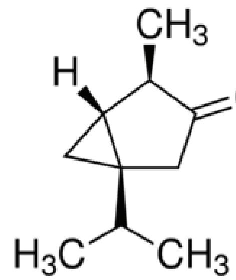
Sage Words About Sage

by: Dan Willis, Co-Editor

Sage is an underrated herb. Even in the places where it is a dominant flavor—breakfast sausage, certain popular perfumes—it rarely goes recognized. That's why we have Thanksgiving. One day out of the whole year, the leaves of this woody shrub are responsible for flavoring the turkey and stuffing which form the centerpiece of the classic American Thanksgiving feast. Its soft, savory aroma is the very scent of the holiday; cracking open a bottle of rubbed sage is just about the closest you can get to a late-Autumn day in your childhood home without hopping on a Greyhound.

Common sage, salvia officinalis, has been around for a very long time. It's been used for medicinal and spiritual purposes by Europeans since the 3rd century BC. Since then, Greek scholars, monastic poets and Charlemagne himself have all praised its unique flavor and supposed healing properties. But once post-Civil War America settled into the Thanksgiving traditions we now take for granted, sage really took off. But what is it about the chemistry of sage that makes it so appealing?





The answer might be terpenes. Terpenes are organic compounds which contain contiguous isoprene (C_5H_8) units. They are found in the highest concentrations in the resins of coniferous trees. Many of the smells we would describe as 'piney', as well as 'woody' or 'minty' are the result of terpenes. And it's a particularly savory blend of terpenes that gives sage it robust and homey sent.

Now, 5:8 is a very high C:H ratio, but surprisingly few terpenes are aromatic. Most actually achieve this either through intense conjugation, or the formation, fusion, and bridging of rings. This can result in some bonkers geometry. The three most important terpenes, if not the three most important chemicals for sage's flavor are borneol and eucalyptol (each of which contains a bridged six-carbon ring) and thujone (which contains a three-carbon ring bridged to a five-carbon ring). It's these bizarre-looking molecules that give everything from eucalyptus to rosemary to wormwood their powerful, herbaceous scents.

But despite these aromatic power-players, sage has a very mellow flavor, thanks to its finely tuned chemical composition. It's strong enough to stand up to big flavors like onion and poultry, but unlike some similarly terpenated plants, it won't make your turkey taste like a Christmas tree trimmed with toothpaste. It's a crucial part of classic American Fall favorites like pumpkin soup, creamed onions, and of course turkey & stuffing. It's an underrated herb, but at least we give it one day out of the whole year. Happy sage appreciation day.

References:

http://chemwiki.ucdavis.edu/Organic_Chemistry/Lipids/Properties_and_Classification_of_Lipids/Terpenes

http://www.herbwisdom.com/herb-sage.html