A Time for Reflection & Looking Ahead

This will be the last issue of the DelChem Bulletin published before we go on break for the summer. As we begin to wind down, I would like to take a look back at the events from this past spring and a look forward to some of the exciting events coming up in the fall.

In January, Dr. Sarah Jane Ward from the Lewis Katz School of Medicine at Temple University came and gave a talk to us about the uses of Cannabis as medicine. We held this event at the DuPont Country Club in Wilmington. The meeting was a great success, and we had over 30 members and non-members in attendance.

February brought us to Newark, to the campus of University of Delaware. There, the Delaware ACS and the UD Women in Chemistry group co-hosted Christie McInnis from Dow Microbial Control, who spoke to us about new product development in industry. We saw many new, young faces at this meeting, and it generated a good amount of conversation.

Continuing southward, we held our March meeting in Dover, where we hosted Ian Farrell, an analytical chemist at Dogfish Head Brewing. Ian spoke to us about quality control at Dogfish Head, and he gave a very interesting talk about different aspects of quality control when it comes to beer. Everyone in attendance had a good time, despite the fact it was St. Patrick’s Day weekend, and we had to compete with the noise from a parade.

Spring is awards season for us, with the Carothers Award Banquet in April and the Section Award in May. The Wallace H. Carothers Award is an international award given to a chemist who has made significant contributions to chemistry in industry, and our 2019 recipient is Robert (Bob) Gore. As I write this, we have not yet held our April meeting, but it looks as though we will have over 100 people in attendance! Our section award winner this year is Dr. Mary Watson from University of Delaware, and she will be giving a presentation titled “Re-Imagining the Role of Amines in Organic Synthesis” on Saturday, May 18 at the DuPont Country Club in Wilmington. We will also be honoring our 50-, 60-, and 70-year members at this event.

Our section also continues to be engaged in community outreach. Several of our members will be representing our section at the City of Wilmington’s annual Earth Day event this year and running an interactive activity with groups of children. We also recently sent members to judge the annual Delaware Valley Science Fair and to present some special awards on behalf of the section.

This year we will once again be having an end-of-the-semester happy hour and networking event with the UD Women in Chemistry. This will be on Thursday, May 2 from 5:30-7:30 at Iron Hill Brewery in Newark. This event was a huge success last year, and several of the attendees were invited to give summer talks at UD by the Women in Chemistry group. Members in industry are particularly encouraged to attend.

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Polymers are fundamental to every part of our society, and they have all kinds of amazing properties. This cartoon depicts a merger of chemicals being discussed by two businessmen (at least they look like businessmen since there are vests and ties; no lab coats) to create a polymer. The timing for this cartoon couldn’t be more appropriate given the recent merger of Dow and DuPont, two of the oldest and largest polymer companies in the world. Polymers are a great example of this — given all they have done for the world. But then again, Dow DuPont merged with the intention to separate into three new entities. Just like chemistry, we may ask, “What will the (perhaps unstable) equilibrium look like?

Robert Langer
Massachusetts Institute of Technology
Spring Wrap Up

As I write this in early April, warmer weather is causing thoughts of lawn care, the grill, beach trips and the tearing up of Main Street in Newark. I predict a crazy summer!

Al Denio
Delaware ACS Bulletin Contributor

Medical Marijuana

Newark now has its very own supply at the Compassionate Care Research Institute, located just a mile from the UD campus. This location makes sense when you consider the number of students suffering pain and anxiety in their organic and physical chemistry courses. Add in those students trying to cope with math and physics courses and you can understand why Newark is such an attractive location.

The new facility, called “Fresh Cannabis,” is located at 800 Ogletown Road. They now offer 10 strains of cannabis at present but will soon offer 30 strains of the plant. A licensed pharmacist is on the staff to help with dispensing. Several of the staff members hold degrees in horticulture, plant sciences and agriculture. Zach Lee left his job at DuPont to work here. He is a UD grad with his degree in plant sciences.

I have not yet visited this new business but plan to do so. I shall explore the possibility of a tour for ACS members. This is a new kind of plant based chemical industry that also buys chemical products to cope with insects and fungus problems. When you also consider the number of states that permit the sale of recreational marijuana, this is indeed a growth industry.

The March 1 issue of Science magazine reported on a study of medical marijuana use by elderly people to control pain. The report stated that this enabled some senior citizens to return to work full-time. Let’s hope they are not driving school buses!

Neat Chemistry

The March 25 issue of C & E News includes a brief article about C60, often referred to as buckyball. Professor Richard J. Whitby at the University of Southampton and his group managed to insert a methane molecule inside the cage! They now will try to trap O2 and NH3 within C60.

“Forever Chemicals” No More?

This is the title of an article in the same issue of C & E News about methods to remove nonpolymer per- and polyfluoroalkyl substances from drinking water. You will soon get rich if you develop a cheap and effective method of solving this serious problem.

The article includes a map of the U.S. (lower 48) with problem areas indicated. Our region obviously has lots of contamination! Only a few states are without this problem, such as Iowa and Nebraska.

I worry about the contamination of beer which is about 95% water. Are there breweries in Iowa and Nebraska?

The Ethylene Oxide Problem

You may recall the huge leak at the Croda plant on the Sunday after Thanksgiving. Motorists were stranded on the Delaware Memorial Bridge for 8.5 hours. Luckily there was no fire or explosion at the scene but many citizens were exposed to a known carcinogen.

I fear that Croda will soon restart the plant to produce this very dangerous compound. My proposal to move the plant to a remote location has been ignored. When you drive across that bridge, keep your fingers crossed!

Have a great summer, free of sunburn and insects!
Abstract

Factor V and its close cousin Factor VIII circulate in plasma as procofactors. Their importance in blood coagulation is illustrated by the bleeding diseases associated with deficiencies in either of the procofactors. They are inactive precursors that require proteolytic activation to yield the corresponding cofactors Va and VIIIa. In the case of factor V, activation results from the proteolytic release of an 835-residue central B domain to yield heterodimeric factor Va which can bind the proteinase, factor Xa, on membranes exposing phosphatidylserine to assemble prothrombinase. The incorporation of factor Xa into prothrombinase yields a profound increase in the rate at which its cognate substrate, prothrombin, is converted to thrombin. Factor V cannot bind Xa and function as a cofactor. In contrast to the extensive literature on the subject, it is not cleavage per se that activates the procofactor, but rather the disruption of a tripartite inhibitory structure constituted by a basic region (BR) centrally located in the B domain and two acidic regions AR1 and AR2 flanking the B domain. Structural work with Xa reveals that AR1, retained in Va, contributes in a major way to the proteinase-cofactor interaction. BR and AR2 in uncleaved factor V constrain AR1 in such a way as to prevent Xa binding. A new structure of a truncated form of human factor V reveals that AR1 and AR2 are positioned adjacent to each other, despite being separated by 835 residues, to form a putative extended surface for BR binding. This idea is consistent with FRET studies and confirmed by HDX. Functional studies reveal that it is the single cleavage after AR2 that disrupts the inhibitory structure and exposes AR1 and other surfaces for high affinity Xa binding and the assembly of prothrombinase. This combination of structural and functional approaches unexpectedly provides new insights into long-standing and poorly understood aspects of coagulation biochemistry. It also reveals novel strategies to down-regulate cofactor function or up-regulate procofactor function for therapeutic gain.
Abstract
Amines enjoy a privileged place in the heart of organic chemists. Alkyl amines are widely available, and easily prepared in high enantiomeric purity. In addition the amino group (NH2) can be carried through multi-step syntheses in protected form, and enables straightforward purification. These features are well appreciated in the use of alkyl amines for the preparation of nitrogen-containing products, including a plethora of natural products and medicines. We are expanding the toolkit of reactions of alkyl amines by developing cross-coupling reactions via cleavage of their carbon–nitrogen bonds. Capitalizing on the robust methods to prepare enantio-pure benzylic amines, we have developed stereospecific cross-couplings of benzylic ammonium salts to deliver highly enantioenriched diaryl and triaryl alkanes, as well as benzylic boronates. This method was the first example of either an enantioselective or stereospecific cross-coupling of a benzylic electrophile with an aryloboronic coupling partner.

Recognizing the abundance of primary alkyl amines with unactivated alkyl groups (not benzylic, allylic, or strained), we have also developed cross-couplings of Katritzky pyridinium salts. These reactions efficiently convert alkyl amine derivatives into alkyl arenes, and provide new opportunities for the use of amines in synthesis. Our method is the first example of the cross-coupling of an alkyl amine derivative in which the C–N bond is not electronically or strain-activated. We have also extended this chemistry to cross-couplings of benzylic pyridinium salts to enable transformation of benzylic amino groups to aryl or vinyl substituents. Our more recent work with new coupling partners and new classes of alkyl pyridinium salts will also be presented.

Brief Bio
Born in 1977, Mary P. Watson grew up in Tampa, FL. She completed an A.B. in Chemistry at Harvard University in 2000, where she performed undergraduate research with Prof. David A. Evans at Harvard, as well as with Prof. Kenneth B. Wagener at the University of Florida. She earned a Ph.D. in organic chemistry in 2006 from the University of California, Irvine, under the direction of Prof. Larry E. Overman. Her doctoral thesis focused on the development and mechanistic investigation of the palladium(II)-catalyzed asymmetric allylic imidate rearrangement. During the course of this work, she had the opportunity to collaborate with Prof. Robert G. Bergman at the University of California, Berkeley, where she performed kinetic and computational studies. From 2006–2009, she was a National Institutes of Health NRSA postdoctoral fellow at Harvard University with Professor Eric N. Jacobsen. During her postdoc, she developed a nickel-catalyzed method for olefin arylcyanation via activation of C–CN bonds. In July 2009, she joined the faculty at the University of Delaware. She was promoted to Associate Professor in 2016, and to Professor in 2018. Her research focuses on developing new transition metal-catalyzed methods for the synthesis of organic molecules, with a particular emphasis on controlling stereochemistry and identifying new classes of substrates for cross-coupling reactions. Her research accomplishments have been recognized with a NSF Early Career Award, a Thieme Chemistry Journal Award, a Rising Star Award from the ACS Women Chemists’ Committee, a Wavefunction Presentation Award, and inclusion in the 2017 J. Am. Chem. Soc. Young Investigator issue. In addition to her passion for research, Watson is also the proud mom of twin kindergarteners.
Rob Mishur's
On the Horizon

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We already have several exciting events planned for the fall, so be sure to mark your calendar now! Our first speaker of the fall will be Melissa Newell, Lab Manager of the Delaware State Police Forensic Chemistry Unit. This talk is scheduled for Thursday, September 19. On October 17, we will be at the Tri-State Bird Research and Rescue in Newark, where we look forward to a talk by Dr. Erica Miller, DVM. Finally, in November, we will have two events. The first is a section meeting, tentatively scheduled for Tuesday, November 19, and the speaker will be Mecky Polschröder, professor of biology at University of Pennsylvania. Dr. Polschröder’s work involves structure and function of bacterial and archaeal cell surfaces. Also, in November is the annual Ullyot Public Affairs lecture held at the Science History Institute in Philadelphia. Following the lecture, the Ullyot Award is jointly presented by the Delaware and Philadelphia sections of the ACS. This year’s award recipient is Roald Hoffman, Nobel laureate in chemistry. Recent recipients of this illustrious award include Jennifer Doudna, discoverer of CRISPR technology, Marcia McNutt, 22nd President of the National Academy of Sciences, and Sir James Fraser Stoddart, 2016 winner of the Nobel Prize in Chemistry.

The Delaware Valley Mass Spectrometry Discussion Group (DVMSDG) is sponsoring two travel awards for students who plan to present at the 67th American Society for Mass Spectrometry (ASMS) Conference, June 2nd – 6th, 2019 in Atlanta, GA. Applicants must be enrolled full-time in either a graduate or undergraduate program at a college/university in the greater Philadelphia/Delaware Valley region.

Interested applicants should submit the following information:

• Copy of their ASMS abstract
• 1-2 page supplementary description of their research project
• 1 page curriculum vitae
• Applications should be submitted electronically in Word or PDF format

by May 3rd, 2019 to

Steven.Mark.LaMonaca@dupont.com

Applications will be judged by DVMSDG Board, and the winners will be announced at our annual Vendors’ Night meeting on May 7th, 2019.

Further information about DVMSDG can be found at our website: http://dvmsdg.org

Contact if you have any questions regarding the award or the application process.

Steven M. LaMonaca
Awards Chair, DVMSDG
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ASMS Travel Award
67th American Society for Mass Spectrometry Conference
June 2-6, 2019 • Atlanta, Georgia

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Delaware Competitive High School Chemistry Exam
Friday, May 3, at 8 am McKean High School, Wilmington

The DE ACS will award cash prizes to the top scorers. Teachers who are interested in sending students to the exam should email Mike Stemniski at mastem@udel.edu no later than April 25.
**UD Women in Chemistry group (Newark)**
**Happy hour/social event**
**Thursday, May 2 5:30-7:30 PM**
Iron Hill, 147 E Main Street, Newark, DE 19711

**Delaware Valley Enzymology Club**
*DE & PHIL. ACS Enzymology Topical Group*

**Thursday, May 9th**
Chennai Corner, 145 S Gulph Rd, King of Prussia, PA 19406
Social Hour 6 pm | Dinner 7 pm | Seminar 8:15 pm

**Structural Correlates of Procofactor and Cofactor Function:**
*A Final Frontier in Blood Coagulation Biochemistry*
Dr. Sriram Krishnaswamy
Perelman School of Medicine at the University of Pennsylvania and The Children’s Hospital of Philadelphia, PA.
Dinner is $30, student $20. The seminar is free.
Dinner reservations must be made *by Friday May 3rd*. Reservations not canceled by Monday, May 6th will be billed. Email Yixuan Qiu at dvenzymec@gmail.com for reservations and more information.

**Delaware Valley Mass Spectrometry Discussion Group Vendors Meeting**
**Monday May 13, 2019. 5 PM**
Radnor Hotel, Wayne, PA.

**Mass Spectrometry: Power and Beauty**
R. Graham Cooks, Purdue University

5 pm Vendor Show, 6:30 pm Free Buffet-Style Dinner, 7:30 pm Business (Election of Officers, etc), 7:40 pm Talk
Please RSVP to rshomo@adaptas.com by Tuesday, May 7 at 5 pm.


**ACS Awards Ceremony**
Section Award, 50 and 60 year member awards
**Saturday, May 18 1:00-4:00 PM**
Dupont Country Club, 1001 Rockland Rd, Wilmington, DE
* Awards committee selected
* Mary Watson, UD Biochemistry Department
* Re-imaging the Role of Amines in Organic Synthesis

**New Conference:**
*1st Annual Empowering Women in Organic Chemistry 2019*
**Friday, June 28, 2019**
University of Pennsylvania, Philadelphia, PA.
This one-day event will include talks from organic chemists in industry and academia, a dynamic poster session, panel discussions, and many opportunities for networking. Professor Geraldine (Geri) Richmond (University of Oregon), past-president of AAAS, National Medal of Science awardee, and co-founder of COACH, will give the keynote lecture. Madeleine Joullie (UPenn), Emma Parmee (Merck), Lisa Jarvis (C&EN), Malika Jeffries-El (Boston University), and Catherine Leimkuhler Grimes (UDelaware) will also give invited talks. Graduate students, postdocs, faculty, and professionals are invited!
See [https://ewochem.org/EWOC/ewoc-2019/](https://ewochem.org/EWOC/ewoc-2019/) for more information and to register.

**Delaware ACS Section Meetings**
**Thursday, September 19**
Melissa Newell, Lab Manager
Delaware State Police Forensic Chemistry Unit
**Thursday, October 17**
Dr. Erica Miller, DVM
Location: Tri-State Bird Research & Rescue, Newark, DE