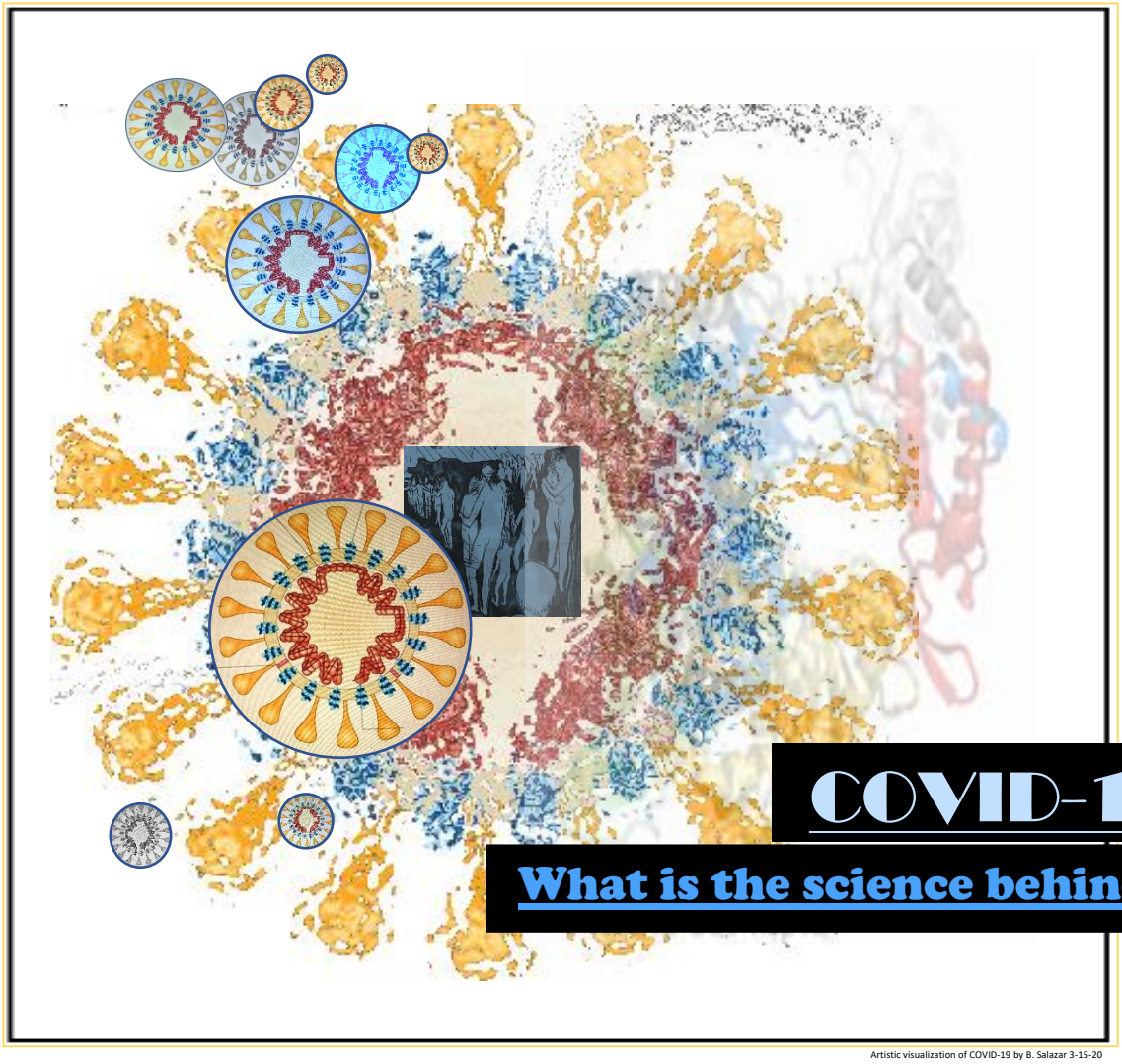
Chesapeake Chemist
Maryland Section American Chemical Society

Local Section Newsletter
March 15, 2020

STUDENT AWARDS 2020



Artistic visualization of COVID-19 by B. Salazar 3-15-20

Chesapeake Chemist
Maryland Section American Chemical Society

Maryland Local Section Newsletter

Editor in chief: Beatrice Salazar

Policy
Pumtiwitt McCarthy, Chair-2020
Sarah Zimmerman, Web Master
Jennifer Schmitt, Social Media Liaison

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Cover

Illustration: COVID-19 by Beatrice Salazar

CHAIR'S MESSAGE

Dear colleagues:

Welcome to another new year with the ACS Maryland Section! As your new chair, I look forward to engaging with you this year through our upcoming events. Our section aims to reflect you and to serve your needs as a member of the chemistry community in this region. I have three major goals this year:

- More effective communication with our membership. We seek to relay information about our events in a timely manner using multiple platforms including *The Chesapeake Chemist*, our recently updated website, email, and social media platforms (Facebook and Twitter).
- Increasing membership participation in our events. I would love to see more of you at our events. By improving our communication, I hope that this will lead to more members being involved in our section.
- Developing a sustainable method to reach out to and engage participation of younger chemists. We are fortunate to reside in an area where there are many colleges and universities. Our region also has many young professionals working areas of government, industry, non-profit organizations and academia. I know you have much to say and your voices need to be heard. Please consider becoming more involved in our section.

In closing, I am hoping that all our members feel that the ACS Maryland Section serves them well. Of course, we are not perfect so I would appreciate an opportunity to learn how we can work for you and with you better. Please consider sending an email to us (acsmarylandsection10@gmail.com) if you want to be more involved and if you would like to provide general comments and/or suggestions.

Pumtiwitt McCarthy

Editor's Comments

The 2020 started with and interesting direction toward a more structured Maryland Section's local events. Shortly after taking office, Chair Dr. P. McCarthy created a **Communication Team** that will bring the best information to all active ACS Maryland members. I, would like to encourage all members to take advantage of this resource for your own career advancement. Send your most recent published article, tell the scientific community about your research, your job, your interesting activities, your experience at an ACS meeting, let us help you connect and flourish in your career.

Beatrice Salazar

2020 Maryland ACS Student Award Luncheon

Guest Speaker

MIKE ADELSTEIN

President and CEO of Potomac Photonics

CONTACT:

George Farrant

gfarrant@yahoo.com

Chair of Student Awards Committee

Student Awards Speaker

The speaker's presentation and Student Award Ceremony has been cancelled due to COVID-19

*

Learn more about

the science of this virus,

what to do if get sick,

and find articles from ACS

Pages 18 /19

*

Biography

Mike Adelstein PRESIDENT AND CEO

Mike Adelstein has spent his career at Potomac working with industry leaders, inventors, researchers and entrepreneurs to quickly bring new products to market through digital rapid prototyping that can then ramp up to high volume production manufacturing. Integrating a wide range of digital fabrication technologies such as laser micromachining, 3D Printing, factory automation, micro-CNC precision machining, machine vision and more, he has enabled Potomac to optimize designs for manufacturing by working iteratively with customers.

Degrees in **Biochemistry and Molecular Biology from the University of Maryland, Baltimore County [UMBC]** allow Mike Adelstein to understand the science-based intricacies required to bring microfluidics, biotech and medical device ideas to life. His more than 20 years experience working with Potomac's digital fabrication pioneers, bridges engineering and biological systems for the best solutions to today's multi-disciplinary challenges.

Quality performance is a central platform in Mr. Adelstein's strategy. He has brought Potomac into compliance with ISO13485 standards. **With an MS in Technology Management and as a Certified Public Accountant [CPA],** all aspects of Potomac's infrastructure are integrated to ensure quality across functions. Source

Chesapeake Chemist
Maryland Section American Chemical Society

Student Award Luncheon

RSVP George Farrant, gfarrant@yahoo.com
at least two weeks before the event (Please inform of any dietary restrictions)

AWARD

The ACS Student Award is given to one student at each college or university that participates in the Maryland Section of the ACS. The meriting students are nominated by their own research or academic advisor. This year we will celebrate awardees from 21 local colleges and universities. This meeting is one of the more popular meetings we hold each year and we expect approximately 100 or more attendees.

The Maryland section of the ACS will be holding the Annual Student Awards Ceremony at Notre Dame of Maryland University. All are invited to come to see the best and the brightest of our 2020 new group of students as they start on their careers in Chemistry and related fields.

The speaker for this event will be Mike Adelstein, President and CEO of Potomac Photonics, UMBC graduate in Chemistry and a founder of a very successful-cutting edge scientific company. He is a very good speaker and will have some interesting things to impart. *George Farrant*

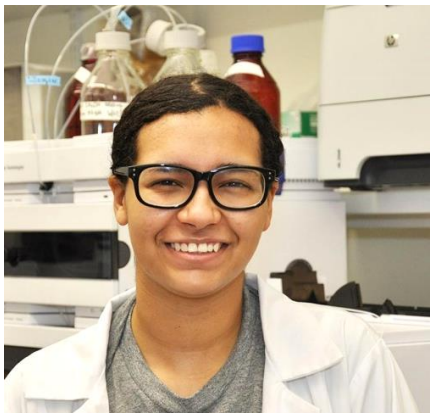
LOCATION and AGENDA

Where……. Doyle Formal Lounge, Notre Dame of Maryland University, Baltimore, MD
https://www.ndm.edu/
When……Sunday, March 29, 2020 at 12:00 noon
Directions: https://www.ndm.edu/admissions-aid/visit-campus/map-directions-/Parking
Cost…… Awardees have a complimentary lunch
$20 members and non-members
$10 students
Payment... Cash or check made payable to Maryland ACS Pay at registration

2020 STUDENT AWARDS AGENDA:
Sunday March 29th, 2020

12:00-12:30 P.M.	Registration and viewing of the posters of the student who presented at the ACS National Meeting in Philadelphia Hors d'oeuvres and seating
12:30-1:30 P.M.	Luncheon
1:30-2:00 P.M.	Awards ceremony
2:00-3:00 P.M.	Lecture and Q&A

CONGRATULATIONS
2020 Student Awardees



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CONGRATULATIONS
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2020 Student Awardees Criteria for Nomination

Excellence in Research Practices
Creativity
Outstanding GPA
Completion of Selective Chemistry, Biochemistry and Organic Chemistry Courses
Faculty and Staff Group Reviews

HISTORY CORNER…

2020 marks the 42nd anniversary of the Student Awards Ceremony

By George Farrrant,

George Farrant, SAC Chair

This is the 42nd anniversary of the Student Awards Ceremony (SAC).

This event began in March 1978, under the direction of Dr. Carl Minier from Essex Community College of Baltimore County (CCBC). He was chair of SAC for several years. The program was part of the Maryland Section of the American Chemical Society (ACS) effort to promote the study of chemistry by recognizing outstanding achievement early in a student's career.

The selection for the awardees is left up to 21 individual chemistry departments of the local colleges and universities. Each college and university are contacted to submit one nominee each year. Each University or college has total autonomy to design their own nomination criteria. SAC has been one of the most popular celebrations of the Maryland Section over the years, often generating more than 100 attendees. In the past years we have increased the number of awardees. The award is a significant recognition of a student's record and often helpful in the pursuit of a career in the sciences.

Since 2018 we are including a poster section of the students' recipients of travel awards, another successful program of the ACS Maryland Section. The poster presentation is open for discussion with the respective presenter 30 min. to 45 min. before the award ceremony, during lunch and few minutes after the ceremony. Please join us and connect with young promising students.

2020 STUDENT TRAVEL AWARD

Young Scientists Research and Poster Abstracts

The Maryland Local Section of the ACS supports the Student Awards Program designed to encourage the student advancement of chemistry in all its branches, to support research in chemical science and industry, and to promote the careers of chemists.

CONTACT

Student Travel Awards Chair

Dr. Louise Hellwig
Morgan State University

Information from ourwebsite…

Undergraduate and Graduate Student Travel Grants

Undergraduate and Graduate students may apply to the ACS Maryland Section to receive up to $500 for travel and expenses to attend a national ACS Meeting or a MARM (Mid-Atlantic Regional meeting). This is open to ACS members who are enrolled full time in a college or university in the Maryland Section.

The application should include:
- The meeting you plan to attend along with location and dates
- Your ACS membership number
- An estimated budget (cost for travel, registration, lodging, and meals)
- A 250 word essay describing your motivation for attending the meeting
- A copy of your abstract and the abstract number ACS gave it when your abstract was accepted
- A letter of support from your faculty advisor
- Please state what would be the most convenient way for the check to be made out, in the event you are awarded a travel grant.

Application Dates:
__Spring National ACS meeting - December 1st, previous year (decisions will be announced by January 20th)
__Fall National ACS meeting - April 2nd. (decisions will be announced May 10th.
Special consideration will be given to the first student who applies from each college/university. We especially encourage schools which have never had a student apply for a travel grant, to consider applying for a travel grant this year.

Louise Hellwig

TRAVEL AWARDEES

ACS AND THE MARYLAND SECTION MAKE AVAILABLE TRAVEL AWARDS FOR THOSE ATTENDING SCIENTIFIC MEETINGS TO PRESENT THEIR WORK OR THEIR RESEARCH.

CONTACT:

DR. LOUISE HELLWIG

LOUISE.HELLWIG@MORGAN.EDU

The Maryland Section of the American Chemical Society is pleased to announce the following grants of $400.00 each for students attending the ACS National Meeting in Philadelphia. March 26, 2020.

*Hood College

Amber Meyers
McKenzi Weatherhogg

McDaniel College

*Alena Villanueva
Jonah Ruskin

Stevenson University

* Lemane Namarra
Sara Bonfils

*Towson University

Lynn Krushinski
Gabrielle Lembo
Pierce Brown

*UMBC

Jahir Andrade
Yang Liu

*UM School of Pharmacy

Alexandria Chan
Ivie Conlon

*St. Mary's College of Maryland

Hana Yarbrough

*Abstracts presented and published in CCNL

Poster presentation will be at the Student Awards Ceremony on Sunday, March 29, 2020 starting at 11:30 A.M. Students presenter and families are invited. For more information see page 8.

Towson University Travel Awardees Abstracts

Pierce Brown, **SYNTHESIS OF QUANTUM-CONFINED Au25SG18 NANOCLUSTERS FOR CANCER THERAPY**

The primary objective of this research is to synthesize stable, robust 1.1 nm gold nanoclusters (Au25SG18) with glutathione (GSH) as the ligand efficiently and in high yields. These alterations enable the clusters to exhibit unique optical, catalytic, biomedical and electrochemical properties, which have made these nanoclusters desirable in various fields of study. In addition to these unique and invaluable properties, these nanoclusters containing 25 gold atoms are extremely stable even amongst its other magic numbered counterparts due to the stability of the icosahedral core and sulfur-gold bonds. The synthesis of these gold clusters and characterization with the ligand glutathione will be presented. To quantify the viability and stability of these nanoclusters for biological applications, the nanocluster systems are tested for (i) their stability in different ionic strengths and (ii) their stability in biological media of varying concentrations which is analyzed through both its zeta potential and DLS profiles. Furthermore, the stability of these systems are analyzed through UV-vis to identify if any aggregation of the nanoclusters occur. Once confirmed of their stability, these gold nanoclusters can be used to study their effectiveness in theranostics.

Gabrielle Lembo, **CHEMICAL SIGNATURES FROM UPLC/MS FOR COCOA PROVENANCE DETERMINATION**

The production of chocolate products is a global industry that needs a method to determine the geographic origins of its most essential component, cocoa. Traceability of cocoa is becoming more important for quality control in the chocolate industry, so that consumers can know they are purchasing products that adhere to fair-trade regulations, organic farming practices, etc. Many of the steps in the process of producing cocoa can influence the chemical makeup of the different aspects of the final product including the flavor profile and aroma. Each region where cocoa is gown has variations in soil composition, weather and farming practices that influence the cocoa bean development. Additionally, differences in post-harvest treatments including fermentation and roasting conditions influence the overall chemical composition of the resulting cocoa liquor used to make finished chocolate products. These differences result in unique chemical signatures that can identify cocoa liquors by their country of origin. Many studies have employed GC/MS, ICP/MS, and HPLC to quantify and detect the presence of certain classes of compounds in cocoa, but there are fewer studies focused on provenance determination via chemical signatures. Previous work by this group has been able to accurately determine the country of origin of a cocoa using ICP/MS to construct a unique elemental profile for each country. Use of LC/MS provides an opportunity to use a wide variety of molecules to generate chemical signatures. The cocoa sample preparation and conditions for UPLC/ESI-TOFMS used to obtain unique chemical signatures from cocoa liquor samples are described. Several classes of compounds were identified from the mass spectral data, and the semi-quantitative analysis method was verified with a cocoa standard reference material. Discriminate analysis was used to identify cocoa liquor samples from five different countries. The method was able to accurately group and identify country of origin in 95% of samples. Future directions include moving beyond country level provenance determination, to regional discrimination within countries, and potentially differences in signatures due to genetic strains of cacao.

Lynn Krushinski,

In recent years, magnetic nanoparticles have become increasingly attractive to researchers for their wide scope of applications across numerous fields. For this reason, there is no shortage of literature available on magnetic nanoparticle synthesis and characterization. Iron Cobalt nanoparticles cannot be found in such an abundance due to their tendency to quickly oxidize when exposed to air, but these specific nanoparticles offer relatively high magnetization values so if they could be synthesized reliably they could have a great potential impact across many fields. This project aims to synthesize these nanoparticles in such a way that they become the base for biocompatible ferrofluid for the specific application of magnetic drug targeting. Surfactants allow for air stabilization and biocompatibility to be achieved in the FeCo nanoparticles. In this project, oleic acid and oleylamine are used as surfactants to result in a carbon coating around the nanoparticles. Chloro(triphenylphosphine) gold is used following and in addition to the carbon surfactants to create a gold layer. The resulting particles therefore should have air stabilization and biocompatibility achieved through the use of carbon and gold surfactants. These resulting particles are taken through size separation methods such as centrifuge and fractionation in order to achieve uniform size distributions at the desired particle diameter. UV-Vis spectroscopy, EDX imaging, and ICP-MS will be used to characterize the particles by confirming and quantifying surfactant ratios to iron and cobalt and magnetization values will determine the relation between particle diameter and magnetic field strength.

Hood College Travel Awardees Abstracts

Amber Meyers, **ULTRAFAST LASER SPECTROSCOPY TO STUDY PHOTODYNAMICS OF ASYMMETRIC HYDROGENASES**

In nature, some bacteria are able to efficiently produce hydrogen gas. [FeFe]-hydrogenases are the enzymes that generally catalyze the reduction of hydrogen in nature. These enzymes, which contain iron in their active site, are of great interest because of the increasing need to develop a cheaper substitute for platinum as a catalyst for hydrogen production. Symmetric model compounds containing all CO ligands or mixed CO/CN and CO/PMe3 ligands on both irons in the active site have been studied extensively. However, asymmetric compounds have not been the focus of as much work. This work examined two asymmetric molecules containing both CO and CN ligands: [Fe2(μ-S2C3H6)(CO)5(CN)1]1- (**1**) and [Fe2(μ-S2C2H4)(CO)5(CN)1]1− (**2**). The asymmetry of these model compounds makes the redox potentials of the two iron atoms different, changing the catalytic properties of the compounds. The molecules were studied using 400 nm and 266 nm UV pump-infrared probe spectroscopy in order to better understand the ultrafast dynamics of the active site. So far, **1** has been studied using 400 nm and 266 nm pump pulses, and **2** has been studied using 400 nm pump pulses. In **1**, distinct bleaches are observed around 1930, 1979, 1999, and 2038 cm-1. There are also new absorptions at 1899, 1964, and 2023 cm-1. The bleaches and absorptions decay with a time constant of 23 +/- 6.6 ps. There is some evidence of residual signal remaining out to 300 ps, especially with the bleach at 1979 cm-1. Similar bleaches and absorptions are observed in **2** due to the similarity in structure. Additionally, density functional theory (DFT) calculations are being used to simulate possible photoproducts.

McKenzi Weatherhogg **DETECTION OF COCAINE IN UNITED STATES PAPER CURRENCY USING ELECTROSPRAY MASS SPECTROMETRY**

Liquid chromatography- electrospray ionization mass spectrometry (LC/ESI-MS) is used to help identify substances based in both physical separation and determination of mass. LC/ESI-MS is often used in forensic chemistry to aid in the determination of substances of abuse. Cocaine is a drug of abuse known to be found in trace amounts in United States paper currency. This study focused on optimization of conditions for extracting cocaine from currency and study of LC/ESI-MS parameters that influenced detection of the target analyte. Extraction conditions under study were length of time of sample extraction, type of extraction method (vortex or sonication), and the use of a sample filter. LC/ESI-MS conditions of capillary and cone voltages were also studied. It was found that cone voltage had a significant impact on intensity of the cocaine molecular ion in MS detection. Additionally, higher capillary voltages were found to enhance cocaine ion formation. Cocaine was detected in a wide range of currency tested.

UMBC Travel Awardees Abstracts

Jahir Antonio Batista-Andrade, **ANALYSIS OF DISSOLVED ORGANIC MATTER AND CONTAMINANTS OF EMERGING CONCERN TO DETECT LEAKING SEWERS IN URBAN STREMS**

Analysis of dissolved organic matter and contaminants of emerging concern to detect leaking sewers in urban streams
Sanitary sewer overflows (SSOs) are common in urban areas due to aging infrastructure. SSOs can introduce wastewater contaminants directly to urban watersheds, threatening public healthand ecological systems. With approximately 550,000 residents, the Gwynns Falls and Jones Falls watersheds cover the western and central areas of Baltimore City. The Baltimore City Department of Public Works tracks SSOs in these watersheds; however, the impacts of SSOs and other unidentified sewer leaks on urban streams are not well understood. We propose that characterization of dissolved organic matter (DOM) and measurement of contaminants of emerging concern (CECs) in urban streams can be used to locate leaking sewers. The objective of this work was to investigate DOM fluorescence signatures and CEC concentrations in urban streams and assess the potential input of raw wastewater. DOM was analyzed in water samples collected each month from 27 sites in these streams from March to December 2019. Absorbance spectra and fluorescence excitation-emission matrices (EEMs) were used to understand changes in DOM composition across the watersheds, and a parallel factor analysis (PARAFAC) was conducted with the 270 EEMs to identify fluorescent components. CECs were measured in water samples from four sites, including one urban and one suburban from each watershed, for July to December 2019. The investigated CECs included antibiotics, hormones, sucralose, and UVfilters. Sucralose, oxybenzone, and octocrylene were detected at concentrations as high as 417, 116, and 48 ng L-1, respectively, and the highest concentrations occurred at urban sites in the Gwynns Falls. The EEM-PARAFAC component scores and regional volumes (*e.g.*, tyrosine, tryptophan, fulvic acid, soluble microbial product, and humic acid like-fluorescence) were compared to CEC concentrations and SSO data. Overall, this work will combine municipal data on SSOs with spatiotemporal analysis of DOM and CECs to improve identification of leaking
sewers and their effects on urban streams.

Yang Liu

Chromatofocusing is a specialized liquid chromatography method that employs an ion-exchange column packing. The method utilizes an internally generated, retained pH gradient (or a retained simultaneous pH and ionic strength gradient) and combines the best features of ion-exchange chromatography and isoelectric focusing. This work investigates the computer-aided design of the buffers that create the chromatofocusing pH gradients. The design method is based on either local-equilibrium theory and the coherence condition (the mechanistic model approach) or a machine-learning, linear regression model (the non-mechanistic model approach). For simplicity, a three-buffer system is used, with one buffering species in common between the starting and elution buffer. By performing a stepwise change from the starting buffer to the elution buffer, a four front pH gradient is formed inside column and used for antibody purification. A buffer pool consisting of five buffering species is employed, and the computational method automatically selects the optimal set of three buffering species (out of 10 such sets) that produces the best fit to the target pH gradient. Results indicate that chromatofocusing is useful for several important types of bioprocessing applications. This study employs Julia, which is a new programming language designed for high-performance computing and machine learning applications.

UM School of Pharmacy Travel Awardees Abstracts

Alexandria M. Chan, **DUAL INHIBITION OF HDAC6 AND THE PROTEASOME AS A POLYPHARMACOLOGIC METHOD FOR TREATMENT OF HEMATOLOGICAL MALIGNANCIES**

Polypharmacology has become a promising method of targeting cancer cells because of their adaptiveness to use multiple pathways for survival; this is also the method of resistance to many current treatments. Proteasome inhibitors are among these approved therapies for hematological malignancies. The proteasome is responsible for the degradation of proteins that are either no longer needed, misfolded, or damaged. In cancer cells, there is an increased amount of ineffective proteins that are produced. When the proteasome is inhibited, there is an accumulation of these proteins that cause the cell to burst. One method of resistance to proteasome inhibition is the aggresome pathway, controlled by histone deacetylase-6 (HDAC6). Using this pathway, the cell trafficks unwanted proteins into aggresomes where they are stored until degradation by lysosomes. HDAC6 is upregulated in cancer cells, making it an ideal target for chemotherapy. Significantly, recent literature demonstrated that HDAC6 knockout mice did not present any defects. Typically, HDAC inhibitors comprise three parts: a zinc binding group, a linking group, and a capping group. Increasing the size of the linking group, in particular, or capping group of the inhibitor, increases the specificity of the inhibitor towards HDAC6. Indeed, the wider binding pocket of HDAC6 permits the accommodation of larger, aryl linker groups, which are less readily accommodated by other family members. This increase in specificity also helps decrease the off-target effects that are observed with pan-HDAC inhibitors. Recent literature has shown that the dual inhibition of both the proteasome and HDAC6 has a synergistic effect leading to cell death and decreased cell proliferation. Therefore, we are assembling a library of dual proteasome and HDAC6 inhibitors by enhancing existing proteasome inhibitors with different hydroxamic moieties to act as a zinc binding group for HDAC6 specific inhibition in the treatment of hematological malignancies.

Ivie Conlon, **A POLYPHARMACOLOGY APPROACH TO DESIGN DUAL INHIBITORS AGAINST ONCOPROTEINS Mcl-1 and HDM2 WITH DENSELY FUNCTIONALIZED INDOLE SCAFFOLDS**

Protein-protein interactions (PPIs) govern key processes within the cell, including proliferation, differentiation, and cell death. The Bcl-2 protein family, which includes anti-apoptotic proteins Bcl-2, Bcl-xL, Mcl-1 and Bcl-w, and their binding partners pro-apoptotic proteins Bim, Bad, Bak, and Bax, among others, are key regulators of the intrinsic apoptosis pathway. Dysregulation of these PPIs, which is often caused by upregulation of pro-apoptotic proteins, can lead to cell immortality and cancer. Tumor suppressor protein p53, which is involved in regulating numerous cell processes including apoptosis and senescence, is negatively regulated by its E3 ubiquitin ligase HDM2, which is often overexpressed in numerous cancers. There is cross-talk between these two protein families, with p53 a regulator of the Bcl-2 family via its transcription-independent apoptosis pathway during mitochondrial translocation. The Mcl1/Bim and HDM2/p53 interactions are governed by α-helices, with the PPI helical domains of Bim and p53 offering similar recognition faces; specifically Leu62(i), Ile65 (i+3), Phe69 (i+7) in the Bim-BH3 α-helix and Phe19 (i), Trp23 (i+4), and Leu26 (i+7) in the α-helix of the p53 transactivation domain (TAD). Although multiple clinical trials are on-going with new Mcl-1 and HDM2 inhibitors, a prevalent theme amongst the failures of newer cancer drugs is the development of resistance, and so multi-target drugs may be more clinically viable. We hypothesize that a single, dual inhibitor that functions to mimic both the Bim-BH3 and p53TAD helical recognition faces will

simultaneously target both Mcl-1 and HDM2, affording a particularly efficacious drug through anticipated synergistic effects. Recently, triply-substituted indoles have elicited significant and selective inhibition of Mcl-1 and, in independent research, of HDM2. Therefore, we are leveraging these findings towards the discovery of dual Mcl-1/HDM2 inhibitors based on densely-functionalized indole cores, and our progress will be reported.

McDaniel College Travel Awardees Abstracts

Alena Villanueva, **EXPLORING THE KINETICS OF THE TRAFFIC LIGHT REACTION: COMPLEX AND POORLY DEFINED SYSTEM**

The traffic light reaction is an example of an oscillation chemical reaction that is typically used for demonstration purposes. The reaction is ideal for chemical education since it uses cheap and ubiquitous reagents, is simple to assemble, and produces vibrant ad easily observable color changes (hence the name). The initial idea of this project was to create a simple and effective lab to demonstrate kinetics in a general chemistry lab environment. However, we found that the traffic light reaction, though ubiquitous, is mechanically complex and is poorly documented literature. In the end, this study focused on refining a previously used chemical traffic light lab procedure, which produced inconsistent results and unnecessarily long reaction times, and deeply exploring the reaction kinetics. The procedure, which uses a mixture of glucose, sodium hydroxide, and indigo carmine dye, was controlled to study the independent effect of each reagent, as well as pH, on the overall reaction time and intermediate reaction stages. In doing so, we created a newly refined and reliable experiment, and we discovered some new and interesting mechanistic details about a decades old reaction.

St. Mary's College of Maryland Travel Awardees Abstracts

Hana Yarbrough,

The ability to produce dyes that absorb and emit within the near-infrared (NIR) region is of value to the material science and biomedical fields. Boron difluoride chelates of the aza–dipyrromethene core structure (aza–BODIPYs) have received a recent resurgence of interest in the chemical literature due to their high photostability and tunability. This poster presents a facile and reproducible method to the synthesis of a series of symmetrically and asymmetrically nitrated aza–BODIPYs as well as an evaluation oftheir photophysical properties.

Stevenson University Travel Awardees Abstracts

Lemane Nesfin Namarra, **DRUG DESIGN OF NUCLEOSIDE REVERSE TRANSCRIPTASE INHIBITORS (NRTIs) USING ABACAVIR AS A LEAD COMPOUND BY COMPUTATIONAL TECHNIQUES**

HIV has been one of the deadliest viruses that heavily influences the immune system by weakening it, resulting in infections and diseases leading to death. Abacavir (brand name Ziagen) is used in the treatment of human immunodeficiency virus (HIV) infection. Abacavir is a nucleoside (and nucleotide) reverse transcriptase inhibitor (NRTI), used in combination with other medications as part of highly active antiretroviral therapy (HAART). Hypersensitivity reactions associated with abacavir can be severe and potentially fatal. In an attempt to find a more effective and safer drug, the purpose of this investigation is to do Structure Based Drug Design (SBDD) on numerous modifications of the energy minimized structures of the lead Co-crystallized structure of the Abacavir-enzyme complex. The co-crystallized structure was found from the existing Protein Data Bank (PDB files). Molecular docking that is commonly used in the SBDD studies predicts the binding mode of the ligand to the appropriate binding site of the target. Various Physico-chemical properties Partition Coefficients, Distribution coefficient at pH 7, Solvation energy and related data using Molecular Operating Environment (MOE) as a software were computed for the different modifications of the Abacavir structure in the binding site of the co-crystallized structure. In addition to these properties the docking results show binding affinities for various conformations determined using London dG and (Generalized -Born Volume Integral) GBVI/Weighted Surface area) WSA dG. These studies will probably shed more insight into predicting the mechanism and to select possibly a more suitable compound with minimal side effects.

REPORTS

Executive Committee Meeting

The first executive committee meeting of the Maryland Local Section of the American Chemical Society took place at Morgan State University last February 24, 2020. All ACS members residing in Maryland are welcomed to these meetings where they could share concerns, bring new ideas and connect with scientist from the Maryland area.

Courtesy of Beatrice Salazar taking picture

The minutes are available and will be discussed and approved in the second executive committee meeting. For further information on the minutes contact Secretary of the ACS Maryland Section Louise Hellwig. Major points: Welcoming of two new members Dr. Linda Gonzales from McCormick Co., Dr. Lee Lefkowitz and the new Maryland Section's chair-2020 Dr. Pumtiwitt McCarthy from Morgan State University.

MISCellaneous Distillery Tour

On Saturday, February 22, 2020, ACS Maryland reported a successful tour of the Miscellaneous Distillery at 114 S. Main Street, B103, Mount Airy, MD 21771. The event was attended by 34 people who learned the process of making spirits and having fun with chemistry.

The tour became an inspiration for more tours of the kind and coordinators are seeking possible future wine tours to create a more entertaining networking activities. We are looking forward for these upcoming events.

SUCCESFUL ACTIVITY REPORT

CONTACT

Beer Tour Events Coordinators

Louise Hellwig
and
Michele Foss

Maryland Local Section

General meetings information

CANCELLATION! **National Meetings** American Chemical Society, March 22-26, 2020. Interested in attending future national meetings, apply to your Local Section for support. Contact louise.hellwig@morgan.edu

CANCELLATION! **Student Awards Ceremony**

CANCELLATION! **Senior Awards Ceremony**

Announcement

Chemistry in the Library

Designed for students ages 7 and above Events will be at the

Savage Branch	Saturday, @ 2 PM, 14 Mar
Central Branch	Saturday, @ 2 PM, 21 Mar
Glenwood Branch	Saturday, @ 2 PM, 28 Mar

Other events will be at the following libraries in the near future (see Vol. 77 Feb. Issue No. 1)

- Howard County Library System East Columbia Branch
- Carroll County Library System, Eldersburg Branch

April Events

April 18, 2020 US. National Chemistry Olympiad takes place at CCBC see invitation and details on page 20

April 22, 2020 Chemist celebrate Earth Day see event invitation on page 21 this program offers a tour of the Montebello Water Filtration Plant in Baltimore.

April 22, 2020 Earth Day celebration at the Pub. Featuring speaker Dr. Lee Blaney (UMBC) on environmental issues, see invitation on page 18

Braude Award

The George L. Braude Award, presented at the October meeting, Nominations will be accepted May 1, 2020 to May 31, 2020 https://acsmaryland.org/braude-award/
Contact: Louise Hellwig, louise.hellwig@morgan.edu

Cancellation NEWS

ACS Chemistry for Life®

MEETINGS & EVENTS

Philadelphia Meeting Cancellation Registrants and Presenters

Safety is a core value of the American Chemical Society, and as such the health and well-being of our members, community and staff are paramount. As a result, we are cancelling (terminating) the ACS Spring 2020 National Meeting & Expo scheduled for March 22-26, 2020, in Philadelphia.
Our decision was based on several factors, including, but not limited to:

- The Governor of the Commonwealth of Pennsylvania signed an emergency disaster declaration as a result of the COVID-19 global outbreak and several COVID-19 cases have now been reported in the greater Philadelphia area.
- Input received from Philadelphia city officials and continued review of recommendations from the U.S. Centers for Disease Control and Prevention (CDC) and other governmental bodies.
- Watching the rapidly expanding trajectory of the COVID-19 virus using tools such as the Johns Hopkins Center for Systems Science and Engineering COVID-19 tracking system to monitor the ever expanding outbreak of COVID-19 domestically and globally.
- Concern from our attendees and presenters, domestic and global, about safety of travel to and mass assembly in Philadelphia…

Please visit the ACS Spring 2020 National Meeting & Expo webpage for additional details or reach out to us at NationalMeetings@acs.org .

Thank you for your patience, understanding, and support as we move forward.

Kate Fryer,

Executive Vice President, Membership & Society Services

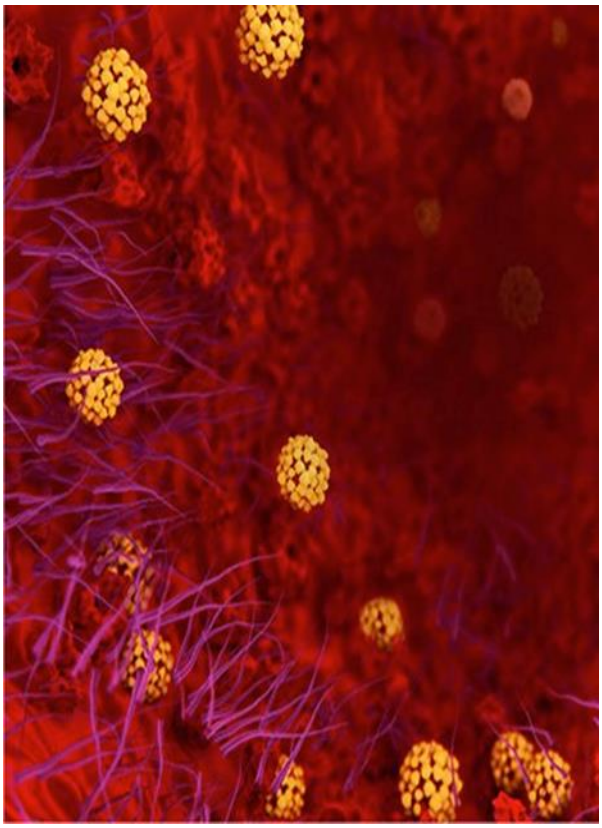
Coronavirus (COVID-19)

https://pubs.acs.org/page/vi/chemistry_coronavirus_research
(ACS Resources)

Chemistry in Coronavirus Research: A Free to Read Collection from the American Chemical Society

In light of the current outbreak of a novel coronavirus (2019–nCoV), ACS Publications would like to share this Virtual Issue that features a collection of articles on coronavirus research. Chemistry has a key role to play in understanding everything from viral structure to pathogenesis, isolation of vaccines and therapies, as well as in the development of materials and techniques used by basic researchers, virologists and clinicians. This Virtual Issue aims to provide a brief overview of the important contributions of chemistry to understanding and controlling the spread of coronaviruses and includes articles from *ACS Infectious Diseases*, *ACS Chemical Biology*, *Journal of Medicinal*

Chemistry, *Biochemistry*, *Chemical Reviews*, and *ACS Applied Materials & Interfaces* as well as the preprint server ChemRxiv. We hope the research contained in this Virtual Issue will provide you with important insight into challenges and approaches in virus research.



COVID-19 statistical data:
https://gisanddata.maps.arcgis.com/apps/opsdashboard/index.html#/bda7594740fd40299423467b48e9ecf6

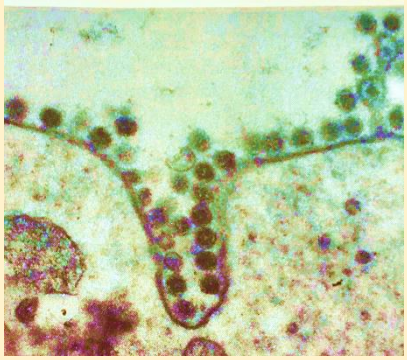
What to if we get sick: https://www.hopkinsmedicine.org/health/conditions-and-diseases/coronavirus/coronavirus-what-if-i-feel-sick

What is the science behind COVID-19 D.Wrapp etal., Science 10.1126/science.abb2507 (2020)

(see commentary in next page)

What is the science behind COVID-19?

The coronavirus is in everyone's mind nowadays. We hear all kinds of good advice in the news: wash your hands, limit your travels, don't shake hands, practice social distance, etc., From one scientist to another, don't you wish there was a little more science on the subject? Like: what's the basis of the measurement of the virus using the kits that are not widely available and that everybody is clamoring for? What do we know about the virus? Well, all you need to do is google a little and read a little.



EM Showing coronavirus particles attaching on the plasma membrane of a cell. The cell begins to form an endocytic vesicle engulfing the virus particles. Design from the book "Viruses" by Arnold J. Levine 1991. Courtesy of B.S.

As far as the answer to the first question, what is the basis of the measurement? The answer is: Reverse Transcriptase – Polymerase Chain Reaction (RT-PCR). The earlier basic version of this technique, PCR, was devised by Kary Mullis in 1984. He shared the 1993 Nobel Prize in chemistry with Michael Smith for this work. Kary Mullis was a somewhat eccentric scientist who died last year. PCR and the related protocol that uses reverse transcriptase to carry out the conversion of RNA to the corresponding coding DNA and subsequent DNA amplification allows for a very sensitive technique that has revolutionized molecular biology. This is truly worth learning about; you can find more about it by simply checking out a standard biochemistry or molecular biology textbook (for an older guy like me) or a Wikipedia / google search (for a young person like you).

If you want to know more about the formally called novel betacoronavirus (2019-nCoV) there is a recent article in Science (February 19, 2020, exact ref on p18 above). A team of scientists from The University of Texas at Austin and from the Vaccine Research Center, National Institute of Allergy and Infectious Diseases, National Institutes of Health, have published the structure of the 2019-nCoV spike and a few additional tidbits. This is less than a three-page article not counting references and figures; the article is packed with excellent science and even if you are not the structural biochemist type it is well worth reading. Among the interesting things I learned: scientists used cryo-Electron Microscopy (cryo-EM) to determine the structure of the CoV spike (S) glycoprotein at 3.5 A-resolution. This is of interest because S is a target for treatments that include vaccines, antibodies and diagnostics. Another piece of interesting information: S from 2019-nCoV and S from SARS-CoV share the same receptor in host cells: angiotensin converting enzyme (ACE2). The difference in the kinetics of the interaction, determined by use of Surface Plasmon resonance (SPR), between S from each virus and host cells may account for why the 2019-nCoV can more easily spread from human-to-human. In short, state-of-the art physico-chemical methods to address a major health problem. Science at its best!

Camilo Rojas, PHD, Johns Hopkins University,

March 15, 2020

cThe Maryland Section of the American Chemical Society is Sponsoring a

Special Earth Day Seminar:

"The Environment is on Drugs!"

Professor Lee Blaney

Department of Chemical, Biochemical and Environmental Engineering, UMBC

Our environment is on drugs. Literally! Think about it. What happens to the caffeine in the coffee that we drink? What about the fragrances and sunscreens in our shampoos, lotions, and cosmetics? What about the antibiotics and other medicine that we take when we are sick? Where do these chemicals go after we use them? It turns out that many of these compounds get discharged into the sewer system and, ultimately, make their way to a wastewater treatment plant. Our wastewater treatment plants have been designed to remove traditional contaminants, such as carbon, nitrogen, and phosphorus. Specialty chemicals like antibiotics and sunscreens often pass through the treatment plant and get released into the environment. In this talk, Lee Blaney will share some of his concerns about the presence of these chemicals in our water and discuss his lab's ongoing work to measure these 'contaminants of emerging concern' in Baltimore streams and the greater Chesapeake Bay watershed.

At Heavy Seas Taproom, 4615 Hollins Ferry Rd. Baltimore, MD

Tuesday, April 21st from 6-9PM

Seminar and Q&A from 7:15-8:30

Snacks will be Served, Admission is $5

2020 ADMINISTRATION OFFICERS

2020 SECTION OFFICERS

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Vice-Chair 2020..... Eric C. Cotton, Community College, of Baltimore County, cccotton2@ccbcmd.edu
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..... Beatrice Salazar, Chair-2018, beatricesalazar1@gmail.com
..... Sara Narayan, Stevenson University, SNARAYAN@stevenson.edu

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4. 2018-2020 Sarah Zimmerman Web Master, Chair of Member Assistance Committee,* scatzim@gmail.com

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An Invitation to U.S. National Chemistry Olympiad USNCO-2020

From February to May 3, 2020

February: Invitation to all high schools
March: Maryland Local Section pre-qualification exam
April: U.S. National Chemistry Olympiad, USNCO
Coordinator: Beatrice Salazar


USNCO at Notre Dame


USNCO at CCBC

Welcome to the 2020 Chemistry Olympiad. We are very enthusiastic about this year's competition at the Community College of Baltimore County, CCBC.

The Maryland Local competition is now open to all participants. All high school students 9-12 taking chemistry are encouraged to register for the pre-qualification exam or USNCO-Maryland. Use the USNCO-Maryland website to get all forms and all the information needed to participate. The local exam is administered from March 1st to April 14th. Nominees will be selected by April 16th.

The USNCO competition will be on April 25 – May 3, 2020.

USNCO MARYLAND URL: http://www.beatricesalazarusncocoordinator.webs.com

Chemists Celebrate Earth Day

An Invitation to Celebrate Earth Day
with the Maryland Section of the American Chemical Society

April 20, 2020

Coordinator Beatrice Salazar

The Maryland Section of the American Chemical Society will have a tour of the Montebello Water Filtration Plant-I in Baltimore

The tour is designed for high school students, the scientific community and university and college students to learn the chemistry involved in the treatment and purification of surface water to produce safe drinking water. The tour includes the history of the plant. It was built in 1915, due to public health concerns, disease and deaths. The community's health improved after cleaning water was used for domestic consumption. The tour includes an explanation of the water sources, the reservoirs in the Chesapeake area and the clean water distribution network.

In addition, a visit to the facilities showing the different steps in the process of water treatment with emphasis on the chemicals added and the chemical reactions that occur during water treatment. Instructional material is available for students and their chemistry teachers involving the chemical reactions that take place as different chemicals are added to water. We also include a discussion of the byproducts formed and the potential harm of these byproducts. All high schools in the Baltimore area are invited please make a reservation.

http://www.acsmarylandevents2016.webs.com/

In addition, this STEM resource is available in an
Engineering APP to learn about Engineering projects nationwide:

http//www.repicture.com

CHEMISTRY IN THE LIBRARY

50th Anniversary of Earth Day

Ages 7 & up (7-8 year olds must be accompanied by an adult); 60 min. Registration required.

Savage Branch	Saturday, @ 2 PM, 14 Mar
Central Branch	Saturday, @ 2 PM, 21 Mar
Glenwood Branch	Saturday, @ 2 PM, 28 Mar
Eldersburg Branch	Saturday, @ 1 PM, 04 Apr
Elkridge Branch	Saturday, @ 2 PM, 11 Apr
East Columbia Branch	Saturday, @ 2 PM, 18 Apr
Miller Branch (for Adults & Families)	Wednesday@7 PM, 22 May
Miller Branch:	Saturday, @ 2 PM, 25 Apr
Jarretsville Branch	Saturday, @ 2 PM, 02 May
APG Discovery Center*	Saturday, @ 2 PM, 09 May
Light Street Branch	Saturday, @ 2 PM, 16 May
Govans Branch	Saturday, @ 2 PM, 11 Jul

* Ripkin Stadium

To register for programs, please see website of appropriate library website:

- Howard County Library System https://hclibrary.org/
- Enoch Pratt Free Library https://www.prattlibrary.org/
- Carroll County Public Library https://library.carr.org/
- Harford County Public Library https://www.prattlibrary.org/

CONTACT:

Rose A. Pesce-Rodriguez, rose.a.pesce-rodriguez.civ@mail.mil

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- **Contacting the National ACS membership division: 800-333-9511 (US only)** or service@acs.org

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