

The Reaction Times

VOLUME III

MAY 2019

Spring Edition

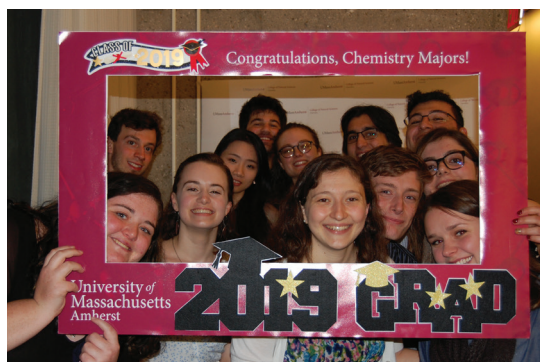
Congratulations, 2019 Senior Chemistry Majors!



Spring 2019
Gisele Andree
Jean Arnaud
Benjamin Avramidis
Allison Burke
Dominique Carey
Sara Chedid
Christopher Chinman
Alexander Demokritou
Bianca Edozie
Nicolas Gupta
Jessica Jones
Kyle Koczera
Mark Leon-Duque
Zhaoxia Li
Madison Montagna
Amber Nehring
Julie Novelli
Francisca Perez
Alexandra Sahagian
Alexander Santoro
Dana Sebestyen

Fall 2019
Minji Kim
Xavier Sanchez-Felix
Andreas Valle

BS Concentration in
Chemistry
Tushar Bahl
Richard Maxson



Vicki Hubby Wins CNS Outstanding Staff Award

The CNS Outstanding Staff Award recognizes the crucial role played by staff members in facilitating the success of the College of Natural Sciences. As the Business Manager for the Chemistry Department, Vicki Hubby is responsible for managing the department's instructional and general operating budget. The new glassware for the organic labs, those amazing new instruments in the upper level labs, events honoring our wonderful students, graduate student fellowships—she figures out how to pay for all of it! Vicki also sets up laboratory startup funds for new faculty and helps faculty manage budgets from external and internal grants. If it's related to purchasing, budgets, and balances, Vicki knows how to do it. Her responsibilities are very significant undertakings, given that our student enrollments and faculty research funding has more than doubled in the last 10 years. The scale of the operation in the Chemistry Department has increased dramatically since Vicki arrived in 1999, and she has met the challenges with incredible ability, creativity, and grace. Congratulations, Vicki!



The impetus for *The Reaction Times* newsletter was a series of discussions members of the Equity & Diversity Committee had with undergraduates, graduate students, postdocs, faculty, and staff, who indicated that they would like to learn more about others in the UMass Chemistry community.

2019 Undergraduate Award Winners

Academic Awards

American Chemical Society (ACS) Hach Scholarships

Olivia Pietrobuono and George Ryan

ACS Undergraduate Award in Analytical Chemistry

Ryan Thai

CRC Press Chemistry Achievement Award

Laura Casey, Ethan Goulart, and Obinnaya Okereke

Edward Shapiro Fund

Allison Burke, Nicholas Heller, Samuel Knight,
Mark Leon-Duque, and Ryan Pham

George R. Richason, Jr. Scholarship

Bryanna Lexus Freitas

Jay A. Pirog Scholarship

Eliadine Desir

John A. Chandler Memorial Scholarship

Yankai (Mark) Xiang

Robert Maxwell Williams Memorial Scholarship

Jacob Carroll, Sinclair Emans, and Jennifer Marino

Royal Society of Chemistry Certificate of Excellence

Ryan Thai

Thomas R. "Casey" Stengle Scholarship

Olivia Pietrobuono

Research Awards

ACS Undergraduate Award in Inorganic Chemistry

Ruby Nelson

ACS Undergraduate Award in Organic Chemistry

Francisca Perez

ACS Undergraduate Award in Physical Chemistry

Tristan Heck

Chemistry Undergraduate Research Fund

Samuel Stroup

Dr. Uche Anyanwu Memorial Fund

Gisele Andree

Benjamin Avramidis

Tiernan Kennedy

J.F.B. Fund for Undergraduate Research

Taylor Garrey

Mr. Tompkins Award

Cameron Kaminsky and Mark Leon-Duque

Oliver Zajicek Memorial Scholarship Award

Sara Chedid

Professor Jack Ragle Endowed Fund in Chemistry

Tristan Heck

Roger G. Bates Chemistry Fund

Gillian Willcox

Sir Harold W. Kroto and Steve F.A. Acquah GEOSSET Award

Dominique Carey

Tarselli Family Research Award

Tiernan Kennedy and Jason Biundo

Departmental Awards

ACS-Connecticut Valley Section Student Award

Mark Leon-Duque

American Chemical Society Membership Awards

Luke He

Tiernan Kennedy

American Institute of Chemists Award

Gisele Andree

Departmental Recognition Award

Gisele Andree

Sara Chedid

Distinguished Undergraduate Instructor Award in Honor of Earl J. McWhorter and George R. Richason, Jr.

Lara Al-Hariri

Distinguished Graduate Teaching Assistant Award in Honor of George R. Richason, Jr.

Yanfeng Li

Distinguished Undergraduate Teaching Assistant Award in Honor of George R. Richason, Jr.

Luke He

Positron Award

Gisele Andree

Richard W. Fessenden Award

Gisele Andree

Senior Class Award

Gisele Andree



Senior & Awards Dinner



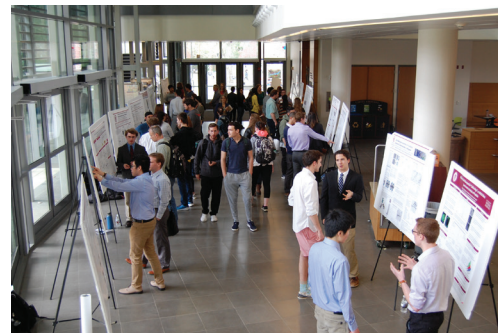
Senior Reception



Undergraduate Research Poster Award Winners

The Dr. Uche Anyanwu Memorial Fund recognizes the top three posters by chemistry majors. It was established by Dr. Ucheoma O. Akobundu to honor her late husband, who was a former graduate student of DV.

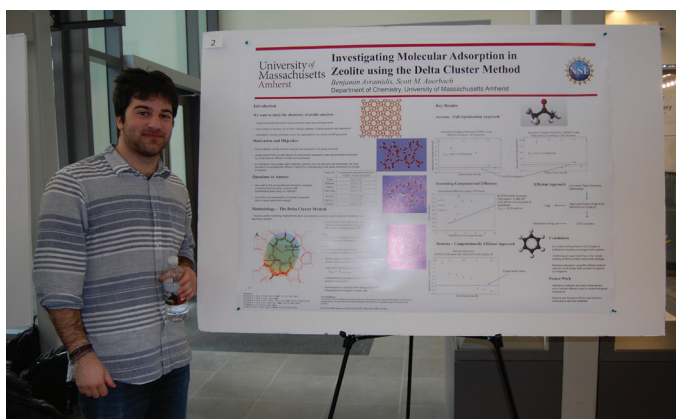
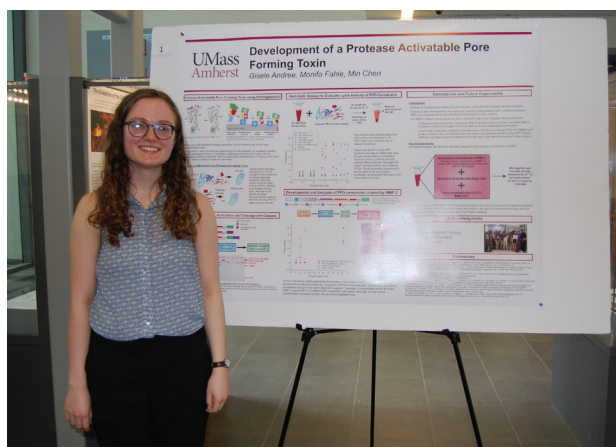
Of the sixteen posters presented in the ISB atrium this year, the three award recipients were Gisele Andree, Benjamin Avamidis, and Tiernan Kennedy.



Development of a Protease Activatable Pore-forming Toxin

by Gisele Andree

Cancer is an incredibly difficult disease to treat as it will often evolve and advance beyond the initial treatment methods; thus, finding new ways to eradicate cancer cells is tremendously important. The development of protease activatable pore forming toxins that target cancer cells is one way to tackle this problem. Using the cytolysin, perfringolysin O (PFO), large proteins are attached to the C-terminus of PFO thus inhibiting its normal cytotoxic activity. These inhibitor proteins are attached via an amino acid linker that contains a cleavage sequence of a specific protease. Once in the presence of this protease, the inhibitor proteins are cleaved off and PFO can regain its cytotoxic ability. Constructs can be designed to only be activated by proteases that are over-expressed and secreted from cancer cells, so these proteins would only be toxic towards these types of cells. My studies with Prof. Min Chen aim to develop a PFO-fusion protein that can be cytotoxically activated through proteolysis by matrix metalloprotease-2 (MMP-2), a protease overexpressed and secreted in many types of cancers. Different protease-activatable PFO-fusion proteins were designed using green fluorescent protein (GFP) and maltose binding protein (MBP) as the inhibitor proteins and the cytotoxic activities of cleaved and un-cleaved constructs are tested via hemolytic assays.



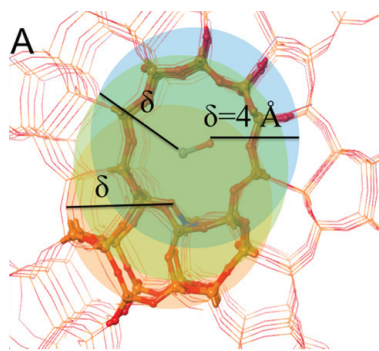
Using a Cluster Method to Computationally Describe Adsorption Processes in HZSM-5 Zeolite

by Benjamin Avamidis

Zeolites are solid, nanoporous crystal-structured aluminosilicate catalysts that are used widely in industry as aids in processing and separating fuel from crude oil. Given our society's insatiable hunger for energy as well as the restrictions and faults associated with the burning of fossil fuels, our lab focuses on the possible contributions zeolites may have in synthesizing reusable green biofuels. To investigate this possibility, we use computers to aid in the heavy quantum computations required to model interactions occurring within

zeolite pores which eventually produce biofuel precursors. A question concerning computational chemists when faced with modeling a large system like zeolite is, "How many atoms do we include in our model?" My role as a researcher in Prof. Scott M. Auerbach's group has been to ask that same question in regard to single molecule adsorption within HZSM-5 zeolite.

The adsorption process, taken to be the energy associated for a molecule to sit comfortably within a pore, is arguably the most important step in all zeolite catalysis. Utilizing a previously developed cluster method, the atoms required to properly describe adsorption are determined to be the adsorbate molecule and the few essential atoms involved at the zeolite active site. By having each atom emit a sphere of radius δ chosen by the user, the surrounding atoms of zeolite which fall within collective spheres determine which atoms represent the model. The importance of this method lies within the idea that by systematically increasing δ , we eventually reach a point where energy change is independent of δ , therefore obtaining the least number of atoms required to describe our system. Our hope is that this delta cluster method will make computation of adsorption processes easier, saving time and computational resources.



A schematic of how the delta cluster algorithm works. A δ -distance (Å) is chosen by the user and spheres of specified δ -radius encapsulate the zeolite atoms which are considered in the model. Zeolite atoms that fall within overlapping spheres are chosen.

A. N. Miguez, Q. Sun, S. Vaitheeswaran, W. Sherman, S. M. Auerbach, *J. Phys. Chem. C* **2018**, 122(40), 23230–23241.

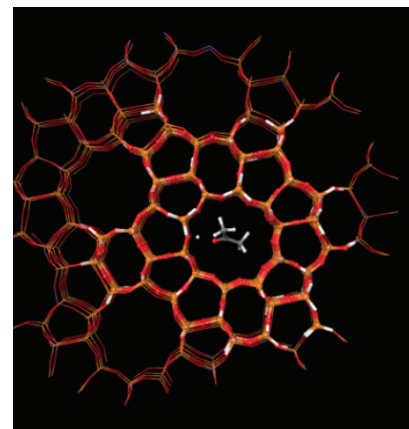


Image of a 9.5 Å delta cluster superimposed on the original master cluster which is used to carve out specified delta clusters. Highlighted atoms make up the 9.5 Å cluster.

DNA-Mediated Assembly of Bacterial Chemoreceptor Complexes

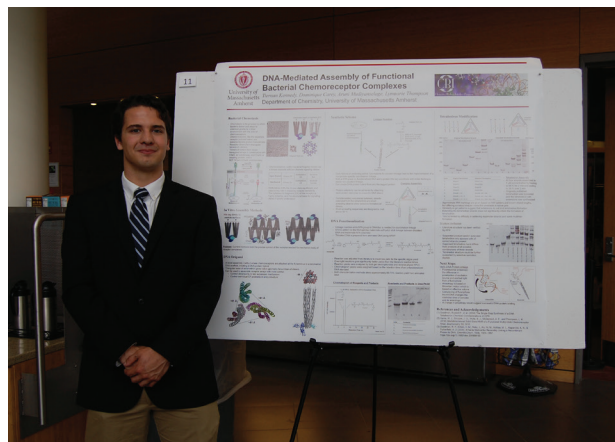
by Tiernan Kennedy

Our research in the Thompson Lab focuses on uncovering the signal propagation mechanism in bacterial chemotaxis receptors. This highly conserved class of transmembrane proteins binds attractant



Figure 1.

and repellent ligands and in turn controls the activity of the bacterial flagellar motor, but the physical mechanism for the process is poorly understood. However, our research is complicated by the fact the chemoreceptors form highly complicated signaling arrays that are difficult to replicate and control in vitro.



Over the past year and a half, I have worked toward developing a novel in vivo assembly of these receptor complexes using a DNA origami scaffold. We believe that attaching our protein complexes to the base of a DNA tetrahedron will provide the control over receptor geometry needed to test some of our most critical hypothesis. To date I have optimized a key DNA modification reaction needed to attach the tetrahedron to our protein and have shown that the necessary DNA origami scaffold can be synthesized. We hope that when this assembly method is completed it will provide the control needed to gain a much deeper understanding of our protein. Figure 1 shows our proposed assembly constructs. Attaching protein dimers to the vertices of a DNA tetrahedron (top) provides native-like trimers-of-dimers of chemoreceptors. Each protein dimer is depicted in gray with accessory proteins for complex formation in blue and teal.

Graduate Student Awards

Riddha Das Wins People's Choice Award in Three Minute Thesis Competition

Graduate student Riddha Das was one of ten finalists in this year's Three Minute Thesis Competition and won the People's Choice Award for her presentation "Nanoparticles: New Weapons to Combat Cancer." In a general audience talk, she described her PhD research with Prof. Vincent Rotello on developing techniques to use nanoparticles to selectively deliver a protected form of an anti-cancer drug to tumor cells, and then activate the drug. This greatly reduces the harmful side effects of chemotherapy. <https://www.umass.edu/gateway/feature/three-minutes-genius>



Faculty Achievements

Our outstanding faculty continue to be recognized for their contributions and achievements, including:

Trisha Andrew was selected to present the Kavli Foundation Emerging Leader in Chemistry Lecture at the ACS National meeting. (<https://www.acs.org/content/acs/en/pressroom/newsreleases/2019/march/kavli-lectures-smart-garments-for-sensing-human-behavior-and-the-search-for-extraterrestrial-life.html>)

Lara Al-Hariri was awarded a Senior Lecturer Professional Improvement Fellowship for Fall 2019.

Lila Gierasch was elected to the National Academy of Sciences and received the Merrifield award for her outstanding contributions to peptide science.

S. "Thai" Thayumanavan was awarded the Mahoney Life Sciences Prize for his paper "Shrink-wrapped Proteins as Next Generation Biologics" and received the Distinguished Graduate Mentor Award from the UMass Graduate School.

Gabriela Weaver has been named American Council on Education Fellow for 2019-2020.

Richard Vachet won the College of Natural Sciences Outstanding Research Award.

Mingxu You won a Sloan Research fellowship and received a CAREER Award from the National Science Foundation.

New Staff

Laura Sedberry is the Seminar/Safety/Alumni Coordinator for the Chemistry Department and Co-receptionist for the main office. She works with seminar faculty and student hosts, speakers, and many others to ensure the weekly seminars run smoothly. She also helps with donor thank you letters, follows up with those whose safety trainings are due, and much more.

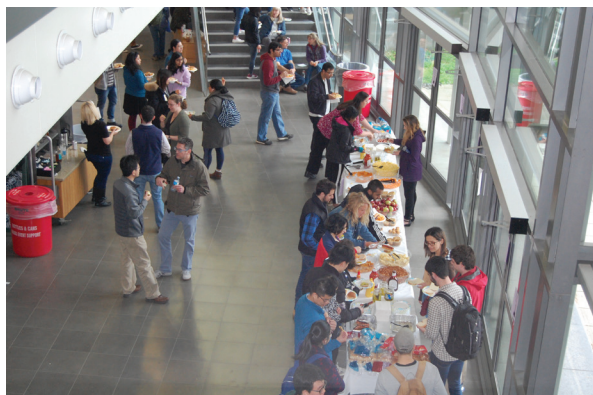
Laura recently moved from Indiana with her husband and two cats. She obtained a BS in Business Management and a Master's in Social Work from Indiana University-Purdue University Indianapolis. She has previously worked as a therapist to children and families and in office roles for non-profits and small organizations. Laura is excited to be a part of the Chemistry Department and loves the energy of being in an academic setting!

Sovann-Malis Loeung is the Program Coordinator for the NIH-funded Chemical-Biology Interface Training Program (CBI) and the Biotechnology Training Program (BTP). In addition to organizing events such as the CBI Chalk Talks and Biotech tAles, she helps with grant renewal preparation, compiles trainee applications for review, and prepares graduate student appointments. Previously, she was an Administrative Assistant in the College of Education and earned a Bachelor's degree in Social Justice Studies from University Without Walls in 2017. She has enjoyed interacting with the graduate students and faculty in CBI and BTP!

Pi(e) a Professor



Chemist(r)y's Cake & Coffee Social and the Departmental BBQ



Building Bridges Art Exhibit Spring 2019

The Building Bridges <https://www.umass.edu/diversity/building-bridges> Showcase event was held April 9 in the Fine Arts Center atrium, and featured visual arts, poetry and music from artists across campus, including art by Chemistry's own Karen Hakala, Marvin Ellin, Margaret MacDonald (retired), and music by Julian Tyson (chemistry), and John Donoghue (physics).



John Donoghue and Julian Tyson



Violet Sabrewing (above) and Blue-Crowned Motmot (below) both photographed by Marvin Ellin while in Costa Rica



Karen Hakala's mixed media piece came about as a result of a talk she heard about St. Jane Frances de Chantal and her memoir in which she discusses the 'Martyrdom of Love.'



Watercolor rooster by Margaret MacDonald

"The beauty of nature inspires me to paint and embrace the challenge of recreating it with watercolor."

Physical Sciences Building Ribbon Cutting

The PSB ribbon cutting ceremony included speeches by Governor Charlie Baker, State Senator Jo Comerford, State Representative Mindy Domb, as well as UMass system President Martin Meehan, Trustee Mary Burns, UMass Amherst Chancellor Kumble Subbaswamy, CNS Dean Tricia Serio, and Chemistry Head Richard Vachet.



Editorial staff: Amanda Bennett, Christie L. C. Ellis, Ricardo Metz, and Mahdiah Yazdani. Design and editing: Brigette McKenna

Thank you to everyone who sent in accomplishments and story ideas. Please email comments, achievements, and ideas for our next issue to reaction-times@chem.umass.edu.