The New Haven Local Section of the American Chemical Society Presents The Third Annual Student Research Symposium

Saturday, April 28, 2018

Hosted by Quinnipiac University Department of Chemistry & Physical Sciences

Open to Graduate and Undergraduate Students



http://newhaven.sites.acs.org

Symposium Schedule

8:15 - 9:00 Registration Main Lobby Welcome and introductions 9:00 - 9:10 MNH 105 9:10 - 10:00 Keynote speaker MNH 101 (Auditorium) 10:00 - 10:15 Break **MNH 105 Oral presentations** 10:15 - 11:40 MNH 101 (Auditorium) 11:45 - 12:30 Lunch **MNH 105** 12:30 - 1:30 **Poster Session** MNH 105 Awards ceremony 1:45 - 2:00 MNH 101 (Auditorium) 2:00 Symposium close

Keynote Speaker Professor Vincent T. Breslin Southern Connecticut State University

Factors Controlling the Distribution of Contaminant Metals in Connecticut Coastal Harbors

Since 2001, Werth Center for Coastal and Marine Studies student and faculty researchers have collected and analyzed the chemical and physical characteristics of surface sediments from fourteen Connecticut harbor and river estuaries. The goal of this research was to conduct a high spatial resolution sampling within each harbor to determine factors contributing to variations in sediment composition and metal contamination. Harbors examined in this study represent a range of demographics, land use, urbanization and industrialization, and are geographically located in eastern Long Island Sound.

Sediment metal concentrations (iron, copper, zinc, arsenic, cadmium) were determined using flame or graphite furnace atomic absorption spectrometry following acid digestion using US EPA Method 3050B. Mercury analyses were performed on sediment directly using a DMA-80 mercury analyzer.

Measured sediment metal concentrations within each harbor are highly variable, and for many harbors, crustal abundances of contaminant metals are exceeded by 5-20 fold of natural abundances. Sediment organic carbon content (loss on ignition), mean grain-size and iron content are strongly correlated with metal concentrations in all harbors/rivers studied. Knowledge of the spatial variation of contaminant metals within harbors is important for assessing current and future impacts to commercial activities and living marine resources.



Biography:

Vincent T. Breslin, Professor of the Environment, Geography and Marine Sciences at Southern Connecticut State University (SCSU), teaches undergraduate courses in Marine Studies, Environmental Studies, the SCSU Honors College, and the graduate Environmental Education MS program. Dr. Breslin received the J. Phillip Smith Award for Outstanding Teaching at SCSU and was elected a SENCER Leadership Fellow for his work in science and civic engagement. He is co-founder and coordinator of the Connecticut State Colleges and Universities Werth Center for Coastal and Marine Studies that promotes Marine Science Study especially having to do with the Long Island Sound environment. Dr. Breslin's laboratory research and field-based studies examine the biogeochemical behavior of contaminant metals in coastal sediments. His research studies have been important in understanding the spatial distribution of contaminant metals in Connecticut harbors and the potential accumulation of these metals in living marine resources.

Corporate Sponsors



Gaussian, Inc. Gaussian.com



Contor Colburn LLP www.cantorcolburn.com

Oral Presentations

Time	Authors	Academic Institution
10:15 - 10:35	David Stevens Exploring the Role of the Third Active Site Meta Eta with Quantum Mechanical/Molecular Mech Simulations.	2
10:35 - 10:55	Daria Kim & Suzanne Szewczyk Joint Safety Teams and Safety Culture.	Yale University
10:55 - 11:15	Yue Qian Enhanced Monte Carlo Methods for Modeling Pr Energies of Binding Calculations.	Yale University oteins and Absolute Free
11:15 - 11:35	Stefanie Kickinger Elucidating the Molecular determinants for the Betaine/GABA Transporter 1 (BGT1) Inhibitors.	
11:35 - 11:55	Nicole Langlois Progress Towards the Synthesis of Cadiolides an	University of New Haven ad Analogs.

Poster Presentations

Number	Presenter Academic Institution
1	Isaac Wendler Yale University Kinematic and Thermodynamic Effects of 3-10 Helical Dipole on PCET.
2	Joshua Green Southern Connecticut State University A Comparison of Acid Digestion Methods for Marine Sediment to Optimize Metal Recovery.
3	Melissa JagrosseSouthern Connecticut State UniversityApplication of Ketones in Petasis Reaction for the Synthesis of Amino Acids andOther Novel Molecules.
4	Jessica Freeze Yale University What is Safety Culture – Chemistry Joint Safety Team.
5	Cory WilliamsSouthern Connecticut State UniversitySynthesis and Antibacterial Assessment of Oxazaborolidine Derivative.
6	Brandon Miller University of New Haven Studies Toward the Total Synthesis of Spiromastixone J.
7	Justin Pantano University of New Haven Progress Towards the Synthesis of Usnic Acid and its Analogs.
8	Julia Harrison Southern Connecticut State University Stereoselective Synthesis of Amino Acids.
9	Alexandra Goriounova University of New Haven Collection and Chemical Analysis of Micrometeorites.
10	Yo Ng University of New Haven The Effect of Solar Eclipse on Ground Level Ozone Concentration.
11	Imran TariqQuinnipiac UniversityAn Electrochemical Investigation into the Unorthodox Redox Properties of Gadolinium Bridged Polyoxometalates.

12	Amanda Fawver Fish DNA Barcoding	Southern Connecticut Sate University
12	Kolly Kruyeman	Quinniniac University

- 13Kelly KruysmanQuinnipiac UniversityOptimizing Expression and Purification of a Cytoskeletal Protein from
Archaea.
- 14Mikayla MclaughlinSouthern Connecticut State UniversityIsolation and Characterization of Potential Antibiotic Compounds.

Abstracts: Oral Presentations

Presentation #1

Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase Eta with Quantum Mechanical/ Molecular Mechanical Free Energy Simulations

David Stevens (Yale University)

david.stevens.drd73@yale.edu

Human DNA polymerase η (Pol η) is an enzyme involved in the repair of DNA mutations that cause skin cancer. Recent experimental work suggests that a third Mg2+ ion plays an essential catalytic role, in addition to two well defined Mg^{2+} ions that align the active site for catalysis. These experiments were interpreted to imply that this metal ion enters the active site prior to the phosphoryl transfer reaction. In addition, a specific hydroxyl group has been proposed to protonate the pyrophosphate leaving group. We investigate this reaction mechanism using quantum mechanical/molecular mechanical (QM/MM) free energy simulations that combine a finite temperature string method with umbrella sampling. Our simulations address these key issues by providing critical information regarding the impact of the transient third metal on the reaction mechanism and the proposed proton transfer. The results provide evidence that the third metal ion not only acts as a shuttle for the pyrophosphate leaving group, but also thermodynamically drives the phosphoryl transfer reaction. Moreover, the simulations suggest that the presence of this third metal ion prevents the proposed proton transfer reaction to this leaving group.

Presentation #2

Joint Safety Teams and Safety Culture in Academia

Daria Kim & Suzanne Szewczyk (Yale University) daria.kim@yale.edu & suzanne.szewczyk@yale.edu

The Joint Safety Team (JST) is a group of graduate students and post-doctoral fellows that work with the Department of Environmental Health and Safety (EHS) and the Department of Chemistry to cultivate a culture of safety. The main goals of the JST are to improve the safety awareness and literacy in chemical laboratories, provide safety related skills and resources to assist researchers, and establish a

network of communication. Recently, the JST has developed a system to collect and curate near miss reports. A near miss is an incident that does not cause serious injury or property damage. Near misses occur much more often than more serious accidents and are therefore a better resource for safety precautions. Other endeavors include a database of safety moments, resources for safety officers, and informational safety posters. The JST hosts a number of safety events each year in collaboration with the EHS including safety talks given by faculty, instructional laboratory safety walkthroughs for first-year students, a summer field trip to an industry sponsor, and a large safety event where students, post-doctoral fellows, and faculty can watch laboratory safety demos, obtain PPE, participate in fire extinguisher training, and more.

Presentation #3

Enhanced Monte Carlo Methods for Modeling Proteins and Absolute Free Energies of Binding Calculations

Yue Qian (Yale University)

yue.qian@yale.edu

In this study, an Monte Carlo (MC) statistical mechanics algorithm is presented to explore the protein-ligand conformational space with emphasis on the motions of the protein backbone and side chains. The parameters for each MC move type were optimized to better reproduce conformational distributions of 18 dipeptides and the well-studied T4 lysozyme L99A protein. Next, the performance of the improved MC algorithms was evaluated by computing absolute free energies of binding for L99A lysozyme with benzene and seven analogs. Results for benzene with L99A lysozyme from Molecular Dynamics (MD) and the optimized MC protocol were found to agree within 0.6 kcal/mol, while a mean unsigned error of 1.2 kcal/mol between MC results and experiment was obtained for the seven benzene analogs.

Presentation #4

Elucidating the Molecular determinants for the subtype-selectivity of Betaine/GABA Transporter 1 (BGT1) Inhibitors

> Stefanie Kickinger (Yale University) stefanie.kickinger@yale.edu

As a member of the GABAergic system, the GABA transporters (GATs) play a critical role in the regulation and termination of the GABA-mediated signaling as they function as key proteins in neurotransmitter uptake. We have previously identified 2-amino-1,4,5,6-tetrahydropyrimidine-5-carboxylic acid (ATPCA) as the most potent substrate-inhibitor of the betaine/GABA transporter 1 (BGT1) reported to date. In order to characterize the molecular basis of GABA-transporter subtype selectivity, a series of ATPCA analogues were synthesized and pharmacologically characterized in radioligand-based uptake assays at the four human GABA transporters (hGATs) recombinantly expressed in mammalian cells. Overall, the analogues retained subtype-selectivity for hBGT1, though with lower inhibitory activities compared to ATPCA. Further characterization of five BGT1-active analogues in a fluorescence-based FMP assay revealed that the compounds are substrates for hBGT1, suggesting that they interact with the orthosteric site of the transporter. In silico-guided mutagenesis experiments showed that the nonconserved residues Q299 and E52 in hBGT1 potentially contribute to the subtypeselectivity of ATPCA and its analogues. Computational docking studies and molecular dynamics simulations suggested that these residues form stable hydrogen bonds with the guanidine or amidine moieties of ATPCA and its derivatives. Overall, this study provides new insights into the molecular interactions governing the subtype-selectivity of BGT1 substrate-inhibitors.

Presentation #5

Progress Towards the Synthesis of Cardiolides and Analogs

Nicole Langlois (University of New Haven) nlang3@unh.newhaven.edu

Cadiolides are a class of marine natural products that have been found to possess antibacterial potency against the growth of Methicillin-Resistant Staphylococcus aureus (MRSA) at minimum inhibitory concentrations similar to, or lower than current leading antibiotics. The mechanism by which these structures act to kill or inhibit bacterial growth, and the extent of their potency in other applications, have not been elucidated at this time. In order for such studies to be conducted, a costeffective and efficient synthesis must be accomplished and scaled up to yield multigram quantities of the cadiolides. Our research was designed in order to make progress toward an efficient, simple synthesis of the cadiolides and analogous structures to allow for further studies to reveal their potential as antibiotics. The method involves the utilization of an acylated Meldrum's acid adduct to form the initial step toward the key intermediate structures. This allows for the use of costeffective reagents in a relatively simple fashion. The synthesis examined follows a six-step process toward the production of Cadiolide B – a basic form among the most potent of the cadiolides. The synthetic route studied is unique in that it allows for two major points of divergence for creating a variety of analogs, differing in the presence of solubilizing groups on the aromatic rings to enhance positive "drug-like" characteristics. We have succeeded in completing reactions toward the synthesis of Cadiolide B, with confirmation pending further analytical data. Currently the project has moved toward the synthesis of cadiolide analogs to explore structure alterations and to generate a potential library of compounds to submit for assessment of antibacterial activity.

Abstracts: Poster Presentations

Poster #1

Kinematic and Thermodynamic Effects of 3-10 Helical Dipole on PCET

Isaac Wendler (Yale University) isaac.wendler@yale.edu

Proton-coupled electron transfer (PCET) reactions are a class of chemical redox reactions in which a proton and electron move simultaneously or with some degree of synchrony. Oftentimes, the PCET reactions are more favorable than the stepwise transfer of electrons and proton. This advantage is utilized extensively in biology, and PCET reactions are prevalent in enzyme action, cellular respiration, and photosynthesis. A key question in biological PCET research is how protein and enzyme structure affect PCET reactions. A particular protein secondary structure, alpha-helices, have been thought to play a key role in many protein functions, and much of that control has been attributed to the presence of an overall dipole, with negative charge on the C-terminus and positive charge on the N-terminus. No studies have explored how an alpha-helix dipole effects PCET reactions. We hypothesize alpha-helix dipoles could be used in biology to fine-tune a PCET reaction occurring in an enzyme. I am synthesizing small alpha-helix models to eventually measure the effect of the helical dipole on the kinetics and thermodynamics of a PCET reaction. These studies may inform how biology controls this important class of reactions. My project focuses on the kinetic and thermodynamic effects of a helical dipole on a PCET reaction. More specifically, I plan to determine the kinetic and thermodynamic character of a PCET reaction involving a substituent attached to the N-terminus of an alpha-helical peptide and compare these results to a similar PCET reaction involving the same substituent in solution, unaffected by a helical dipole.

A Comparison of Acid Digestion Methods for Marine Sediment to Optimize Metal Recovery

Joshua Green (Southern Connecticut State University) joshuagreen1444@yahoo.com

Students and faculty of the Werth Center for Coastal and Marine Studies at Southern Connecticut State University have been examining the trace metal contamination in sediment in coastal embayments along the Connecticut coastline. Since 2001, the spatial variation in sediment trace metals has been determined in thirteen harbors. Researchers have employed a nitric acid-hydrogen peroxide wet digestion protocol for the extraction of metals from harbor sediment (US EPA Method 3050B). Elements including copper, iron, zinc, cadmium and arsenic yield recoveries exceeding 85% compared to values certified for NIST SRM 2702 Estuarine Sediment. The HNO3-H2O2 digest is not a total sediment digest. Hydrofluoric acid would need to be employed to achieve a total acid decomposition of the sediment. As such, many elements are not fully recovered from the sediment including chromium, lead, nickel and manganese. Recoveries for these elements using the USEPA Method 3050B in our laboratory range from 55-75%. Recent work by Winters et al., 2013 suggests that trace metal recoveries from estuarine sediment may be improved by using closed vessel systems and optimizing acid ratios. This study seeks to develop a closed system sediment digest protocol using combinations of nitric acid, hydrochloric acid, hydrogen peroxide, and perchloric acid to increase trace element recoveries from estuarine sediment. Recoveries of elements using modified digest protocols will be assessed using recoveries for NIST SRM 2702 estuarine sediment and also compared to current digest recoveries for US EPA Method 3050B used in our laboratory.

Poster #3

Application of Ketones in the Petasis Reaction for the Synthesis of Amino Acids and Other Novel Molecules

Melissa Jagrosse (Southern Connecticut State University) jagrossem1@southernct.edu

Multicomponent reactions have received significant attention from the organic chemistry community as a means to synthesize a diverse range of products in an economically and environmentally efficient fashion. The Petasis reaction is one such example of a multicomponent reaction and involves a vinyl- or arylboronic acid, an amine, and an aldehyde as the reagents. In principle, the carbonyl component can also be a ketone instead of an aldehyde, however only a few scattered examples of this kind have been reported in the literature to date. This research seeks to investigate the scope of the Petasis reaction using ketone substrates with a variety of different boronic acids and amines. In particular, we report the synthesis of a novel Petasis product in 67% isolated yield and several related examples in somewhat lower yield.

Poster #4

What is Safety Culture – Chemistry Joint Safety Team

Jessica Freeze (Yale University) jessica.freeze@yale.edu

The Joint Safety Team (JST) is a group of graduate students and post-doctoral fellows that work with the Department of Environmental Health and Safety (EHS) and the Department of Chemistry to cultivate a culture of safety. The main goals of the IST are to improve the safety awareness and literacy in chemical laboratories, provide safety related skills and resources to assist researchers, and establish a network of communication. Recently, the JST has developed a system to collect and curate near miss reports. A near miss is an incident that does not cause serious injury or property damage. Near misses occur much more often than more serious accidents and are therefore a better resource for safety precautions. Other endeavors include a database of safety moments, resources for safety officers, and informational safety posters. The JST hosts a number of safety events each year in collaboration with the EHS including safety talks given by faculty, instructional laboratory safety walkthroughs for first-year students, a summer field trip to an industry sponsor, and a large safety event where students, post-doctoral fellows, and faculty can watch laboratory safety demos, obtain PPE, participate in fire extinguisher training, and more.

Poster #5

Synthesis and Antibacterial Assessment of Oxazaborolidine Derivatives

Cory Williams (Southern Connecticut State University) corywilliams528@gmail.com

Oxazaborolidine compounds are characterized as heterocyclic compounds containing a boron-nitrogen and boron-oxygen bond. These compounds are synthesized via the reaction between a boronic acid or boronic acid derivative, and a 1,2-amino alcohol. The first goal of this project was to synthesize, characterize, and purify these compounds. Once synthesized, the biological activity of these compounds was assessed.

Studies Toward the Total Synthesis of Spiromastixone J

Brandon Miller (University of New Haven) bmill8@unh.newhaven.edu

The Synthesis of Spiromastixone J was studied for two main aspects. The first being that Spiromastixone J has only been isolated in extremely low yield from Spriomastix sp. Fungus roughly 3,000 meters below sea level.1 The second is the molecule's antibacterial activity on Gram-positive bacteria and comparable inhibition of bacterial growth to commercial antibacterial drugs.1 These two factors combined make Spiromastixone J a practical target for organic synthesis. On the path to the synthesis of Spiromastixone J, our synthetic scheme highlighted three key intermediates. The first being a resorcilate derivative. Three synthetic pathways have so far been studied on the route to this intermediate. These pathways consist of three main themes: consecutive Claisen Condensations followed by ketene trapping and dehydration, the Diels-Alder 4+2 Cycloaddition and a pseudo-Robinson Annulation followed by elimination.3,4,5,6,7 The three outlined synthetic pathways have proven thus far to be ineffective at obtaining gram-scale quantities of the resorcilate intermediate. Further research is aimed at more recently reported Diels-Alder approaches in combination with Lewis Acid catalysis.

Poster #7

Progress Towards the Synthesis of Usnic Acid and its Analogs

Justin Pantano (University of New Haven) jpant3@unh.newhaven.edu

Usnic acid is a naturally occurring product that has antibacterial properties against Streptococci, Staphylococci, and Mycobacteria. Syntheses of usnic acid have traditionally been quite low yielding, but it's readily available by extraction from lichens. We attempted to synthesize usnic acid via the use of a template. Along the way, macrocyclic analogs could be made that could be candidates for biological testing as novel antibacterials. The first part of the synthesis was to synthesize large quantities of methyltrihydroxyacetophenone to use in later steps. Following that, the second part was the create the template, which could couple to the acetophenone derivative. The syntheses of the pieces of the template stalled due to not being able to meet reported standards for some reactions. Also investigated was the reaction of a readily synthesized analog of usnic acid (dehydrogenated usnic acid) and its reaction with various aldehydes to create new, more complex, and potentially bioactive molecules.

Poster #8

Stereoselective Synthesis of Amino Acids

Julia Harrison (Southern Connecticut State University) harrisonj6@southernct.edu

Synthetic amino acids have a wide range of use as pharmaceuticals. Of particular interest are a-amino acids, which have an amine and a carboxylic acid group attached to the same carbon. A subset of a -amino acids has a second R-group at the a-carbon in place of the hydrogen atom. These a,a-disubstituted amino acids have a variety of interesting biological properties. Despite their relatively simple structures, amino acids present significant synthetic challenges, specifically the selective installation of a stereocenter to obtain the desired compound as a single enantiomer. We are investigating nucleophilic additions to optically active N-sulfinylketiminoesters derived from the Ellman sulfinamide auxiliary. Numerous combinations have been tested by varying the ester group, substituent R-group, and the Grignard reagent. The best results were obtained when non-branched Grignard reagents were used with isopropyl and tert-butyl ester substrates.

Poster #9

Collection and Chemical Analysis of Micrometeorites

Alexandra Goriounova (University of New Haven) agori3@unh.newhaven.edu

Rain water and snowfall were collected in traps designed with piping and magnets. The optimal magnet to use in terms of strength and shape was determined from preliminary testing. The collection was done in order to obtain the micrometeorite pieces that are falling to the Earth's surface everyday and conduct chemical composition analysis on the collected micrometeorites. The focus was placed on metal alloy micrometeorites as they can easily be isolated from other materials by strong magnets and analyzed using chemical instruments available on campus. The physical appearance of the collected particles were examined using an optical microscope as a preliminary screening method for a spherical shape, size in the micrometer range, and relative hardness. Potential micrometeorite candidates were analyzed by X-Ray Fluorescence (XRF) and X-Ray Diffraction Crystallography (XRD)

instruments (both available at University of New Haven) for the iron and nickel content analysis and crystal structures to confirm their space origins. The potential candidates tested thus far have been excluded as micrometeorites thrugh instrumentation techniques, so further collection is being performed. Confirmed micrometeorites will be sent to Prof. Don Brownlee at University of Washington to be sliced by an Ultramicrotomy instrument for Transmission Electronic Microscope (TEM) analysis. We have involved K-12 students in the rainwater collection and optical microscope screening steps to broaden the impact of our project.

Poster #10

The Effect of Solar Eclipse on Ground Level Ozone Concentration

Yo Ng (University of New Haven) yng1@unh.newhaven.edu

High exposure of ground ozone could trigger or worsen health conditions. Ground ozone is created by chemical reactions between nitrogen oxides and volatile organic compound in the presence of solar radiation. As a result, the intensity of the solar radiation should have a significant impact on the ground ozone concentration. This project investigated the effect of solar radiation on the ground ozone concentration at the University of New Haven and other universities. A portable ozone monitor was deployed for such purpose. Periodical measurements were conducted at the University of New Haven's West Haven campus to study the ozone concentration in relation to UV index throughout the day. Periodical outdoor ozone measurements on campus revealed a diurnal trend, and the peak of ozone concentration was onehour later than that of the UV index. Ozone measurements were performed every minute during and after the solar eclipse event in Newark, New Jersey on August 21st, 2017. The processed data revealed that ozone concentration during the solar eclipse was significantly lower than that immediately after the eclipse. Such drastic change did not occur on the day after the eclipse. This research serves as a foundation of future studies on the impact of seasonal solar radiation on ground ozone concentrations.

An Electrochemical Investigation into the Unorthodox Redox Properties of Gadolinium Bridged Polyoxometalates

Imran Tariq (Quinnipiac University) iktariq@quinnipiac.edu

Polyoxometalates are complex inorganic ions self-assembled from multiple metals and oxygen. Electrochemical analysis of certain moieties in solution have demonstrated unusual redox properties. The investigation was to discern whether different cations or different proportional concentrations would affect the redox potential, which was tested using Cyclic Voltammetry. The actual samples tested were prepared using the polyoxometalate [P2W17061]10- bridged by Europium and Gadolinium. Previous testing has already demonstrated a shift in potential when the concentration of lithium and potassium ions has been varied, and research has been done verifying the importance of the pH of the solutions. The overarching goal of this investigation, and past research, is to identify what properties impact the redox potential of these complex ions and discern the optimal conditions to observe this phenomenon.

Poster #12

Fish DNA Barcoding

Amanda Fawer (Southern Connecticut State University) fawvera1@southernct.edu

The purpose of this project was to test different species of fish samples available to the retail market in New Haven and Fairfield County to identify there DNA code and see if the label that is given to the sample in the retail market is correct. This process was done using the polymerase chain reaction (PCR) to test to see if the DNA that was extracted from the sample was amplifiable by the COI gene-specific primers. If the band had appeared then the sample was sent for sequencing, once the sequencing was returned a bioinformatics assessment was done to obtain the genus and species of the sample. Out of the 25 samples that were sequenced and processed the 5 came back as mislabeled. The Zoarces gillii was one of the mislabeling found its origin comes from the Koreas and the yellow sea. The experiment yielded results that fish are being mislabeled by 20% in the retail market and the fish are coming from all over the world.

Optimizing Expression and Purification of a Cytoskeletal Protein from Archaea

Kelly Kruysman (Quinnipiac University) klkruysman@quinnipiac.edu

Archaea is a domain of single-celled prokaryotic organisms. These microorganisms can be extremophiles, meaning they can survive in harsh conditions such as extreme temperatures or acidity. Currently there is limited research about the cytoskeleton of Archaea compared to the cytoskeleton of eukaryotes and bacteria. One goal of this research was to find an actin homolog in Archaea and express it in E. coli. Actin is an important cytoskeleton protein in eukaryotes because it plays a significant role in cell structure and motility. Crenactin is an actin homolog that has many similarities to actin in eukaryotes. To study crenactin it first must be expressed in E. coli and then purified. Growth conditions for the cells are currently being optimized to determine what conditions express the most crenactin. After the cells grow at 37°C they are induced with a reagent abbreviated IPTG, which helps the cells focus on protein production rather than cell replication. Factors such as IPTG concentration, temperature after induction, and amount of time after induction are being studied to determine which conditions express the most crenactin that can be purified. Running SDS gels is a useful method to determine if crenactin is being expressed in the samples, or if it is being lost during the purification process. An affinity purification using the FPLC can be performed to isolate crenactin from other proteins. After crenactin is purified, the next steps would be to verify that it forms polymers and characterize the polymerized crenactin.

Isolation and Characterization of Potential Antibiotic Compounds

Mikayla Mclaughlin (Southern Connecticut State University) mclaughlinm7@southernct.edu

In the past, natural product screening has proven to be an effective method for finding new antibiotics. Most antibiotics in use today were found through this process. The problem being encountered now however, is the growing rate of drugresistance in pathogenic bacteria is diminishing the effectiveness of these drugs, creating a new urgency for novel drug discoveries. This research is an attempt to extract, isolate, and analyze novel compounds with antibiotic activity produced by bacterial strains provided by colleagues in the SCSU biology department. Three main steps are required for this process: First, extraction of compounds is carried out using multiple solvents of varying polarities. Next, the extracted components are separated by thin layer-chromatography and screened for the active compound via bioautography. Finally, analytical methods such as mass spectrometry and nuclear magnetic resonance spectroscopy are used to interpret the structure of the active compound.

Participants

Name

Institution

Email address

Adiel Coca Alexandra Goriounova Alexandra Savino Amanda Fawver Ana S. Newton Brandon Miller **Camille Solbrig** Carlos Quimbaya Chong Qiu **Cory Williams** Daniel Halloran Daria Kim Dave Stiwell David Stevens Dennis J. Jakiela Frank Gasparro **Gregg** Crichlow Imran Tariq Isaac Hon Isaac Wendler James K. Kearns James Kirby **Jane Snell Copes**

Southern Connecticut State University University of New Haven Yale University Southern Connecticut State University American Chemical Society University of New Haven American Chemical Society Southern Connecticut State University University of New Haven Southern Connecticut State University Albertus Magnus College Yale University Quinnipiac University Yale University Cantor Colburn LLP American Chemical Society Sacred Heart University **Quinnipiac University** Albertus Magnus College Yale University Southern Connecticut State University **Quinnipiac University** Science Outside the Box

cocaa2@southernct.edu agori3@unh.newhaven.edu alexandra.savino@yale.edu fawvera1@southernct.edu ana.newton@yale.edu bmill8@unh.newhaven.edu camsol@comcast.net rfermat39@gmail.com cqiu@newhaven.edu corywilliams528@gmail.com dhalloran@albertus.edu daria.kim@yale.edu dstil1355@yahoo.com david.stevens.drs73@yale.edu djakiela@cantorcolburn.com fgasparro@hamdenhall.org gregg.crichlow@gmail.com iktariq@quinnipiac.edu ihon@albertus.edu isaac.wendler@yale.edu kearnsj3@southernct.edu james.kirby@quinnipiac.edu profsepoc@scienceoutsidethebox.com

	Jenny Wahl	Quinnipiac University	jenny.wa
	Jerry Putterman	American Chemical Society	jerry_pu
	Jessica Freeze	Yale University	23jessic
	Jimmy Rogers	Yale University	james.m
	JiongDong Pang	Southern Connecticut State University	pangj1@
	Joshua Green	Southern Connecticut State University	joshuag
	Julia Harrison	Southern Connecticut State University	harrisor
	Justin Pantano	University of New Haven	jpant3@
	Kap-Sun Yeung	American Chemical Society	kapsun.
	Kelly Kruysman	Quinnipiac University	klkruysı
	Leela Dodda	Yale University	leela.do
	Maddie Hoffmann	Yale University	madelin
	Mahir Abouaassi	Albertus Magnus College	maboua
	Manette J. Macias	Hampford Research Inc.	mmaci2
	Maria-Elena Liosi	Yale University	maria-e
	Mark Buford	Unilever	mark.bu
	Matthew Hesson-	Illinois State University	doctor.n
	McInnis Max Reeve	American Chemical Society	maxreev
	Melissa Jagrosse	Southern Connecticut State University	jagrosse
	Natasha Shah	Quinnipiac University	natasha
	Naudin van den Heuvel	Yale University	naudin.v
	Oh Sang Kweon	Yale University	ohsang.l
	Olivier Nicaise	American Chemical Society	olivier.jo
	Pier Cirillo	University of New Haven	pcirillo@
Rajintha Bandaranayake Robert Collins		Quinnipiac University	rajintha
		Quinnipiac University	collins.r
Stefanie Kickinger		Yale University	stefanie
Suzanne Szewczyk		Yale University	23suzan
	Todd Ryder	Southern Connecticut State University	rydert1
	Toru Sato	Yale University	toru.sate
		-	

vahl@quinnipiac.edu utterman@hotmail.com ca.freeze@yale.edu n.rogers@yale.edu @southernct.edu green1444@yahoo.com nj6@southernct.edu @unh.newhaven.edu .yeung@bms.com sman@quinnipiac.edu odda@yale.edu ne.hoffmann@yale.edu aassi@albertus.edu 2@unh.newhaven.edu elena.liosi@yale.edu urford@unilever.com matthew@gmail.com eve@comcast.net em1@southernct.edu a.shah@quinnipiac.edu .vandenheuvel@yale.edu .kweon@yale.edu jc.nicaise@gmail.com @newhaven.edu a.bandaranayake@quinnipiac.edu r.e@gmail.com e.kickinger@yale.edu nne.szewczyk@yale.edu

rydert1@southernct.edu toru.sato@yale.edu

Vincent T. Breslin	Southern Connecticut State University	breslinv1@southernct.edu
Vladimir Moskalenko	University of New Haven	danosaursasha@gmail.com
Xiaoshen Ma	Yale University	xiaoshen.ma@yale.edu
Yo Ng	University of New Haven	yng1@unh.newhaven.edu
Yue Qian	Yale University	yueqian@yale.edu

Thank you!

A special thanks to:

The faculty and staff at the Quinnipiac University for hosting this symposium on your campus

All student presenters

The wonderful student volunteers

Our judging panel: Dennis Jakiela, Cantor Colburn LLP Robert Collins, Quinnipiac University Rajintha Bandaranayake, Quinnipiac University Mark Buford, Unilever Kap-Sun Yeung, American Chemical Society

Symposium Committee: Jim Kirby, Quinnipiac University Camille Solbrig, American Chemical Society Ana Newton, American Chemical Society Mark Burford, Unilever Max Reeve, American Chemical Society Dennis Jakiela, Cantor Colborn LLP Frank Gasparro, American Chemical Society