New York's American Chemical Society

69th Annual

Undergraduate Research Symposium

Of the Student Activities Committee

May 7th, 2022

ACKNOWLEDGMENTS

We would like to express our sincere thanks and gratitude to those institutions and individuals that have supported our continuing efforts:

Medgar Evers College

Dean of Science at Medgar Evers, Dr. Mohsin Patwary

2022 Chair, ACS NY Section, Dr. Kathleen Kristian

American Chemical Society

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The following deserve special recognition for the time and effort they have given to make this meeting possible:

Dr. Brian R. Gibney – NY ACS Webmaster
Sam Groveman, Zoom Coordinator – Medgar Evers College

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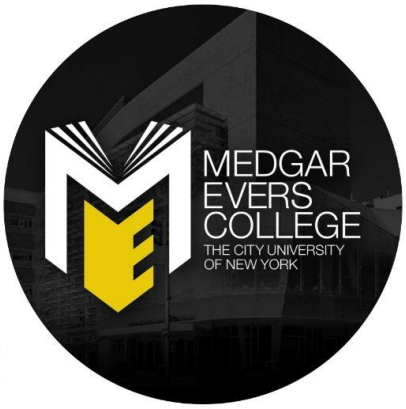

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CITY UNIVERSITY OF NEW YORK

May 7th, 2022


MEDGAR EVERS COLLEGE

New York's American Chemical Society
Student Activities Committee

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May 7th, 2022

Welcome to the 69th Annual Undergraduate Research Symposium, organized by the Student Activities Committee of the New York Section of the American Chemical Society. For the past 69 years, this meeting has given undergraduate chemistry students an opportunity to present the results of their research and learn about the work carried out by their peers.

The New York Section of the American Chemical Society is proud of acknowledging the hard work and dedication of our undergraduates and celebrating their achievements. To every student, congratulations!

Naphtali O'Connor
Dr. Naphtali O'Connor, Co-chair

Michele Vittadello
Dr. Michele Vittadello, Co-chair

Pratikkumar Rathod
Dr. Pratikkumar Rathod, Co-chair

Kevin Mark
Dr. Kevin Mark, Co-chair

NEW YORK'S AMERICAN CHEMICAL SOCIETY

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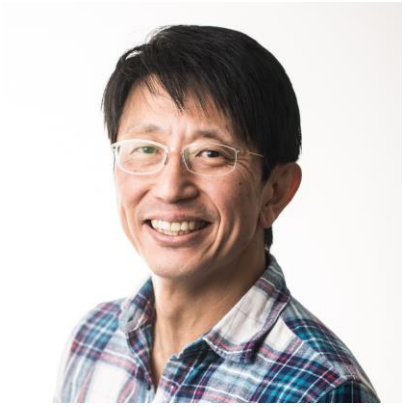
New York's American Chemical Society – Student Activities Committee
69th Annual Undergraduate Research Symposium
Medgar Evers College - CUNY

Saturday, May 7th, 2022

2022 NY ACS Undergraduate Research Symposium	
9:30 am	**Welcoming Remarks** Dr. Rita Upmacis, 2022 Chair, ACS NY Section Dr. Mohsin Patwary, the Dean of Science at Medgar Evers College Dr. Michele Vittadello, Co-Chair, ACS NY Section, Student Activities Committee
9:45	**Keynote Address** Dr. Hiroshi Matsui, Hunter College City University of New York
10:30	**Instructions for the day** Dr. Michele Vittadello, Co-Chair, ACS NY Section, Student Activities Committee
10:35	**Presented Papers -** Analytical Chemistry Biochemistry I Biochemistry II Environmental Chemistry Inorganic Chemistry and Biochemistry Nanochemistry and Surface Chemistry Organic Chemistry Physical Chemistry and Chemical Education Polymer Chemistry
12:05	**Virtual Lunch with our sponsors** • Christian Andrews, Cathy Culver, Christina Daniels and Marlena Sheridan, **PepsiCo** **Graduate Programs** • Dr. Ruth Stark, Graduate School Research Opportunities in Biochemistry, Biophysics, and Biodesign at The City University of New York • Dr. Brian Gibney, CUNY M.S. in Nanoscience • Dr. Sebastien Poget CUNY PhD Biochemistry • Dr. Yolanda Small CUNY PhD Chemistry **Raffle** **Networking Breakout Sessions**
1:00 pm	**End of Program**

KEYNOTE SPEAKER



Dr. Hiroshi Matsui

Hunter College, City University of New York,

Weill Cornell Medical College

By using nanobiotechnolgy, we are developing new strategies to overcome practical issues in clinical translations of some medical fields. This presentation consists of two parts. The first part is to use Brownian motion of superparamagnetic nanoparticles controlled by magnetic fields to improve the efficacy of drug/RNA delivery as such motion enhances the escape of drug-loaded nanoparticles from endosomes before degradation in lysosomes. The second theme is to develop the strategy to amplify the generation of therapeutic extracellular vesiclenanoparticles generated in cells by the stimulus of synthetic peptides self-assembled in donor cells, mimicking prion and amyloid.

ANALYTICAL CHEMISTRY
Moderator:

10:35 DETERMINATION OF THE REFRACTIVE INDEX OF SODIUM ACETATE BY THE EXTENSION METHOD. Jonathan Lee and Jun Shin Department of Chemistry, Queensborough Community College, Bayside, NY 11364

10:50 DEVELOPMENT AND VALIDATION OF SOLID PHASE EXTRACTION AND LIQUID CHROMATOGRAPHY/MASS SPECTROMETRY METHODS FOR THE CONCURRENT DETECTION OF SELECT ANTIBIOTICS IN NEW YORK TECH'S WASTEWATER PLANT. Michael Maino, Jole Fiorito, and Bryan Gibb Department of Biological and Chemical Sciences, New York Institute of Technology, Old Westbury, NY 11568

11:05 BEE POLLEN FROM THE PHILIPPINES: AN ANALYSIS OF FLAVONOID, PHENOLIC CONTENT, AND ANTIOXIDANT ACTIVITY. Carly Sullivan, Fernando Salcedo and Elmer-Rico E. Mojica Department of Chemistry, Pace University, New York, NY 10038

11:20 THERMODYNAMIC STUDY OF ESTERIFICATION OF PROPIONIC ACID USING A MICROWAVE REACTOR: DETERMINATION OF ENTHALPY, ENTROPY AND FREE ENERGY CHANGES. Lijie Wan and Jun Shin Department of Chemistry, Queensborough Community College, Bayside, NY 11364

11:35 Zn PROMOTED CARBON NANOSPHERE ENCAPSULATED Fe-Co CORE-SHELL CATALYST FOR CO_2 CONVERSION TO VALUE ADDED CHEMICALS. Daniel Weber and Cheng Zhang Department of Chemistry, Long Island University Post Campus, Greenvale, NY, 11548

11:50 BIOFUEL PRODUCTION FROM WASTE PLASTIC BY PYROLYSIS. RoseLanda Solon, Ji Kim, PhD Guttman Community College, and Lawrence Pratt, PhD, Medgar Evers College. 50 W 40th st , New York , NY 10018

BIOCHEMISTRY I
Moderator:

10:35 BACH1 INHIBITOR AS A DIRECT ACTIVATOR OF ANTIOXIDANT GENETIC PROGRAM. Katarina Douglas-Blake, Dr. Irina Gazaryan. Department of Chemistry, Pace University, Pleasantville, NY 10570

10:50 DEVELOPMENT OF A FLUORESCENT ASSAY TO MEASURE THE EFFECT OF NEW COMPOUNDS ON HISTONE ACETYLTRANSFERASE ACTIVITY. Jennifer Gattus, Jacqueline Keighron, Jole Fiorito New York Institute of Technology, Northern Boulevard, Valentines Ln, Old Westbury, NY 11568

11:05 DESIGNING SHORT-PEPTIDE CONJUGATES FOR TARGETED THERAPEUTICS AGAINST TUMOR CELLS. Beatriz G. Goncalves and Ipsita A. Banerjee Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx NY 10458

11:20 CHARACTERIZATION OF SMALL RNA STEM LOOPS USING A COMPUTATIONAL APPROACH. Emilee Haines and Maria C. Nagan* Chemistry Department, Stony Brook University, Stony Brook, NY 11794

11:35 SCREENING FOR THE CORRELATION BETWEEN CELL AGE AND HEALTH WITH STRUCTURE AND SOLUBILITY OF HUNTINGTIN INCLUSION BODY IN *S. CEREVISIAE*. Ibrahim Khandakar, Joderick Castillo and Lesley Emtage Department of Biology, York College, City University of New York, Jamaica, NY 11451

11:50 *IN-SILICO* SIMULATIONS OF RNA FOLDING ANALYZED THROUGH HELICAL PARAMETERS, TORSIONS, AND BASE STACKING. Aditya S. Iyer, Mark K. Khalil, Matthew A. Xie, Sophie Huang and Maria C. Nagan* Department of Chemistry, Stony Brook University, Stony Brook, NY 11794

BIOCHEMISTRY-II
Moderator:

10:35 ASSESING CELL HEALTH IN SACCHAROMYCES CEREVISIAE WITH HUNTINGTIN INCLUSION BODIES. Joderick Castillo, Ibrahim Khandakar and Lesley Emtage Department of Biology, York College, City University of New York, Jamaica, NY 11415

10:50 WATER RESPONSIVENESS OF SELF ASSEMBLING PROTEIN TRIBLOCK COPOLYMER CEC. Maria J. Kulapurathazhe, Jacob Kronenberg, Yeojin Jung, Xi Chen, Ray Tu, and Jin Kim Montclare Department of Chemical and Biomolecular Engineering, NYU Tandon School of Engineering Brooklyn, NY 11201

11:05 IN SILICO AND IN VITRO STUDIES OF PEPTIDE-1-LINEAR AND IL13Rα2 RECEPTOR TO DEVELOP ANTITUMOR PEPTIDE CONJUGATES. Charlotta G. Lebedenko, E. Josephine Boder, Diego S. Perez, Ipsita A. Banerjee. Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, NY 10458

11:20 AN INVESTIGATION OF OPIOID RECEPTORS AND THEIR IMPLICATIONS IN ADDICTION. Moll E. Murray, Charlotta G. Lebedenko and Ipsita A. Banerjee Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, New York 10458

11:35 CELL SURVIVAL KINETICS UPON EXPOSURE TO OXIDATIVE STRESS AND DETERMINATION OF CATALASE ACTIVITY. Sapir Sharoni, Anooshqa Bazmi, Jalal Haidery, Anna Li, Jorge Ramos, Uri Samuni, Department of Chemistry and Biochemistry, Queens College, 65-30 Kissena Blvd, Queens, NY 11367

11:50 DAP5 FUNCTION UNDER OXIDATIVE STRESS AND ITS ROLE IN TNBC METABOLISM. Hanna Rosenstock[1] and Columba de la Parra. Department of Chemistry, Herbert H. Lehman College, City University of New York, 250 Bedford Park Boulevard West, Bronx, NY 10468 **[VIRTUAL PRESENTATION]**

ENVIRONMENTAL CHEMISTRY
Moderator:

10:35 THE PHOTOCATALYTIC DEGRADATION OF 2-MERCAPTOBENZOTHIAZOLE (2-MBT) USING FUNCTIONALIZED TiO_2/PAA NANOPARTICLES. Connor Heaney, Giselle Guzman, Caroline Nguyen, and Dr. Yosra Badiei Department of Chemistry, Saint Peter's University, Jersey City, NJ, 07306

10:50 TAILORING THE PROPERTIES OF IMIDAZOLIUM-THIOETHER IONIC LIQUIDS THROUGH STRUCTURAL MODIFICATION. Ho Martin Yuen and Sharon Lall-Ramnarine, Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA

11:05 IMIDAZOLIUM AND PYRROLIDINIUM THIOETHER FUNCTIONALIZED IONIC LIQUIDS. Mehreen Mughal,[1] Sharon Lall-Ramnarine,[1] James F. Wishart,[2] Gopal Subramaniam,[3] and Edward W. Castner Jr.[4] [1]Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA, [2]Chemistry Division, Brookhaven National Laboratory, Upton, New York 11973, USA, [3]Department of Chemistry & Biochemistry, Queens College of the City University of New York Flushing, NY 11367, [4]Department of Chemistry and Chemical Biology, Rutgers University, The State University of New Jersey, Piscataway, NJ 08854

11:20 BIOSORPTION OF CU(II) IONS BY GREEN TEA AND PEPPERMINT TEA WASTE. Armin Osmanovic[1], Daniel Sanchez[2], Jesus Hernandez[2], Dr. Abel E. Navarro[2] [1]Chemistry Department, New York University College of Arts and Sciences, 32 Waverly Pl, New York, NY 10003. [2] Science Department, Borough of Manhattan Community College, CUNY, 199 Chambers St, New York, NY 10007

11:35 CARBON DIOXIDE CONVERSION BY Mn PROMOTED CARBON NANOSPHERE ENCAPSULATED Fe-Co CORE SHELL CATALYSTS. Alexa Saporita and, Cheng Zhang* Department of Chemistry, Physics and Mathematics, Long Island University (Post), Greenvale, NY, 11548

11:50 USING WASTE FOOD TO FUEL THE FUTURE: PRODUCING ETHANOL FROM STARCHY LEFTOVER FOODS. Nina Björkman and Dr. Yelda Hangun-Balkir Department of Chemistry and Biochemistry, Manhattan College, Riverdale, NY, 10741 [**VIRTUAL PRESENTATION]**

INORGANIC CHEMISTRY and BIOCHEMISTRY
Moderator:

10:35 INVESTIGATING DEGRADATION PRODUCTS OF A RUTHENIUM COORDINATION COMPOUND HIGHLY EFFICACIOUS IN TRIPLE NEGATIVE BREAST CANCER Aiman Hafeez,[1,2] Javier Lopez-Hernandez,[1,2,5] Maria Contel.*,[1-5] [1]Brooklyn College Cancer Center, [2]Department of Chemistry, Brooklyn College, The City University of New York, Brooklyn, NY, 11210, US. [3]Biology, [4]Chemistry, and [5]Biochemistry PhD Programs, The Graduate Center, The City University of New York, 365 Fifth Avenue, New York, NY, 10016, US.

10:50 INVESTIGATION OF CHELATING AGENTS FOR THE REMOVAL OF THORIUM FROM HUMAN TEETH UPON NUCLEAR CONTAMINATION. Malika Alamova[1], Chloe Chong [1], Michelle Ma [1], Felicity Liu[1], Jafar Sunga Ali[1], Samuel Groveman[2], Spiro Alexandratos[1], Ali Younes[1]. Department of Chemistry, Hunter College of CUNY, New York, NY, 10065. Department of Chemistry and Environmental Science, Medgar Evers College, Brooklyn, NY 11225

11:05 TOWARDS GOLD-BASED TARGETED THERANOSTIC AGENTS: SYNTHESIS AND CHARACTERIZATION OF CATIONIC Au(III)-NHC IODO COMPLEXES. Roberto De Gregorio,[1,2] Hiwa K Saeed,[1,2] Maria Contel.*,[1-5] [1]Brooklyn College Cancer Center, [2]Department of Chemistry, Brooklyn College, The City University of New York, Brooklyn, NY, 11210, US. [3]Biology, [4]Chemistry, and [5]Biochemistry PhD Programs, The Graduate Center, The City University of New York, 365 Fifth Avenue, New York, NY, 10016, US.

11:20 PISTACHIO SHELLS AS REMEDIAL AGENTS FOR EXTRACTING THORIUM FROM DRINKING WATER. Dihara Hossain[1], Tanja Tane[1], Jafar Sunga Ali[1], Samuel Groveman[2] Spiro Alexandratos[1], Ali Younes[1]. Department of Chemistry, Hunter College of CUNY, New York, NY, 10065. Department of Chemistry and Environmental Science, Medgar Evers College, Brooklyn, NY 11225

11:35 INVESTIGATING THE CONSEQUENCES OF MECHANICAL AND CHEMICAL EROSION OF DENTAL AMALGAM. Liza Isayeva[1], Tanja Tane[1], Dihara Hossain[1], Jafar Sunga Ali[1], Samuel Groveman[2], Spiro Alexandratos[1], Ali Younes[1]. Department of Chemistry, Hunter College of CUNY, New York, NY, 10065. Department of Chemistry and Environmental Science, Medgar Evers College, Brooklyn, NY 11225

11:50 OMEGA-3 SUPPLEMENTS AS ACTIVATORS OF ANTIOXIDANT GENTIC PROGRAM. Najaé Campbell and Irina Gazaryan. Department of Chemistry and Physical Sciences, Dyson College of Arts and Sciences, Pace University, NY 10570.

NANOCHEMISTRY AND SURFACE CHEMISTRY
Moderator:

10:35 LIGHT-DRIVEN WATER-OXIDATION USING NANOSTRUCTURED METAL-BASED POLYMER COMPOSITE FILMS. Oshane Annon, Abril Flores, Christina Rivera and Yosra M. Badiei*. Department of Chemistry, St. Peter's University, Jersey City, NJ 07306

10:50 NOVEL PEPTIDE BOLAAMPHIPHILE IONIC LIQUID GELS FOR THE DEVELOPMENT OF NERVE GUIDANCE CONDUITS. Diego S. Perez, Charlotta G. Lebedenko and Ipsita A. Banerjee Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, NY 10458

11:05 A COMPARATIVE STUDY ON THE INTERACTIONS BETWEEN SINGLE-WALLED CARBON NANOTUBES AND IMIDAZOLIUM AND PYRROLIDINIUM IONIC LIQUIDS. Bethva Robert, Ho Martin Yuen, Sharon Lall-Ramnarine and Tirandai Hemraj-Benny. Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, NY, 11364.

11:20 POLYRHODANINE METAL NANOPARTICLES, SYNTHESIS, AND ANALYSIS. Nickayla Spence[1], Moni Chauhan[1], Arnab Sharma[1], Saleh Jaser[1], Samantha Nieves[2], Qiaxian Johnson[2], Bhanu P. Chauhan[2], [1]Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, [2]Department of Chemistry, William Patterson University, Wayne, NJ

11:35 EFFECT OF INITIAL SOL-GEL PH ON RELEASE KINETICS OF TEMPOL Daniel Goldstein, Sara Lifshitz, Hannah Ariel, and Uri Samuni Department of Biochemistry, Queens College, CUNY, Queens, NY 11367 **[VIRTUAL PRESENTATION]**

11:50 CATALYTIC ACTIVITY OF ENZYMES IN SOL-GEL MATRIX/NANOGELS VS IN SOLUTION. Nataniel Natanov, Kahtan Alsaedi, Sara Lifshitz, Jalal Haidery, Anna Li, Angela Fried, Jorge Ramos, and Uri Samuni. Department of Chemistry and Biochemistry, Queens College, 65-30 Kissena Blvd, Queens, NY 11367 **[VIRTUAL PRESENTATION]**

ORGANIC CHEMISTRY I
Moderator:

10:35 SYNTHESIS AND CHARACTERIZATION OF NEW FLAVYLIUM COMPOUNDS WITH A PHENYL GROUP. Ketevan Basilashvili and Jeonghee Kang Department of Chemistry, St. Joseph's College, Brooklyn, NY 11205

10:50 MECHANISTIC STUDIES OF TAUTOMERIZATIONS IN GUANINE-CYTOSINE BASE PAIR. Benjamin Herrera,[1] Charles Doubleday[2] and Dr. Edyta Greer[1]; [1]Department of Natural Sciences, Baruch College, New York, NY, 10010; [2]Department of Chemistry, Columbia University, New York, NY, 10027

11:05 COMPUTATIONAL STUDIES OF THE DECARBOXYLATION OF CANNABIDIOLIC ACID TO CANNABIDIOL. Florence Uritsky[1], Dr. Edyta Greer[1], and Dr. Charles Doubleday[2]; [1]Department of Natural Sciences, Baruch College, New York, NY, 10010; [2]Department of Chemistry, Columbia University, New York, NY, 10027

11:20 THE INVESTIGATION OF STRUCTURAL EFFECTS ON THE BINDING STRENGTH OF FLAVONES WITH HUMAN SERUM ALBUMIN. Steven Octaviano, and Jianwei Fan Department of Chemistry and Biochemistry, Manhattan College, Bronx, NY 10471

11:35 DEVELOPMENT OF MULTIPLE TARGET MOLECULES FOR THE TREATMENT OF ALZHEIMER'S DISEASE. Dr. Jole Fiorito and Fawaz Syed New York Institute of Technology, Northern Boulevard, Valentines Ln, Old Westbury, NY 11568

PHYSICAL CHEMISTRY AND CHEMICAL EDUCATION
Moderator:

10:35 WORKING TOWARDS A SOLUTION TO THE TRAVELING SALESMAN PROBLEM USING AN OSCILLATING CHEMICAL REACTION. Jake Bordenca, Hugh H. Cheung, Sabrina G. Sobel, Department of Chemistry, Hofstra University, Hempstead, NY, 11549

10:50 GENERATION OF NITRIC OXIDE IN A CONTROLLED RATE THROUGH THE REACTION OF SNP AND GLUTATHIONE. Erin Gal, Jalal Haidery, Anna Li, Jorge Ramos, and Uri Samuni. Department of Chemistry and Biochemistry, Queens College, 65-30 Kissena Blvd, Queens, NY 11367

11:05 SPECTROSCOPIC STUDY OF THE BINDING INTERACTIONS BETWEEN HSA AND COUMARIN SCAFFOLDS. Katherine Gilmartin and Dr. Jianwei Fan Manhattan College, Department of Chemistry and Biochemistry, Riverdale, NY 10471

11:20 MAG-WALKING SIMULATED ANNEALING MONTE CARLO STUDY OF NANO-SOLVATED AMMONIUM CHLORIDE. Sangjoon Lee, Steven L. Topper and Robert Q. Topper. Department of Chemistry, The Cooper Union for the Advancement of Science and Art, New York, NY 10003

11:35 IMPLEMENTATION OF ELECTRONIC LABORATORY NOTEBOOKS IN THE UNDERGRADUATE ORGANIC CHEMISTRY LABORATORY. Matthew Leshinsky, Vandana Bindra, Nanette Wachter, and Sabrina Sobel Department of Chemistry, Hofstra University, Uniondale, NY 11549

11:50 SCIENCE HEROES GAME FOR K12 STUDENTS. Matthew Mistretta, Scott Buzzolani. Adelphi Department of Chemistry, Adelphi University, 1 South Avenue, Garden City, NY 11501

POLYMER CHEMISTRY
Moderator:

10:35 KINETIC ANALYSIS OF BIODEGRADATION OF GIANT LIPOBEADS IN THE PRESENCE OF REDUCING AGENTS: A PLATFORM FOR "SMART" ANTICANCER DRUG AND GENE DELIVERY. Neslihan Tabaru and Dr. Sergey Kazakov Department of Chemistry & Physical Sciences, Pace University, Pleasantville, NY 10570

10:50 DEGRADATION OF POLY(*O*-TOLUIDINE) POROUS MICROSPHERES FOR PAYLOAD DELIVERY APPLICATIONS. Che Chang and David M. Sarno Chemistry Department, Queensborough Community College, Bayside, NY 11364

11:05 DEVELOPMENT OF ELECTROSPUN IONIC LIQUID-POLYMER MEMBRANES. Elijah Bernard,[1] Domenec Paterno,[2] Sophia Suarez[2] and Sharon Lall-Ramnarine,[1] [1]Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA. [2]Department of Physics, Brooklyn College, City University of New York, Brooklyn, New York 11210, USA

11:20 AN INVESTIGATION INTO BINDING INTERACTIONS OF BRAF RECEPTORS WITH TARGETED LIGANDS. Dominic J. Lambo, Charlotta G. Lebedenko and Ipsita A. Banerjee. Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, NY 10458

11:35 PREPARATION OF IONIC LIQUID–POLYMER GELS FOR GAS SEPARATION. Shameir Nembhard,[1] Nicole Zmich,[1] Jasodra D. Ramdihal,[1] Edward W. Castner, Jr.,[2] James F. Wishart[3] and Sharon I. Lall-Ramnarine[1] [1]Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA; [2]Department of Chemistry and Chemical Biology, Rutgers University, The State University of New Jersey, Piscataway, NJ 08854; [3]Chemistry Division, Brookhaven National Laboratory, Upton, New York 11973, USA

ANALYTICAL CHEMISTRY

DETERMINATION OF THE REFRACTIVE INDEX OF SODIUM ACETATE BY THE EXTENSION METHOD. Jonathan Lee and Jun Shin Department of Chemistry, Queensborough Community College, Bayside, NY 11364

The extension method, which was developed based on the observation of a good linear relationship between the percent mass of solution (solid solute and liquid solvent mixture) and its refractive index, has been used to determine the refractive index of solid compounds such as fatty acids and ionic compounds. In the system, a plot of refractive index vs percent mass was obtained in low concentration ranges (0 - 24%), and the line of the linear plot was extrapolated to 100% mass (*i.e.* pure solid) where the refractive index of the solid was calculated. The extension method has been further applied to measure the refractive index of sodium acetate because it showed good solubility in water and some alcohols such as methanol and ethylene glycol. In the experiment, a linear plot was obtained between the refractive index and % mass of sodium acetate in a solvent, and a first order linear equation was calculated based on the plot. By applying 100 to the % mass variable (100% mass means pure solute, the solid sodium acetate) in the linear equation, the refractive index of sodium acetate was indirectly determined in the solvent. Based on the data measured in aqueous solution of sodium acetate, a linear equation (e.g. y=0.001369x + 1.331166) was obtained, then a value of 100% was applied to get the refractive index of sodium acetate, which was 1.468. After two more trials, 1.469(1) was determined as the refractive index of sodium acetate in water (Lit. Value: 1.464).

DEVELOPMENT AND VALIDATION OF SOLID PHASE EXTRACTION AND LIQUID CHROMATOGRAPHY/MASS SPECTROMETRY METHODS FOR THE ONCURRENT DETECTION OF SELECT ANTIBIOTICS IN NEW YORK TECH'S WASTEWATER PLANT. Michael Maino, Jole Fiorito, and Bryan Gibb Department of Biological and Chemical Sciences, New York Institute of Technology, Old Westbury, NY 11568

Proceeding their consumption or improper disposal, antibiotics tend to accumulate in wastewater, an environment characterized by the presence of microbes, such as bacteria. Bacterial exposure to these antibiotics poses significant consequences, such as the potential development of antibiotic resistance. In the medical realm, as the prominence of antibiotic resistance grows, antibiotic efficacy is reduced, contributing to bacterial infections that are more difficult to treat. The objective of this research is to determine, test, and validate efficient methods for detecting four antibiotics [Ampicillin (AMP), Amoxicillin (AMX), Cephalexin (CPX), Doxycycline (DXC)] in wastewater samples collected from the New York Tech wastewater treatment plant in the Long Island campus. Solid phase extraction (SPE) was used for filtering and concentrating wastewater samples, followed by liquid chromatography/mass spectrometry (LC/MS) analysis to detect the antibiotics according to their m/z values and retention times. Antibiotic standards for each antibiotic were prepared and analyzed using the same LC/MS methods as a reference for the wastewater samples. It is believed that AMP and DXC are detectable in our wastewater samples, while AMX and CPX are believed to be undetected. These results demonstrate that the SPE and LC/MS methods of analysis are sufficient for antibiotic detection and may be useful for further research of antibiotic resistance in bacteria.

BEE POLLEN FROM THE PHILIPPINES: AN ANALYSIS OF FLAVONOID, PHENOLIC CONTENT, AND ANTIOXIDANT ACTIVITY. Carly Sullivan, Fernando Salcedo and Elmer-Rico E. Mojica Department of Chemistry, Pace University, New York, NY 10038

Bee pollen is a hive product that is collected from flowers by honeybees that transport it to the hive and pack in the honeycomb mixing with secretion from salivary glands and honey. It is characterized by its excellent bioactive and nutritional composition. Similar to honey and propolis, it has therapeutic properties containing about 250 substances including sugars, proteins, minerals, vitamins, lipids, and flavonoids. Depending on the season, bee species, vegetation, and the area of collection, the chemical composition of bee pollen are qualitatively and quantitatively variable. In this study, different bee pollen samples from the Philippines were characterized for antioxidant activities using DPPH (22-diphenyl-1-picrylhdrazyl) and correlated with their phenolic content obtained using Folin-Ciocalteu assay and flavonoid content using aluminum chloride. In addition, two extraction methods were compared (soaking for 3 days vs sonication for 30 minutes). Results show variable antioxidant activities of the sampled bee pollens. It is also showed that the phenolic content of the bee pollen has low correlation to antioxidant activity.

THERMODYNAMIC STUDY OF ESTERIFICATION OF PROPIONIC ACID USING A MICROWAVE REACTOR: DETERMINATION OF ENTHALPY, ENTROPY AND FREE ENERGY CHANGES. Lijie Wan and Jun Shin Department of Chemistry, Queensborough Community College, Bayside, NY 11364

Microwave reactor is a new technology and has become an invaluable tool adopted in many areas of science laboratories due to the convenience including temperature, pressure and power controls. Application of a microwave reactor was further extended to the thermodynamic study of esterification reaction with the merit of a convenient temperature control of a microwave reactor. The equilibrium constants of the esterification reaction between propionic acid and isopropyl alcohol at the temperatures of 40 - 90°C were determined from the initial and equilibrium concentrations of propionic acid through the acid-base titration using a 0.5M NaOH solution. Thereafter, the thermodynamic data (ΔH and ΔS) of the reaction were calculated from the linear relationship between the equilibrium constants obtained (lnK) and the equilibrium temperatures (1/T) using a microwave reactor. The obtained data were compared to the data calculated from the acetic acid/isopropyl alcohol reaction to compare the effect of longer acid in the reaction. This result will extend the usage of microwave reactor to a tool of the thermodynamic study which can be easily added to an undergraduate laboratory curriculum. Application a microwave reactor will make the thermodynamic study easy, simple and faster due to the convenience of the temperature control of the instrument and its safety feature.

Zn PROMOTED CARBON NANOSPHERE ENCAPSULATED Fe-Co CORE-SHELL CATALYST FOR CO_2 CONVERSION TO VALUE ADDED CHEMICALS. Daniel Weber and Cheng Zhang Department of Chemistry, Long Island University Post Campus, Greenvale, NY, 11548

Global warming has been one of the biggest issues regarding both the environment and the economy of the world. In recent years, it has been discovered that CO_2 can be catalytically converted into lower olefins (C2-C4), which are valuable in the production of polymers for industrial use. While catalytically activating CO_2, remains to be a challenge, as it is one of the most stable carbon containing molecules, it is a necessary topic to research for the benefit of both the environment and the industry. Prior research has revealed that with the additional use of hydrogen the effectiveness of CO_2 utilization has been improved. Hence, a selective conversion of CO_2 to lower olefins can be accomplished through CO_2 hydrogenation over a bimetallic FeCo catalyst at a 1:2 mole ratio (Fe_1Co_2) encapsulated in a carbon nano-sphere (CNS) shell. In this study, a Zn promoter with varying mole ratios ($Fe_1Co_2Zn_3$, $Fe_1Co_2Zn_1$, $Fe_1Co_2Zn_{0.3}$) was implemented into the Fe_1Co_2 catalyst to potentially enhance its performance in converting CO_2 to light olefins. The catalytic performance of these catalysts were compared with the unpromoted catalyst to determine if the promoter was beneficial to light olefin production, as well as to understand the effect that the mole ratio of Zn has on the performance. The catalysts were prepared by the polymerization of resorcinol and formaldehyde in the presence of Fe and Co metal solutions. The synthesized catalysts were evaluated with CO_2 and H_2 in a plug flow reactor (PFR) at various temperatures using gas chromatography for product determination.

BIOFUEL PRODUCTION FROM WASTE PLASTIC BY PYROLYSIS. RoseLanda Solon, Ji Kim, PhD Guttman Community College, and Lawrence Pratt, PhD, Medgar Evers College. 50 W 40th st , New York , NY 10018

Biofuel is a renewable fuel produced from biomass, brown grease, and waste cooking oil. Most biomasses are from cow dung, human fecal matter, poultry droppings kitchen, and agricultural residue as feedstocks. In this project, we have employed pyrolysis to produce biofuel from waste plastics. As common types of waste plastics, a milk bottle as High-Density Polyethylene (HDPE) and single plastic bags as Low-Density Polyethylene (LDPE) have been pyrolyzed at various temperatures, 350°C to 450°C for 6-12 hrs with and without catalyst. The components of the products are mainly hydrocarbons, it will be further characterized by Gas Chromatography Mass Spectrometry (GCMS).

BIOCHEMISTRY-I

BACH1 INHIBITOR AS A DIRECT ACTIVATOR OF ANTIOXIDANT GENETIC PROGRAM. Katarina Douglas-Blake, Dr. Irina Gazaryan. Department of Chemistry, Pace University, Pleasantville, NY 10570

Aging and neurodegenerative diseases show overexpression of Bach1 transcriptional repressor. One of the most important effects of Bach1 is the repression of Nrf2 target genes due to Bach1 direct interaction with DNA. Heme is a physiological effector of Bach1: heme directly interacts with Bach1 protein resulting in the change of Bach1 protein conformation and its release from DNA and nucleus. Bach1 de-repression results in Nrf2 access to target genes and triggering the antioxidant genetic program. We studied a proprietary Bach1 inhibitor, which chemical structure resembles a half of heme ring, in a cell-based reporter assay screening for Nrf2 activators. Apparently, Bach1 inhibitor is also a powerful direct activator of Nrf2 working via

stabilization of Nrf2 protein. The mechanism of this activation is currently unknown. By challenging Bach1 inhibitor effects with addition of ascorbic acid and zinc, we observed very modest quenching of reporter activation with both treatments. Our working hypothesis is that Bach1 inhibitor is capable of binding divalent metals like zinc and iron. Divalent iron can work as pro-oxidative treatment resulting in stabilization of Nrf2 and activation of antioxidant genetic program.

DEVELOPMENT OF A FLUORESCENT ASSAY TO MEASURE THE EFFECT OF NEW COMPOUNDS ON HISTONE ACETYLTRANSFERASE ACTIVITY. Jennifer Gattus, Jacqueline Keighron, Jole Fiorito New York Institute of Technology, Northern Boulevard, Valentines Ln, Old Westbury, NY 11568

Alzheimer's disease is a neurodegenerative disease that results in memory loss and reduction in cognitive function due to the accumulation of amyloid plaques and fibrillary tangles. According to the CDC 5.8 million Americans lived with Alzheimer's disease in 2020. Previous research has explored the relationship between modulating histone acetyltransferase (HAT) activity and improvement from defects in synaptic function and memory after amyloid plaque development. HAT enzymes add an acetyl group to lysine residues of histone proteins, regulating the expression of several memory-related genes during memory formation and/or consolidation. The HAT enzyme uses an acetyl group from acetyl-coA resulting in the production of the acetylated histone and free coenzyme A (CoA). The purpose of this study is to develop a fluorescence assay to detect any change of HAT enzyme p300 activity on histone 3.3 in the presence of HAT modulators. We use a fluorescent molecule, which binds to the sulfhydryl groups of CoA and generates a fluorescent signal. Our results so far have shown that the assay is working properly with significant differences between the substrate control (in the absence of p300) and positive control (in the presence of p300). Our experimental conditions have confirmed anacardic acid as an inhibitor (20% inhibition at 15μM) and YF2 as an activator (17% activation at 100nM). This enzymatic assay will be used for measuring the p300 activity of newly synthesized compounds.

DESIGNING SHORT-PEPTIDE CONJUGATES FOR TARGETED THERAPEUTICS AGAINST TUMOR CELLS. Beatriz G. Goncalves and Ipsita A. Banerjee Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx NY 10458

The number of cancer diagnoses is forecasted to increase over the years. Most of the current treatments include chemotherapeutics, surgery or radiation, which are harmful not only to tumor cells, but also affect normal cells resulting in undesired, detrimental side effects. For this reason, it is important to develop targeted therapeutics that can specifically target and subside overexpressed receptors in tumor cells. In this work, we designed novel peptide conjugates, consisting of tumor targeting peptides conjugated to plant derived di and triterpene natural molecules with inherent anticancer and antioxidant properties for dual targeting. We carried out extensive in silico studies, and examined the binding affinities, stabilities, physicochemical, pharmacokinetic properties and MMGBSA studies to determine the contributing binding energies involved based on trajectories of 100 ns runs for each conjugate with the Ephrin A2 (EphA2) and Epidermal Growth Factor receptor (EGFR). We also conducted *in vitro* studies to

examine the efficacy of the conjugates at the cellular level. Overall, these studies will not only aid in understanding the mechanism of binding with novel peptide conjugates with the receptors, but also potentially aid in the development of novel targeted therapeutics for cancer treatment.

CHARACTERIZATION OF SMALL RNA STEM LOOPS USING A COMPUTATIONAL APPROACH. Emilee Haines and Maria C. Nagan* Chemistry Department, Stony Brook University, Stony Brook, NY 11794

Ribonucleic Acid (RNA) is expressed as a single-stranded biomolecule, performing a number of critical biological roles in the cell. Many viruses use RNA as their genetic material, which has sparked interest in understanding the link between RNA structure and function. This deeper understanding of RNA structure could lead to a better understanding of RNA viruses, such HIV, as well as other RNAs in cellular function. In the RNA strand, unusual base pairing and hydrogen bonding interactions lead to the formation of secondary and tertiary structures. These include secondary structures such as hairpins, stem loops, and tRNA cloverleafs, while tertiary structures include pseudoknots, 3-way junctions, A-minor motifs and others. The focus of this research is on the stem-loop regions of a variety of small RNAs that are characterized based on their NMR conformers. Computational molecular dynamics simulations were run on several RNA stem loops, and their structures were analyzed for sugar pucker conformations and hydrogen bonding interactions. Structures were visualized using visual molecular dynamics (VMD) software and analyzed statistically. This analysis provides a deeper insight on a variety of small RNA loop structures.

SCREENING FOR THE CORRELATION BETWEEN CELL AGE AND HEALTH WITH STRUCTURE AND SOLUBILITY OF HUNTINGTIN INCLUSION BODY IN *S. CEREVISIAE*. Ibrahim Khandakar, Joderick Castillo and Lesley Emtage Department of Biology, York College, City University of New York, Jamaica, NY 11451

Huntington disease is a neurodegenerative disease caused by the expansion of a glutamine-encoding trinucleotide repeat in the *HTT* gene sequence, resulting in a mutated huntingtin (Htt) protein. Htt protein with an expanded polyglutamine tract causes instability in structure and unfolding. This leads to the accumulation of unfolded Htt protein in large aggregates called inclusion bodies. We are using *S. cerevisiae* expressing a mutated *htt* gene fused to *gfp* in order to study the effect of Htt aggregation on cell health. Previous studies showed that inclusions are dynamic, mobile and have a gel-like structures and they undergo a transformation in structure and solubility with time. We are able to determine the reproductive age of cells by staining for bud scars. In our current study, we assayed bud scar tissues to examine the correlation between cell age and the transformation in structure and solubility of inclusion bodies. We found that the alterations in inclusion structure occur at a wide range of cell ages and is more likely linked to inclusion size. We are interested in ascertaining whether cells with large and insoluble inclusions are associated with cellular senescence and possibly cell death. Therefore, we are investigating potential aspects of cell health that are affected by inclusions by assessing mitochondrial membrane potential and probing cell sensitivities to a variety of stresses, such as heat shock.

IN-SILICO SIMULATIONS OF RNA FOLDING ANALYZED THROUGH HELICAL PARAMETERS, TORSIONS, AND BASE STACKING. Aditya S. Iyer, Mark K. Khalil, Matthew A. Xie, Sophie Huang and Maria C. Nagan* Department of Chemistry, Stony Brook University, Stony Brook, NY 11794

Ribonucleic acid (RNA) is an important biomolecule that plays key roles in coding, decoding, and regulating the expression of genes. Specifically, stem-loops within RNA serve a significant role in physiological systems due to their involvement in translation, enzymatic reactions, and promoting functional fidelity of the RNA strands. To determine if current physics models can accurately fold RNA, three stem-loops solved originally by NMR were simulated on the computer. A suite of structural analysis techniques were employed to compare folded structures to experimentally determined NMR structures. Both the loops and helical regions were examined. Simulations of RNA molecules were carried out with the Amber molecular dynamics package in an implicit solvent environment. Helical parameters, base stacking between adjacent bases in the strand, and torsion angles between nucleotides of RNA generally confirmed that the physics models do fold the RNA into a stem-loop structure. A few more subtle interactions were not properly replicated on the computer and improvements to the physics model will be discussed.

BIOCHEMISTRY-II

ASSESING CELL HEALTH IN SACCHAROMYCES CEREVISIAE WITH HUNTINGTIN INCLUSION BODIES. Joderick Castillo, Ibrahim Khandakar and Lesley Emtage Department of Biology, York College, City University of New York, Jamaica, NY 11415

Accumulations of unfolded protein, or inclusions, are an intracellular phenomenon that are found in all degenerative neurological diseases that we know today. How inclusion bodies act on the cell is still not well understood. The huntingtin protein is a protein that forms inclusion bodies found in individuals that have the degenerative neurological disease known as Huntington's disease. Mutations in *huntingtin* that encode an expanded polyglutamine tract near the N-terminus of the protein cause Huntingtin (Htt) to unfold and form inclusion bodies of different sizes and shapes. We are investigating whether inclusions of Htt affect overall cell health in the yeast *Saccharomyces cerevisiae*, using strains that express Htt fused to GFP. Each strain expresses Htt with a different polyglutamine tract length. *S. cerevisiae* expressing native Htt-GFP have polyglutamine tracts of 25 glutamines (25Q) in length, while the mutant forms 72Q and 103Q are much longer and form inclusions with increasing frequency. The cells were analyzed to observe how expression of Htt with different polyQ tract length affected the health of cells. We have been able to observe a correlation between the presence of very large inclusions of Htt-GFP and the cells' ability to maintain regular levels of mitosis, suggesting that large inclusions are harmful. The number of dead cells also correlates with polyQ length and the frequency of large inclusions. We are also assessing the effect of stressful environmental conditions to determine whether strains with different inclusion frequencies have differences in survival.

WATER RESPONSIVENESS OF SELF ASSEMBLING PROTEIN TRIBLOCK COPOLYMER CEC. Maria J. Kulapurathazhe, Jacob Kronenberg, Yeojin Jung, Xi Chen, Ray Tu, and Jin Kim Montclare Department of Chemical and Biomolecular Engineering, NYU Tandon School of Engineering Brooklyn, NY 11201

Water-responsive (WR) materials exhibit dynamic swelling and shrinking behavior in response to relative humidity (RH) changes in their environment. This allows them to serve as high-energy actuators in a variety of different mechanical systems including soft robotics and sensors. Proteins are promising WR materials because they are essential components of natural structures with high energy performance levels. However, the design parameters for WR protein materials remain poorly understood. Our lab has constructed a protein triblock copolymer with multiple self-assembling domains composed of an elastin (E) domain fused with two flanking cartilage oligomeric matrix protein coiled-coil (C) domains to form CEC. Prior experimentation showed that an L44A mutation in the C domain abolishes the α-helical structure. To investigate the role CEC's coiled-coil domain plays in WR behavior, $C_{L44A}EC_{L44A}$ is used as an unstructured control.
Secondary structure is confirmed by circular dichroism spectroscopy. Protein thin films are then cast onto an inert polyimide substrate and exposed to varying RH levels. Energy densities are calculated from curvature measurements of the bilayer samples. $C_{L44A}EC_{L44A}$ outperforms CEC with an energy density of 647.9 ± 86.8 kJ/m^3 compared to CEC's 119.4 ± 34.3 kJ/m^3. Scanning electron micrographs show that $C_{L44A}EC_{L44A}$ possesses greater porosity as well. This suggests that the higher-order assembly of the protein may contribute to protein WR behavior. With these results, we are now closer to understanding the structural elements involved in WR biomaterial development.

IN SILICO AND IN VITRO STUDIES OF PEPTIDE-1-LINEAR AND IL13Rα2 RECEPTOR TO DEVELOP ANTITUMOR PEPTIDE CONJUGATES. Charlotta G. Lebedenko, E. Josephine Boder, Diego S. Perez, Ipsita A. Banerjee. Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, NY 10458

Due to the extremely low survival rate of glioblastoma (GBM) patients, there is a pressing demand for improved technologies that can target GBM. Tumor-targeting peptides, which target receptors overexpressed on cancer cell surfaces and possess blood brain barrier penetrating abilities, show great promise for the treatment of central nervous system cancers. This study focuses on the interleukin 13 receptor α 2 (IL13Rα2), which is overexpressed on the surface of 75% of GBM tumor cells, and a peptide known to selectively target this receptor known as Pep-1L. The binding mechanism of this peptide to IL13Rα2 has not been previously determined, but it has been shown to effectively target drugs to GBM cells followed by cellular uptake. In this study, we have used a computational approach to model IL13Rα2 for the first time with molecular dynamics simulations to propose a potential binding site for Pep-1L to IL13Rα2 and identify multiple peptides or peptide-conjugates that show significantly higher binding affinity to IL13Rα2 than the original Pep-1L. This computational model and proposed mechanism of Pep-1L and IL13Rα2 binding can be used to further study the role of Pep-1L in cancer treatment, and these novel peptide candidates were examined using further *in vitro* studies to better determine their potential applications in GBM therapy.

AN INVESTIGATION OF OPIOID RECEPTORS AND THEIR IMPLICATIONS IN ADDICTION. Moll E. Murray, Charlotta G. Lebedenko and Ipsita A. Banerjee Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, New York 10458

Opioids are pain mitigating substances which aid in managing invasive procedures and traumatic injuries. Their positive properties with regards to medicine are starkly contrasted with strong addictive properties and toxic side effects, which have led to high rates of abuse and overdose in what has become widely known as the opioid crisis. This project sought to design novel peptide-based conjugates with flavonoids, polyphenols, catechins and triterpenes. The binding mechanisms of receptors implicated in opioid addiction were investigated. The opioids selected to be compared to the novel peptide-based conjugates included fentanyl, and oxycodone, as well as already marketed opioid antagonists such as naltrexone.
ADMET analysis displayed strong blood brain permeability and PgP substrate ability of both opioids and peptide-based conjugates, as well as low toxicity of the proposed conjugates. High binding affinities were also observed for both opioids and peptide-based conjugates with all receptors, with particularly high binding affinities existing between both fentanyl and a gallate-peptide conjugate with the Sigma-1 receptor. Molecular dynamics studies complemented these findings with stable RMSD values of ligands in receptor binding pockets. Hydrophobicity of all compounds was found to play a significant role in the binding mechanisms of all compounds. The peptide-based conjugates notably displayed far more hydrogen bonding. Predictions regarding the agonist or antagonist behavior of conjugates were able to be made based on comparisons of interacting residues in receptor binding pockets with known agonists and antagonists of those receptors.
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CELL SURVIVAL KINETICS UPON EXPOSURE TO OXIDATIVE STRESS AND DETERMINATION OF CATALASE ACTIVITY. Sapir Sharoni, Anooshqa Bazmi, Jalal Haidery, Anna Li, Jorge Ramos, Uri Samuni, Department of Chemistry and Biochemistry, Queens College, 65-30 Kissena Blvd, Queens, NY 11367

Our objective is to perform a kinetic study of the rate and extent of yeast cells (Saccharomyces cerevisiae) survival under different conditions of oxidative stress (e.g. hydrogen peroxide). The cells population is initially monitored using scattered light, direct and indirect UV-Vis absorption (colorimetric assay) and a clonogenic assay (serial dilution and counting on agar plates). In this experimental kinetic setup, when determining the cells population at different time points, catalase is employed as a tool to rapidly consume excess hydrogen peroxide prior to plating. Catalase is an antioxidant oxidoreductase enzyme, which prevents the accumulation of reactive oxygen species (ROS) in organisms, specifically hydrogen peroxide. In this two-step enzymatic reaction, hydrogen peroxide is decomposed to yield one oxygen and two water molecules. Hydrogen peroxide binds to Compound I (Cpd I), which is a high-valent oxyferryl intermediate, resulting from the oxidation of catalase in a precursor step. This leads to the formation of the Cpd I-H2O2 complex, which is then reduced by an electron pair transfer from hydrogen peroxide. This reaction result in the production of oxygen and water, together with the regeneration of catalase. The data collected presents our initial kinetic cell survival studies, as well as the activity rate of catalase, determined by the change in absorbance as a function of time.

DAP5 FUNCTION UNDER OXIDATIVE STRESS AND ITS ROLE IN TNBC METABOLISM. Hanna Rosenstock[1] and Columba de la Parra. Department of Chemistry, Herbert H. Lehman College, City University of New York, 250 Bedford Park Boulevard West, Bronx, NY 10468 [**VIRTUAL PRESENTATION]**

Aggressive cancer cells acquire an altered metabolism in which they switch from oxidative phosphorylation (OXPHOS) to glycolytic phenotype (The Warburg Effect) to increase metabolic pathways that support growth, proliferation, and metastasis. The highly metastatic Triple-negative Breast cancer (TNBC) is characterized by dysregulated metabolism glycolysis and the mechanism for this dysregulation is unknown. Our data shows that the translation initiation protein DAP5 is involved in the modulation of mRNAs related to metabolism. Under oxidative stress translation initiation is stopped in normal cells, but when cancer cells are exposed to oxidative stress translation continues and makes aerobic glycolysis favorable. Our data *in vitro* using MDA-MB -231 and 4T1 TNBC cells shows that DAP5 is resistant to oxidative stress, which may allow cancer cell to continue glycolytic metabolism. The mechanism and importance by which DAP5 regulates breast cancer cell metabolism is the focus of our research.

ENVIRONMENTAL CHEMISTRY

THE PHOTOCATALYTIC DEGRADATION OF 2-MERCAPTOBENZOTHIAZOLE (2-MBT) USING FUNCTIONALIZED TiO_2/PAA NANOPARTICLES. Connor Heaney, Giselle Guzman, Caroline Nguyen, and Dr. Yosra Badiei Department of Chemistry, Saint Peter's University, Jersey City, NJ, 07306

Emerging pollutants (EPs), are a new class of anthropogenic pollutants which can cause adverse effects on human health and the aquatic environment. One of these EPs, 2-mercaptobenzothiazole (2-MBT), is a known carcinogen often found in wastewater streams of pharmaceutical industry and hospitals. To prevent further damage to the environment, new and environmentally safe water remediation techniques must be developed. One photocatalyst that has shown great promise in the cleanup and degradation of organic pollutants, is Titanium Dioxide (TiO_2) nanoparticles. Further studies have also shown evidence of increased catalytic activity with the functionalization of polymers such as polypyrrole, polyacetylene, and polyaniline. Polyacrylic acid (PAA) is one of these polymers that shows promise as an enhancing agent for the catalytic effectiveness of TiO_2. This work aims to investigate and categorize the kinetics of the photo-degradation of 2-MBT in the presence of TiO_2 through UV-visible spectroscopy, and assessing the degradation efficiency of this pollutant by TiO_2 in comparison with functionalized TiO_2/PAA composites.

TAILORING THE PROPERTIES OF IMIDAZOLIUM-THIOETHER IONIC LIQUIDS THROUGH STRUCTURAL MODIFICATION. Ho Martin Yuen and Sharon Lall-Ramnarine, Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA

Ionic liquids (ILs) are attractive as specialty liquids that can be tailored for a wide range of applications as alternatives to traditional solvents. Particularly, in energy storage devices that depend on their ability to transport charge as electrolytic fluids. However, their large-scale adoption is hampered by their relatively high viscosity, which arises from interactions between the ions. Although many researchers focus on reducing viscosity by structural modification of IL ions much remains unclear about the intra- and intermolecular interactions between the side chains on the ions that influence IL properties. We report here on the synthesis and purification of imidazolium ILs where the hydrogen at the C-2 position of the ring was replaced with a methyl group aimed at blocking H-bonding between the side chain, the ring, and neighboring ions. The imidazolium cations were synthesized to bear thioether functionalized side chains recently shown to lower IL viscosity. The ILs were prepared by reacting 1,2-dimethylimidazole with selected (alkylthio)alkyl chlorides followed by metathesis with lithium bis(trifluoromethylsulfonyl)amide. The structures of the ILs were confirmed by 1H and 13C Nuclear Magnetic Resonance (NMR) spectroscopy. This work is part of a larger collaborative project with the Johnson group at Yale University, using spectroscopic studies to assess the role of hydrogen bonding in ether and thioether functionalized ILs as a tool to control ionic liquid viscosities.

IMIDAZOLIUM AND PYRROLIDINIUM THIOETHER FUNCTIONALIZED IONIC LIQUIDS. Mehreen Mughal,[1] Sharon Lall-Ramnarine,[1] James F. Wishart,[2] Gopal Subramaniam,[3] and Edward W. Castner Jr.[4] [1]Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA, [2]Chemistry Division, Brookhaven National Laboratory, Upton, New York 11973, USA, [3]Department of Chemistry & Biochemistry, Queens College of the City University of New York Flushing, NY 11367, [4]Department of Chemistry and Chemical Biology, Rutgers University, The State University of New Jersey, Piscataway, NJ 08854

Ionic liquids (ILs) are promising as safer, alternative electrolytes in electrochemical devices, including rechargeable lithium cells, solar cells, and supercapacitors. However, most ILs have significantly higher viscosities than electrolytes based on conventional solvents, resulting in slower charge transport. Recent reports have shown that replacing IL alkyl side chains with short thioether side chains lowers IL viscosity significantly in imidazolium ILs, but not in pyrrolidinium and phosphonium ILs. We hypothesize that imidazolium NTf_2 ILs with thioether side chains will exhibit lower viscosities in comparison to those with alkyl and ether side chains. Research reveals that data is largely missing from the literature on the synthesis and characterization of thioether-substituted ILs of varying structural types, particularly those with poly-thioether side chains covalently linked to the N atom of imidazolium and pyrrolidinium cation rings. We report here on the synthesis of imidazolium and pyrrolidinium thioether-functionalized ILs. Six ILs, bearing 3-4 atom long thioether side chains, were prepared by reacting methylimidazole and methyl pyrrolidine with selected thioether chlorides followed by metathesis with lithium bis(trifluoromethylsulfonyl)amide to produce the desired ILs. The structures of the ILs were confirmed using H-1 and C-13 Nuclear Magnetic Resonance (NMR) spectroscopy. This work is a part of a larger collaborative project where we seek to examine the atomistic origin of viscosity by comparing ILs with ether and thioether side chains. Results are expected to make important contributions to the design of ILs optimized for larger-scale use in energy storage devices such as batteries.

BIOSORPTION OF CU(II) IONS BY GREEN TEA AND PEPPERMINT TEA WASTE. Armin Osmanovic[1], Daniel Sanchez[2], Jesus Hernandez[2], Dr. Abel E. Navarro[2] [1]Chemistry Department, New York University College of Arts and Sciences, 32 Waverly Pl, New York, NY 10003. [2] Science Department, Borough of Manhattan Community College, CUNY, 199 Chambers St, New York, NY 10007.

Biosorption is a remediation technique that uses natural materials to remove contaminants from an aqueous solution. This study evaluates the potential of biomaterials green tea and peppermint tea to remove Cu(II) ions from wastewater. Parameters such as pH, dose of adsorbent, contact time, salt effect, and crowding effect were studied to investigate their impact on the biosorption efficiency in batch adsorption experiments at room temperature. SEM and EDS studies were used to determine the chemical and morphological traits of the biosorbents. The results indicate that both green tea and peppermint tea maximizes the adsorption at pH 7 with 100mg of adsorbent. Data show that both sorption processes are inhibited by the presence of salts, a metal cation, and an organic dye. Langmuir, Freundlich, Dubinin-Radushkevich, Elovich, Jovanovic, and Temkin isotherm models were used to analyze equilibrium data. Maximum adsorption capacity for green tea and peppermint tea reached 33.91 mg/g and 96.62 mg/g, respectively. Time-dependent data was analyzed with first order, second order, Elovich, and Weber-Morris models to investigate kinetics. Elovich kinetics fit green tea data, and second order fit both biosorbents, indicating that the rate of the reaction is determined by the chemical interactions between the sorbate and sorbent. This data demonstrates the potential of spent tea leaves as inexpensive and eco-friendly candidates for the removal of copper from wastewaters.

CARBON DIOXIDE CONVERSION BY Mn PROMOTED CARBON NANOSPHERE ENCAPSULATED Fe-Co CORE SHELL CATALYSTS. Alexa Saporita and, Cheng Zhang* Department of Chemistry, Physics and Mathematics, Long Island University (Post), Greenvale, NY, 11548

Over the years, increased amounts of greenhouse gases such as CO_2 have caused detrimental effects to the environment. The primary objective of this work is to catalytically convert CO_2 to value-added chemicals, such as carbon monoxide, CH_4, methanol, light olefins, and fuels. Herein, we developed a unique carbon nanosphere encapsulated Fe-Co core-shell catalyst to enable efficient CO_2 conversion by introducing Mn into the catalyst composition. The catalyst was prepared by polymerizing resorcinol and formaldehyde in the presence of iron and cobalt polymeric complex solution and manganese nitrate followed by carbonization. The synthesized catalyst was compressed into uniform particle size and evaluated with CO_2 and H_2 in a plug flow reactor (PFR) at various temperatures using gas chromatography for product analysis. Results shows that Mn plays an essential role in affecting the catalyst performance in terms of CO_2 conversion and selectivity of light olefins, CO and CH_4. To have an in-depth understanding of the relationship between activity and properties, further characterizations are to be conducted using temperature programmed reduction (TPR), in situ ambient-pressure X-ray photoelectron spectroscopy (AP-XPS), in situ X-ray diffraction (XRD), and transmission electron microscopy (TEM). Ultimately, carbon nanosphere encapsulated Mn-Fe-Co core-shell catalyst can provide an ideal and practical model system for the selective reduction of CO_2 regarding environmental catalysis and as a way of providing alternative sustainable energy.

USING WASTE FOOD TO FUEL THE FUTURE: PRODUCING ETHANOL FROM STARCHY LEFTOVER FOODS. Nina Björkman and Dr. Yelda Hangun-Balkir Department of Chemistry and Biochemistry, Manhattan College, Riverdale, NY, 10741 [**VIRTUAL PRESENTATION]**

As the threat of the climate crisis is growing, the need to reduce our carbon footprint has led the demand for alternative fuels to increase drastically. However, biofuel production has also created debates because of the so-called food vs. fuel conflict, where valuable land and resources are used to grow feedstock instead of food. As a result, significant research has been made to create second-generation fuels that use waste materials such as woodchips and left-over straw as feedstock. By using left-over products, the fuel production is not in conflict with food production and furthermore enables us to turn waste into valuable product.
This research focuses on bioethanol production from bread waste, something that could be a potential remedy for two major greenhouse gas emission sources – organics in landfills and fossil fuels. The experiment compares acid hydrolysis for bagels, flour, and cornbread in order to determine their suitability as feedstock for bioethanol production. Yields from the experiment are calculated using gravimetric and volumetric analysis, and then used to estimate the viability of using the feedstocks for large-scale production of bioethanol.

INORGANIC CHEMISTRY

INVESTIGATING DEGRADATION PRODUCTS OF A RUTHENIUM COORDINATION COMPOUND HIGHLY EFFICACIOUS IN TRIPLE NEGATIVE BREAST CANCER Aiman Hafeez,[1,2] Javier Lopez-Hernandez,[1,2,5] Maria Contel.*,[1-5] [1]Brooklyn College Cancer Center, [2]Department of Chemistry, Brooklyn College, The City University of New York, Brooklyn, NY, 11210, US. [3]Biology, [4]Chemistry, and [5]Biochemistry PhD Programs, The Graduate Center, The City University of New York, 365 Fifth Avenue, New York, NY, 10016, US.

TNBC is an aggressive form of breast cancer defined by the absence of the expression of progesterone receptor, estrogen receptor, and human epidermal growth factor receptor 2. Due to the inability to target a receptor, treatment of TNBC is highly limited, with a higher rate of incidence and mortality in pre-menopausal women and women of African ancestry. In this regard, our group has developed a potential chemotherapeutic agent in a ruthenium-based compound (**Ru-IM**) that has shown high efficacy in a TNBC-xenografted mouse model with almost no systemic toxicity.
Ru-IM induces canonical or caspase-dependent apoptosis by a mode of action different from that of cisplatin, and that seems to involve the PI3/AKT pathway. **Ru-IM** accumulates preferentially in mitochondria and displays relevant antimetastatic and anti-angiogenic properties. We are thoroughly investigating the mode of action of this compound with the aim to translate it to the clinic (including upcoming detailed pharmacological assays *in vivo*). **Ru-IM** has a half-life of 2.5 days in water, but when heated or in the presence of Cl, it undergoes cyclometallation producing **Ru-CycloIM**. Here we report on the mechanism and conditions for this cyclometallation process as well as the isolation of Ru-CycloIM and other potential degradation products. Future studies will focus on the biological evaluation of the cyclometallated derivative to assess whether it shows enhanced or decreased specificity and

efficacy with respect to Ru-IM. In doing so, we hope to identify the species responsible for the biological activity (either parent compound or prodrug **Ru-IM**, or evolved product **Ru-CycloIM**).

INVESTIGATION OF CHELATING AGENTS FOR THE REMOVAL OF THORIUM FROM HUMAN TEETH UPON NUCLEAR CONTAMINATION. Malika Alamova[1], Chloe Chong [1], Michelle Ma [1], Felicity Liu[1], Jafar Sunga Ali[1], Samuel Groveman[2], Spiro Alexandratos[1], Ali Younes[1]. [1]Department of Chemistry, Hunter College of CUNY, New York, NY, 10065. [2]Department of Chemistry and Environmental Science, Medgar Evers College, Brooklyn, NY 11225

Thorium-232 (^{232}Th) is a radioactive heavy metal that is of increasing interest as a source of nuclear energy. However, upon nuclear incidents, the ingestion or inhalation of Th in major quantities can contribute to chemical and radiological health problems, including accumulation in the bone tissue and an increased risk of developing pancreatic, lung, and hematopoietic cancers. The major mineral component of the bone is hydroxyapatite (HAP) - also the major mineral component of the teeth. As such, the teeth are the first site of exposure upon oral ingestion of Th contaminated materials, and Th can pose a potential risk to teeth development. In essence, in the case of human contamination, it is critical to identify effective chelating agents capable of removing Th. Using a batch study methodology, this present work investigates the uptake and the removal of Th from synthetic HAP and from teeth samples by diethylenetriamine pentaacetate (DTPA), ethylenediaminetetraacetic acid (EDTA), and other promising chelating agents. Th uptake over synthetic HAP exceeds 98% at physiological pH with <1 min of contact time, and uptake exceeds 90% across the entire pH range. Regarding teeth, over 1 mg Th uptaken per gram of tooth is observed after 24 hours. DTPA is found to be the best chelating agent for the removal of Th from synthetic HAP, and the efficacy of the chelating agents in removing Th from teeth samples is currently being investigated.

TOWARDS GOLD-BASED TARGETED THERANOSTIC AGENTS: SYNTHESIS AND CHARACTERIZATION OF CATIONIC Au(III)-NHC IODO COMPLEXES. Roberto De Gregorio,[1,2] Hiwa K Saeed,[1,2] Maria Contel*,[1-5] [1]Brooklyn College Cancer Center, [2]Department of Chemistry, Brooklyn College, The City University of New York, Brooklyn, NY, 11210, US. [3]Biology, [4]Chemistry, and [5]Biochemistry PhD Programs, The Graduate Center, The City University of New York, 365 Fifth Avenue, New York, NY, 10016, US.

Gold complexes bearing N-heterocyclic carbene (NHC) have shown remarkable promise as potential anti-cancer agents displaying high cytotoxicity (low micromolar to nanomolar range) in vitro against a variety of human cancer cell lines. We have recently reported on the development of gold(I)-phosphane complexes containing linkers amenable to bioconjugation to antibodies. More specifically, we synthesized Trastuzumab–gold conjugates. These bioconjugates were significantly more cytotoxic (sub-micromolar range) to HER2-positive breast cancer cells than the gold complexes and Trastuzumab.
Here we report on the synthesis and characterization of a series of novel cationic gold (I) complexes containing N-heterocyclic carbene ligands with various substitutions, as well as one phosphane-containing linker amenable for bioconjugation towards terminal lysine residues on antibodies. We will also report on preliminary studies for the oxidation of these species with I_2

to gold (III) compounds. The goal of this project is to bioconjugate these gold-linker complexes (1) to antibodies like Trastuzumab and explore their efficacy as ADCs.

PISTACHIO SHELLS AS REMEDIAL AGENTS FOR EXTRACTING THORIUM FROM DRINKING WATER. Dihara Hossain[1], Tanja Tane[1], Jafar Sunga Ali[1], Samuel Groveman[2], Spiro Alexandratos[1], Ali Younes[1]. [1]Department of Chemistry, Hunter College of CUNY, New York, NY, 10065. [2]Department of Chemistry and Environmental Science, Medgar Evers College, Brooklyn, NY 11225

Anthropogenic radioactivity generated by nuclear or chemical events results in the liberation of tons of radioactive heavy toxic materials to the environment. Thorium-232 (^{232}Th) is a long-lived radioactive element that is presented in the aquatic environment because of natural and anthropogenic activities. If ingested from contaminated water, it accumulates to a very high extent in the liver, kidneys, and skeleton. The biological fate of thorium in case of accidental, chronic contamination is, therefore, a pressing public health issue. Previous studies in our lab have focused on identifying pistachio shells as promising eco-friendly candidates for the removal of uranium ions from contaminated seawater. The objective of this study was to further solidify pistachio shells as an efficient remediating agent to remove thorium ions from contaminated drinking water, thus limiting their transport into humans. Using a batch study methodology, the influence of kinetics, pH, and initial thorium ion concentration on the shells' uptake of the ions were investigated. Thorium uptake reaches equilibrium at around 4 hours and increases as a function of initial thorium concentration. The impact of pH was observed to be variable but with a comparatively high uptake occurred at pH 5.5. The shell was demonstrated to be a Freundlich isotherm, and the mechanism followed a pseudo-second-order kinetics model. IR, TEM, and EDX were utilized to characterize the sorption of Th on pistachio shells. With determined trends similar to those attained in the batch studies, the shells were successfully exhibited to be viable adsorbents for thorium from drinking water samples.

INVESTIGATING THE CONSEQUENCES OF MECHANICAL AND CHEMICAL EROSION OF DENTAL AMALGAM. Liza Isayeva[1], Tanja Tane[1], Dihara Hossain[1], Jafar Sunga Ali[1], Samuel Groveman[2], Spiro Alexandratos[1], Ali Younes[1]. Department of Chemistry, Hunter College of CUNY, New York, NY, 10065. Department of Chemistry and Environmental Science, Medgar Evers College, Brooklyn, NY 11225

Dental amalgam has been used for more than a century to repair cavities in teeth. Amalgam is composed of various heavy metals, including copper (Cu), silver (Ag), zinc (Zn), tin (Sn), but most significantly, elemental mercury (Hg), which comprises 50% of the amalgam. Leaching of these metals from the amalgam is a concern due to the acidity of most beverages providing ideal conditions to re-mobilize the metals. For Hg in particular, whose ingestion has been associated with a myriad of symptoms such as memory problems and depression, its effects on the teeth have been widely debated in dentistry for almost two centuries. In this context, there is a need to investigate both the leaching of these metals from the amalgam as well as their uptake onto the surrounding teeth. In the present work, the adsorption of Hg, Ag, Zn, Sn and Cu onto hydroxyapatite (HAP), the major inorganic mineral component of teeth and bone, was investigated. The influences of various environmental parameters (e.g. time of contact with the

metal and pH) were investigated using a batch study methodology. For Hg in particular, over 70% was uptaken by synthetic HAP in <1 min and across the entire pH range, and the mechanism follows pseudo-second order kinetics. Characterization was performed by TEM and EDAX, which demonstrated the uptake of all metals of interest. The leaching of the metals from dental amalgam samples as well as their subsequent uptake over teeth samples is currently being investigated.

OMEGA-3 SUPPLEMENTS AS ACTIVATORS OF ANTIOXIDANT GENTIC PROGRAM. Najaé Campbell and Irina Gazaryan. Department of Chemistry and Physical Sciences, Dyson College of Arts and Sciences, Pace University, NY 10570.

The genetic program of antioxidant defense is activated by transcription factor Nrf2. The major constitutive way for Nrf2 activation is the stabilization of its protein by detachment from Cul III ubiquitin ligase complex. Keap1 is a redox sensing adaptor protein in Cul III complex, and upon oxidative modification of its active cysteines can either release Cul III ubiquitin ligase from the complex or undergo a conformational change resulting in dissociation into monomers and a subsequent release of Nrf2 protein from the complex. In both scenarios, Nrf2 protein is stabilized, translocate to the nucleus and triggers the expression of more than one hundred of antioxidant proteins and enzymes. Omega-3 fatty acids are known for their benefits for lowering cholesterol and keeping biological membranes in good shape. Here, using a cell-based luciferase fusion reporter assay, we show that various commercially available omega-3 supplements (Finest Nutrition, Nature's Made, Nature's Bounty, CVS Omega fish oil supplements) can activate the genetic antioxidant program triggered by Nrf2. The magnitude of activation depends on the content of EPA in omega-3 supplement, and Finest Nutrition supplement is the best supplement, which performance closely matches the prescription strength omega-3 medication. The mechanism of Nrf2 stabilization by omega-3 supplements is pro-oxidative since reporter activation is decreased in the presence of stoichiometric antioxidants such as N-acetyl cysteine or ascorbic acid.

NANOCHEMISTRY AND SURFACE CHEMISTRY

LIGHT-DRIVEN WATER-OXIDATION USING NANOSTRUCTURED METAL-BASED POLYMER COMPOSITE FILMS. Oshane Annon, Abril Flores, Christina Rivera and Yosra M. Badiei*. Department of Chemistry, St. Peter's University, Jersey City, NJ 07306

In the past few decades, there has been a rising concern about severe global environmental issues due to the increase in carbon dioxide emissions from the combustion of fossil fuels. The need to mitigate the effects of increasing CO_2 emissions has resulted in the synthesis of molecular water-oxidation catalysts (WOCs) that would enable water splitting to hydrogen and oxygen via the use of dye-sensitized photo-electrosynthesis cells (DSPECS). The solar fuel hydrogen can be utilized in a fuel cell to generate electricity representing a potential solution for the energy utilization and storage problem. However, the discovery of new and functional strategies for the immobilization of (WOCs) remains a crucial step in developing applicable DSPECS. The traditional approach for the surface attachment of WOCs to transparent conductive oxides, such as fluorine-doped tin oxide (FTO), occurs via the modification of the

WOCs' ligand structures through the addition of anchoring groups such as carboxylic acids or phosphonates. Modifying ligand structures generally results in problems such as catalyst instability and desorption from the surface due to hydrolysis. Herein we report the immobilization of unmodified WOCs onto a poly(acrylic) acid (PAA) film that was UV-grafted onto the surface of an FTO. Both immobilized WOCs|PAA|FTO films and PAA|FTO films were characterized using various techniques, including attenuated total reflectance Fourier transform infrared spectroscopy, Toluidine Blue O (TBO) colorimetric staining, and cyclic voltammetry. These characterization techniques provide evidence for the UV-grafted PAA|FTO films and successful immobilization of WOCs.

NOVEL PEPTIDE BOLAAMPHIPHILE IONIC LIQUID GELS FOR THE DEVELOPMENT OF NERVE GUIDANCE CONDUITS. Diego S. Perez, Charlotta G. Lebedenko and Ipsita A. Banerjee Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, NY 10458

Nerve guidance conduit (NGC) development in the field of neural tissue engineering through means of three dimensional (3D) bioprinting has proven to be effective at addressing issues regarding nerve regeneration. A key challenge that remains in the development of NGC scaffolds is the issue of glial scarring, a unique central nervous system issue where axon tissue regeneration is inhibited by reactive and migrating glial cells creating a barrier-like extracellular matrix chemical composition. While the glial scar has been targeted by some biomimetic peptides capable of reducing the glycosaminoglycan over-expression which highly contributes to glial scarring, the multidimensional nature of the glial scar encourages the development of novel biomaterial scaffolds that incorporate the latest advancements in tissue engineering nanotechnologies to overcome singular approaches. This research computationally investigated the combination of two recent advances in biomaterial design: ionic liquid (IL) interactions with peptide bolaamphiphiles (PbAs) and optimization of PbA cell signaling through enhanced supramolecular motion. Supramolecular self-assembly of the PbAs and ILs coupled with receptor-ligand Molecular Dynamics simulations in Amber afforded insight into the efficacy of the bioactive signals in this novel biomaterial composite. We were able to design novel PbA-IL composites that target two receptors implicated in the mechanisms related to glial scarring, neural cell adhesion molecule (NCAM) and 37-kDa laminin receptor precursor (37LRP), with enhanced supramolecular motion.

A COMPARATIVE STUDY ON THE INTERACTIONS BETWEEN SINGLE-WALLED CARBON NANOTUBES AND IMIDAZOLIUM AND PYRROLIDINIUM IONIC LIQUIDS. Bethva Robert, Ho Martin Yuen, Sharon Lall-Ramnarine and Tirandai Hemraj-Benny. Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, NY, 11364.

Supercapacitors have great potential to serve as efficient energy storage devices. However, to facilitate more widespread usage in practical applications, developing more efficient electrodes and electrolytes is necessary. Carbon nanotubes can serve as effective electrodes due to their high surface area. Additionally, ionic liquids can act as excellent electrolytes due to their expansive electrochemical windows. It is necessary to investigate the specific interactions

between single-walled carbon nanotubes and various ionic liquids to contribute to the development of optimal electrodes and electrolytes for energy storage devices. In this comparative study, mixtures containing single-walled carbon nanotubes and ionic liquids containing imidazolium and pyrrolidinium cations coupled with bis(trifluoromethylsulfonyl)amide (NTf_2^-) anion were investigated by Mid-IR spectroscopy and UV-Visible spectroscopy.

POLYRHODANINE METAL NANOPARTICLES, SYNTHESIS, AND ANALYSIS. Nickayla Spence[1], Moni Chauhan[1], Arnab Sharma[1], Saleh Jaser[1], Samantha Nieves[2], Qiaxian Johnson[2], Bhanu P. Chauhan[2], [1]Department of Chemistry, Queensborough Community College of CUNY, Bayside, NY, [2]Department of Chemistry, William Patterson University, Wayne, NJ

Nanoparticles are extensively researched for new medical diagnostics and targeted treatments for cancer. Core-shell nanoparticles and nanotubes are highly functional materials, and their properties can be modified by either changing the constituting materials or the core to shell ratio. Different applications are performed by coating the core particles, such as surface modification, the ability to increase the stability, functionality, controlled release of the core, dispersibility, and enhancing photoluminescence. In our research, we are investigating core-shell and nanotubular synthesis of polyrhodanine Copper nanoparticles in a single-step oxidation-reduction reaction. In the first step of the reaction, the rhodamine monomer forms a one-dimensional complex with copper ions due to coordinative interaction. In the second step, oxidative, reductive polymerization of rhodamine occurs with the reduction of copper ions. The process is carried out in the microwave at 80^{o}C in ethanol. The morphology of the materials was analyzed *in situ* via infrared (IR) spectroscopy, SEM (Scanning Electron Microscopy), EDX (Energy Dispersive X-ray spectroscopy), and TEM (Transmission Electron Microscopy) analysis. Rhodanine derivatives have been found to control human immunodeficiency virus (HIV), hepatitis C (HCV), and Dengue virus proteins. Detailed background research on these applications and the future treatment of these materials for anti-viral, anticancer, and antimicrobial activity and their efficacy as an adsorbent of heavy metals and dyes will be presented.

EFFECT OF INITIAL SOL-GEL PH ON RELEASE KINETICS OF TEMPOL Daniel Goldstein, Sara Lifshitz, Hannah Ariel, and Uri Samuni Department of Biochemistry, Queens College, CUNY, Queens, NY 11367 **[VIRTUAL PRESENTATION]**

Silica based sol-gels are comprised of cross-linked polymeric networks of Si-O-Si-O that can be initiated by acid or base catalyzed hydrolysis of an alkoxysilane such as tetramethyl orthosilicate (TMOS). When the matrix is bathed in a buffer solution, water molecules can diffuse and fill the porous network resulting in a wet-Gel. Furthermore, during the sol-gel synthesis, it is possible to embed analyte/biomolecules within the matrix, to be used in a variety of applications. Depending on the size, charge and shape of the analyte, it may be able to diffuse out of the sol-gel matrix to the bathing buffer. The objective of this study was to characterize the effect of the initial pH when the sol-gel was cast on the rate and extent of release of a small molecule, 4-Hydroxy-TEMPO (TEMPOL). Here we show the comparison of the rate and extent of the release of TEMPOL for matrices made at either pH 2.3 or pH 7.

CATALYTIC ACTIVITY OF ENZYMES IN SOL-GEL MATRIX/NANOGELS VS IN SOLUTION. Nataniel Natanov, Kahtan Alsaedi, Sara Lifshitz, Jalal Haidery, Anna Li, Angela Fried, Jorge Ramos, and Uri Samuni. Department of Chemistry and Biochemistry, Queens College, 65-30 Kissena Blvd, Queens, NY 11367 **[VIRTUAL PRESENTATION]**

Using alkoxysilanes the sol-gel method allows us to generate a solid amorphous matrix that is structurally stable, chemically inert, optically transparent and highly porous. This matrix can be utilized to encapsulate enzymes such that they remain intact and functional. Moreover, some studies demonstrated that the encapsulated enzymes are rendered more stable than in solution. We explored the catalytic activity of several enzymes when encapsulated in silica based sol-gel matrices and nanogels vs. their activity in solution. Such enzymes include, Glucose oxidase (GOX) and heme proteins such as Hemoglobin and Myoglobin. GOX is an enzyme known to confer antibacterial properties to certain fungi. We performed kinetic measurements of [H_2O_2] evolution for the reaction of beta-D-glucose and oxygen, using an indirect spectroscopic iodide assay. We compared the activity of the enzyme when in a buffer solution vs. when encapsulated within silica-based sol-gel matrices and nanogels.

ORGANIC CHEMISTRY

SYNTHESIS AND CHARACTERIZATION OF NEW FLAVYLIUM COMPOUNDS WITH A PHENYL GROUP. Ketevan Basilashvili and Jeonghee Kang Department of Chemistry, St. Joseph's College, Brooklyn, NY 11205

Anthocyanins are glycosylated derived red-purple-blue flavonoid pigments found in the outer layer of plant structures such as fruits, vegetables, flowers. The core structure of anthocyanins is the flavylium cation. Anthocyanidins are plan pigments formed by the hydrolysis of anthocyanins, characterized by the same flavonoid structure without glucose on the number 3 carbon of the C ring of the flavylium cation. Those colored pigments can be used as a dye in Dye-Sensitized Solar Cells (DSSC) and as a sensor or therapeutic compound for diseases caused by protein aggregation. Flavylium compounds with a phenyl group, 7, 8- dihydroxy-4'-phenyl flavylium, 7,8- dihydroxy-3-phenyl flavylium, and 7-hydroxy-3 phenyl flavylium were synthesized using Aldol condensation. The products were confirmed and characterized by UV/Vis, IR, and NMR spectroscopies. In this presentation, the synthesis and characterization of the flavylium compounds will be discussed.

MECHANISTIC STUDIES OF TAUTOMERIZATIONS IN GUANINE-CYTOSINE BASE PAIR. Benjamin Herrera,[1] Charles Doubleday[2] and Dr. Edyta Greer[1]; [1]Department of Natural Sciences, Baruch College, New York, NY, 10010; [2]Department of Chemistry, Columbia University, New York, NY, 10027

The tautomerization of guanine (G) and cytosine (C) DNA base pair was investigated computationally with wb97xd functional and 6-311+G(d,p) basis set. Tautomerization is a process which involves proton transfers between guanine and cytosine. It produces rare tautomeric forms that may lead to errors in DNA replication, expression and thus cause mutations which could be the cause of many genetic diseases and even cancer. The purpose of

investigating the energy path of the tautomerization reaction is to see how likely the reaction is to take place in a realistic environment. This can be done computationally to consider surrounding molecules to the DNA, particularly water molecules, which can affect stability due to solvation effects. Our study revealed that the energy of activation for G-C tautomerization is 12.9 kcal/mol. The reaction was found to be exergonic by 10.3 kcal/mol. Mechanistic details, including contributions of tunneling will be discussed.

COMPUTATIONAL STUDIES OF THE DECARBOXYLATION OF CANNABIDIOLIC ACID TO CANNABIDIOL. Florence Uritsky[1], Dr. Edyta Greer[1], and Dr. Charles Doubleday[2]; [1]Department of Natural Sciences, Baruch College, New York, NY, 10010; [2]Department of Chemistry, Columbia University, New York, NY, 10027

Cannabidiolic acid (CBDA) is one of the many compounds produced by the cannabis plant, and when decarboxylated, it gets converted to cannabidiol (CBD). The decarboxylation of cannabidiolic acid (CBDA) via loss of CO2 to form cannabidiol (CBD) was studied using computational methods. Computations were carried out with B3LYP/6-31G(d,p). The study of the decarboxylation of CBDA revealed that it involves acid catalyzed keto-enol tautomerization, which was found to be the rate-limiting step. A second derivative of the cannabis plant, delta-9-tetrahydrocannabinol (THC), is also obtained through decarboxylation, but the two compounds have differing effects on the body. While THC produces psychoactive effects when absorbed into the body, CBD produces calming effects, and has various anti-inflammatory and anticonvulsant properties. Decarboxylation reaction energies will be discussed and compared to the decarboxylation of THC.

THE INVESTIGATION OF STRUCTURAL EFFECTS ON THE BINDING STRENGTH OF FLAVONES WITH HUMAN SERUM ALBUMIN. Steven Octaviano, and Jianwei Fan Department of Chemistry and Biochemistry, Manhattan College, Bronx, NY 10471

Human Serum Albumin (HSA) is the most abundant protein found in human blood. It is composed of 585 amino acids with three domains, each with two subdomains, A and B. HSA has the ability to bind with drug molecules, allowing for a given drug to be transported across the body. The binding strength of a drug to HSA is an important factor to consider when designing a drug molecule, as a higher or lower binding strength affects the active concentration or the delivery rate of a drug. HSA has two primary binding sites. Site 1 is on domain IIA, and site 2 is on domain IIIA. Binding site 1 is generally non-polar, preferring to bind with hydrophobic molecules. As such, drug molecules with aromatic rings generally bind themselves to site 1. Flavone is an example of a drug scaffold, being the base for drugs such as Rutin and Hidrosmin. The binding strength of flavone is dependent on its polarity, which can be affected by the addition of certain functional groups. Analysis of binding strength can be determined via spectrofluorometry, as binding site 1 contains the amino acid Tryptophan which has strong fluorescent properties. The fluorescence property of HSA will be altered or quenched upon the binding of a molecule to the binding site. The level of quenching can determine the binding strength of a given molecule. It was found that flavone more strongly binds with HSA with the addition of non-polar functional groups, while it binds less strongly with the addition of polar functional groups.

DEVELOPMENT OF MULTIPLE TARGET MOLECULES FOR THE TREATMENT OF ALZHEIMER'S DISEASE. Dr. Jole Fiorito and Fawaz Syed New York Institute of Technology, Northern Boulevard, Valentines Ln, Old Westbury, NY 11568

Alzheimer's disease (AD) is the 7th leading cause of death in the United States according to the NIH and is characterized by the progressive deterioration of cognitive performance. It does not currently have a cure, and treatments aim only to mitigate the symptoms of mild AD. The disease proceeds through the accumulation of improperly processed amyloid β peptides into plaques and intracellular neurofibrillary tangles of tau proteins. AD is a multifactorial neurodegenerative disorder with several target proteins contributing to its etiology. Potential therapeutic strategies to combat AD include the inhibition of phosphodiesterase type 5 (PDE5) and the modulation of histone acetyltransferase, among others. Current drug therapies rely on the administration of a single drug that acts on one specific molecular target or the combination of drugs acting on different targets. In this research study, we propose the development of a multi-target-directed-ligand (MTDL), wherein one drug molecule interacts with multiple targets involved in the disease. To investigate this therapeutic approach, we designed a small library of quinoline derivatives as potential MTDL candidate molecules with biological activity on both PDE5 and HAT enzymes. Thus far, one molecule has been successfully synthesized. Upon finalization of the molecule library, each candidate will be tested via PDE5 and HAT assays to determine their effect on enzymatic function.

PHYSICAL CHEMISTRY AND CHEMICAL EDUCATION

WORKING TOWARDS A SOLUTION TO THE TRAVELING SALESMAN PROBLEM USING AN OSCILLATING CHEMICAL REACTION. Jake Bordenca, Hugh H. Cheung, Sabrina G. Sobel, Department of Chemistry, Hofstra University, Hempstead, NY, 11549

The traveling salesman problem (TSP) is a problem that asks how a hypothetical person, i.e. a traveling salesman, would visit several points of interest once each and return to the starting point in the shortest possible distance. This has applications in many industries such as the transport and delivery of food or mail. The solving of the TSP has been attempted using AI, neural networks and slime molds. The purpose of this experiment is to use an inorganic reaction (the Belousov−Zhabotinsky Reaction or BZ Reaction) as opposed to a biological or computorial method to solve the TSP. Currently, there has been research done on this reaction using a light sensitive ruthenium-catalyzed reaction and extensive light hardware and software, but we came up with another possible solution using a dual-catalyzed recipe of Ruthenium and Ferroin with a simpler light set-up to simulate a grid and potentially make the TSP solvable.

GENERATION OF NITRIC OXIDE IN A CONTROLLED RATE THROUGH THE REACTION OF SNP AND GLUTATHIONE. Erin Gal, Jalal Haidery, Anna Li, Jorge Ramos, and Uri Samuni. Department of Chemistry and Biochemistry, Queens College, 65-30 Kissena Blvd, Queens, NY 11367

Nitric oxide (NO) is a free radical produced naturally by nitric oxide synthase as a byproduct of cellular responses. Sodium nitroprusside (SNP) is an inorganic compound, which in the

presence of glutathione, a tripeptide antioxidant, produces nitric oxide through a redox reaction. The mechanism for this reaction results from the reduction of the glutathione's thiol group by SNP to form a disulfide complex in aerobic conditions, generating nitric oxide as a byproduct. Our objective is to form nitric oxide in a controlled rate to be used in cell survival studies. We used the Griess assay to follow nitrite accumulation as an indirect method to follow the rate of nitric oxide formation.

SPECTROSCOPIC STUDY OF THE BINDING INTERACTIONS BETWEEN HSA AND COUMARIN SCAFFOLDS. Katherine Gilmartin and Dr. Jianwei Fan Manhattan College, Department of Chemistry and Biochemistry, Riverdale, NY 10471

One of the most abundant proteins found in the blood is Human Serum Albumin (HSA). HSA has been studied extensively for its binding interactions with drug molecules in order to transport them to specific target sites within the body. While the binding to HSA increases stability of the drug, it also decreases the free concentration, or the effective concentration of the drug, therefore, optimizing the binding strength between the drug and HSA is an important research area in medicinal chemistry.
HSA is a single chain protein composed of 585 amino acids, whose structure is made up of three domains (I, II, III) with two subdomains each (A and B). HSA has two primary drug binding sites, located in IIA and IIIA. Through this research the binding interactions of drug scaffolds, specifically three families of Coumarin, to the binding site in IIA of HSA were studied. Using fluorescence spectroscopy, the binding interactions between Coumarins and HSA were observed by studying the quenching effects the Coumarins have on the fluorescence of HSA. To determine the strength and favorability of the scaffolds bonding to HSA, parameters such as the Stern-Volmer quenching constant (K_{SV}), the binding constant (K_a), and the number of binding sites (n) on the protein were calculated. These parameters granted insight into how polarity, hydrophobicity and substituent location impact the binding strength of Coumarin scaffolds and HSA.

MAG-WALKING SIMULATED ANNEALING MONTE CARLO STUDY OF NANO-SOLVATED AMMONIUM CHLORIDE. Sangjoon Lee, Steven L. Topper and Robert Q. Topper. Department of Chemistry, The Cooper Union for the Advancement of Science and Art, New York, NY 10003

Airborne ammonium chloride nanoparticles are formed by the reaction of ammonia and hydrogen chloride in the presence of water. Although it is known that the formation can be affected by the humidity, temperature, and the presence of dissolved organic matter, less is known about the mechanism for aerosol particle growth. In the present study, the minimum energy structures of nano-solvated ammonium chloride (surrounded by 2-8 water molecules) were determined using the mag-walking simulated annealing Monte Carlo method. Implemented via the TransRot software, mag-walking uses either a small, optimized stepsize or (randomly) a larger, magnified fixed stepsize, and can be tuned to either find the global minimum structure or, where relevant, higher-energy structures of interest. The method and parameters were benchmarked through the successful replication of literature global minimum energy values of water clusters using the TIP3P, TIP4P, and TIP4P/2005 empirical pair

potentials. In future work, we plan to use ab initio calculations to predict thermodynamic properties, reaction energetics, and infrared spectra of nano-solvated ammonium chloride.

IMPLEMENTATION OF ELECTRONIC LABORATORY NOTEBOOKS IN THE UNDERGRADUATE ORGANIC CHEMISTRY LABORATORY. Matthew Leshinsky, Vandana Bindra, Nanette Wachter, and Sabrina Sobel Department of Chemistry, Hofstra University, Uniondale, NY 11549

Organic chemistry laboratories are often a pivotal part of many students' careers in majors revolving around STEM. There are many students who struggle applying the knowledge that they learn in lecture to laboratory work. Following the COVID-19 pandemic, having gone through remote education, there has been distinct deterioration in student academic performance. Additionally, many students have yet to have any laboratory experience at the university level. Herein we describe one method we began to implement in order to combat these challenges while improving student engagement, performance, and understanding of the lab experience. The method we used was the implementation of an electronic laboratory notebook. We will discuss how we selected our choice for an electronic laboratory notebook, the instructors' perspective in evaluation of student work, and the performance of students during this pilot program.

SCIENCE HEROES GAME FOR K12 STUDENTS. Matthew Mistretta, Scott Buzzolani. Adelphi Department of Chemistry, Adelphi University, 1 South Avenue, Garden City, NY 11501

All students taking chemistry are required to know the names and achievements of some specific scientists to answer questions on standardized exams such as the New York state regents exams and exams from the American Chemical Society. Some figures students learn about are Dmitri Mendeleev, Henry Louis Le Chatelier, Ernest Rutherford, and Marie Curie. Oftentimes the multitude of names and scientific principles confuse students. The Science Heroes game plays similarly to Hedbanz, a family fun guessing game, where the players put a card to their head with a picture and they must ask questions to determine who they are. The character cards in Science Heros are all famous scientists and the players must ask questions, such as "Did I study gasses?" or "Did I do research in Germany?" to determine which scientist they are. Included with the game is a packet of information containing brief biographical information about each scientist's life and achievements. A scientific adaptation of a classic game can be used in classrooms to help students learn scientist's names and related scientific discoveries in a more fun manner compared to something as dull as reading notes or flashcards. This game is a fun way of popularizing science and helping students review basic science knowledge. Teachers can use it in versatile ways in the classroom to introduce and review science topics. The game was created by Adelphi University students Scott Buzzolani and Matthew Mistretta under the mentorship of professor Justyna Widera-Kalinowska.

POLYMER CHEMISTRY

KINETIC ANALYSIS OF BIODEGRADATION OF GIANT LIPOBEADS IN THE PRESENCE OF REDUCING AGENTS: A PLATFORM FOR "SMART" ANTICANCER DRUG AND GENE DELIVERY. Neslihan Tabaru and Dr. Sergey Kazakov Department of Chemistry & Physical Sciences, Pace University, Pleasantville, NY 10570

According to the International Agency for Research on Cancer, approximately 19.3 million new cancer cases and almost 10 million cancer deaths occurred globally in 2020. Chemotherapeutic drugs are highly toxic, killing healthy cells, and causing adverse reactions. The ultimate goal of our research is to develop the so-called bioscopic anticancer chemotherapy with superior tumor response and minimum side-effects even at a greater drug loading concentration. Spherical nanoparticles consisting of a hydrogel core coated by a lipid bilayer known as lipobeads is a good candidate for delivery of chemotherapeutic agents to and their controlled release within targeted organs. In this work, the previously synthesized microgels degradable under presence of reducing agents were used for preparation of lipobeads by mixing microgels with liposomes of different lipidic compositions. Kinetics of degradation of fluorescently labeled lipobeads in the presence of reductants (dithiothreitol and glutathione) was studied by confocal microscopy. Three steps were distinguished in the course of degradation: de-crosslinking by breakage of disulfide bridges, polymer network swelling, and outward diffusion of uncleavable polymer chains. Both decrease in fluorescence intensity and swelling of the hydrogel core during degradation revealed the second order kinetics. The characteristic time (half-life time) of overall changes varied from seconds to minutes depending on pH, origin and concentration of reductants added, and size of microparticles. The results are promising in terms of engineering novel "smart" multifunctional lipobeads, which can provide a number of novel and unique options such as new schemes of drug release and combined drug delivery without adverse side-effects.

DEGRADATION OF POLY(*O*-TOLUIDINE) POROUS MICROSPHERES FOR PAYLOAD DELIVERY APPLICATIONS. Che Chang and David M. Sarno Chemistry Department, Queensborough Community College, Bayside, NY 11364

Porous polymer capsules are of interest for cargo loading and delivery and have biomedical and anticorrosion applications. We have previously developed a single surfactant water-in-oil-in-water double emulsion method that produces porous microspheres of poly(*o*-toluidine), POT, and related polymers. We are now exploring simple methods by which they may be degraded in order to release a potential cargo. SEM images indicate that porous POT spheres are indefinitely stable if left undisturbed in water, but are significantly damaged by stirring, which reveals their interior. The capsules become increasingly fragmented over time and are completely destroyed after one week of stirring. Very similar results are observed in 25% and 50% aqueous acetone; however, exposing them to 25% and 50% aqueous NMP produces mostly irregular aggregates within one hour. Our early results suggest that porous POT spheres could slowly release a payload over time simply by stirring, or more rapidly in the appropriate solvent. In addition to time and solvent, we intend to examine the effects of temperature and pH on capsule degradation.

DEVELOPMENT OF ELECTROSPUN IONIC LIQUID-POLYMER MEMBRANES. Elijah Bernard,[1] Domenec Paterno,[2] Sophia Suarez[2] and Sharon Lall-Ramnarine,[1] [1]Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA. [2]Department of Physics, Brooklyn College, City University of New York, Brooklyn, New York 11210, USA

Ionic liquid (IL)-polymer mixtures are emerging as a class of smart materials, which can be tuned to exhibit both the attractive properties of ILs such as low flammability, low volatility and inherent conductivity and the solid support of polymers. In many devices, liquid electrolytes are problematic and solid electrolytes are more advantageous due to higher thermal stability and lower predisposition to leakage. Electrospinning of IL-polymers mixtures has been reported as an advantageous technique to produce fibers and membranes with advantages over traditional smart nanocomposite materials. In this work, we explore the preparation of IL-Polymer mixtures optimized for producing highly conductive electrospun membranes, by variation of the type of IL and polymer used and the ratios in which they are combined. We report here on the preparation of imidazolium bis(trifluoromethylsulfonyl)amide ionic liquids mixed in varying concentrations with polyvinylchloride (PVC), polyacrylonitrile (PAN) and polyvinylpyrrolidone (PVP). The polymers were dissolved in Dimethylformamide (DMF) and mixed with the ILs dissolved in DMF. Thus far, the challenge in preparing these IL-Polymer mixtures, is finding the optimum ratio of IL:Polymer that can be electrospun without issue. Preliminary results show that using 4:1 or 2:1 weight percent mixtures of BMIM NTf_2 : PVC in DMF created a solid and a gel respectively both of which could not be electrospun. Ongoing and future work will focus on varying the ratios of the IL-Polymer mixtures as well as the type of IL and the type of polymer. We anticipate that highly conducting electrospun IL-Polymer membranes will make important contributions when implemented into energy conversion devices such as Dye-Sensitized Solar Cells.

AN INVESTIGATION INTO BINDING INTERACTIONS OF BRAF RECEPTORS WITH TARGETED LIGANDS. Dominic J. Lambo, Charlotta G. Lebedenko and Ipsita A. Banerjee. Department of Chemistry, Fordham University, 441 East Fordham Road, Bronx, NY 10458

The BRAF V600E receptor has been found to be over-expressed in several types of cancers, making it a target for drug design. In this work, we developed multiple novel peptide-based conjugates to analyze their binding affinity and stability capabilities with both the BRAF wildtype receptor and the BRAF V600E receptor. Both receptors were examined to determine if the peptide conjugates provoke binding specificity toward the BRAF V600E over the BRAF wildtype receptor. The peptide sequence utilized for conjugation is known for targeting tumor neovasculature. We hypothesized that conjugating it with selected polyphenols may further enhance its tumor targeting ability. We used the POCASA server to determine the active sites, and based on the PLIP studies, it was evident that the conjugates with the highest binding affinity were those that formed high number of hydrogen bonds and hydrophobic interactions docked to the active sites of the receptors. Molecular dynamic simulations were carried out to determine the stability of the receptor docked ligands over the course of 100 ns simulations. With each compound, upon conjugation with the peptide sequence, the number of interactions

increased, therefore, the binding stability drastically increased upon conjugation. Additionally, bioavailability was examined using SwissADME which provided the potential in vivo application of these peptide conjugates. These findings provide insight into the molecular interactions of the conjugates and their potential for binding to and targeting the BRAF V600E receptor in developing new therapeutics for targeting cancer.

PREPARATION OF IONIC LIQUID–POLYMER GELS FOR GAS SEPARATION. Shameir Nembhard,[1] Nicole Zmich,[1] Jasodra D. Ramdihal,[1] Edward W. Castner, Jr.,[2] James F. Wishart[3] and Sharon I. Lall-Ramnarine[1] [1]Department of Chemistry, Queensborough Community College of the City University of New York, Bayside, New York 11364, USA; [2]Department of Chemistry and Chemical Biology, Rutgers University, The State University of New Jersey, Piscataway, NJ 08854; [3]Chemistry Division, Brookhaven National Laboratory, Upton, New York 11973, USA

Ionic liquids (ILs), with their characteristic low vapor pressures and tunable properties, are potentially suitable for membrane-based separation of gases under vacuum conditions, but their viscosities are too low. Ion gels prepared from ionic liquid-polymer mixtures have shown promise as solid supports that facilitate the separation of gases while retaining IL properties. However, key attributes of ion gels are still poorly understood, and both the structure of the IL and the IL/polymer ratio need to be optimized to achieve good separation of gaseous mixtures. This project aims to develop improved and energy-efficient separation mechanisms that will reduce hazardous gas releases into our environment. We report on the preparation of selected ion gels. Ionic liquids based on tetraalkyl-phosphonium and ammonium cations and bis(trifluoromethylsulfonyl)amide anions were synthesized and purified in our labs. The alkyl groups on the IL cations were selected by design to form a significant non-polar region, and thus optimized for use as gas separation membranes. The polymeric material used in the ion gels is a common battery development diblock copolymer, PDVF-*co*-HFP. H-1 and C-13 Nuclear Magnetic Resonance (NMR) spectroscopy was used to confirm the structure of the ILs, and they were combined with five weight percent of the di-block co-polymer to produce ion gels. Preliminary results reveal soft, gel-like materials rather than thin membranes. The IL/polymer ratio will be varied to produce membranes optimized for gas separations and the ion gels will be characterized using differential scanning calorimetry, high-energy X-ray scattering and Pulse-Gradient Spin Echo NMR spectroscopy.

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