NORTHERN NEW YORK LOCAL SECTION OF THE AMERICAN CHEMICAL SOCIETY

10TH ANNUAL UNDERGRADUATE AND GRADUATE CHEMISTRY AND BIOLOGY RESEARCH SYMPOSIUM

SUNY PLATTSBURGH
PLATTSBURGH, NY
MARCH 2ND, 2019

Table of Content

NORTHERN NEW YORK LOCAL SECTION
10TH ANNUAL NNY ACS RESEARCH SYMPOSIUM

***Time*:** Saturday, March 2, 2019 from 8:45 am to 3:30 pm

Where: SUNY Plattsburgh, Angel College Centre (Ballroom), Plattsburgh, NY

***Purpose*:** Bring together faculty and students from diverse chemical and biological backgrounds for communicating interdisciplinary research and increase interactions and collaborations.

***Overview*:** Students will present their work in one of two formats: a poster or a short oral presentation. Seven short undergraduate oral presentations (15 minutes each followed by 5 min questions from audience) are scheduled in the morning followed by a plenary lecture, lunch and then a poster session.

Schedule

8:45-9:15 am	Registration and posters set-up (coffee, juices and muffins)
9:20 am	Welcome note from the host institution & NNY local section's chair

Undergraduate Oral Presentations

9:30 am	Rebecca Meacham (Clarkson University)
9:50 am	Nicholas Flint (SUNY Potsdam)
10:10 am	Beza Tuga (SUNY Plattsburgh)
10:30 am	Lisa Kozodoy (St. Lawrence University)
10:50 am	**(10 min) Coffee Break**
11:00 am	Hannah Despres (SUNY Plattsburgh)
11:20 am	John Paliakkara (SUNY Potsdam)
11:40 am	Megan Carhart (Clarkson University)
12:00 pm	**Lunch**

Plenary lecture

12:45 pm	**Dr. Silvana Andreescu (Clarkson University): "Biosensors in Everyday Life"**

Poster Session

1:30 pm	Poster Session & Judging (cookies and cider)
3:00 pm	Final Remarks & Awards Presentation
3:30 pm	Adjourn

NNY ACS LOCAL SECTION OFFICERS

Dr. Fadi Bou-Abdallah – (Chair)
Chemistry Department
SUNY Potsdam
bouabdf@potsdam.edu

Dr. Silvana Andreescu– (Vice Chair)
Chemistry & Biomolecular Science
Clarkson University
eandrees@clarkson.edu

Dr. Dana M. Barry – (Secretary)
Center for Advanced Materials Processing (CAMP)
Clarkson University dbarry@clarkson.edu

Dr. Ewa Pater – (Treasurer)
Chemistry Department
SUNY Plattsburg paterem@plattsburgh.edu

Dr. Rajesh Sunasee – (Councilor)
Chemistry Department
SUNY Plattsburgh
rsuna001@plattsburgh.edu

Dr. Martin Walker – (Alternate Councilor)
Chemistry Department
SUNY Potsdam
walkerma@potsdam.edu

*_

SYMPOSIUM ORGANIZERS:

Dr. Rajesh Sunasee, SUNY Plattsburgh
Dr. Ewa Pater, SUNY Plattsburgh
Dr. Fadi Bou-Abdallah, SUNY Potsdam

POSTER SESSION ORGANIZER:

Dr. Karina Ckless, SUNY Plattsburgh

SPECIAL THANKS:

Ms. MaryNell Bockman, SUNY Plattsburgh

SPONSORS:

Northern New York Local Section
of the American Chemical Society &
SUNY Plattsburgh ACS Student Chapter

PARTICIPATING UNIVERSITIES:

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation # 1**********

Dynamic Covalent Exchange in Polyanhydrides

Presenter's Name: Rebecca Meacham
Faculty Mentor: Dr. Devon Shipp
Co-authors: Ana Witkowski, Kelly Tillman
Clarkson University

In recent years, shape memory polymers have become increasingly popular, due to their ease of fabrication, low production cost, relatively low density, and high recovery of a permanent shape. We are looking to demonstrate the shape memory characteristics of degradable polyanhydrides when heated above and then cooled below their Tm (crystalline melt temperature). Preliminary work has shown that polyanhydride-poly(-caprolactone) composites are capable of exhibiting shape memory properties. However, the shape memory was complicated by the exchange that the anhydride groups undergo at temperatures above ~ 60 ^{o}C which relieves stress in the polymer, causing poor shape recovery. This was overcome by using polymers with Tm ~30-40 ^{o}C. Furthermore, at elevated temperatures this exchange process can lead to new permanent shapes because of the anhydride exchange. In the present work, we are looking to create all-anhydride polymers made using a monomer combination that also has low Tm values to form a polymer that will successfully exhibit shape memory behavior. Additionally, at temperatures of 80-90 ^{o}C, we expect the exchange to occur quickly, which will allow for self-healing to occur. Stress relaxation in polymers with various monomer compositions will be measured to determine temperature ranges that can be used for either shape memory or self-healing.

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation # 2**********

Probing the Interactions Between the Nuclear Receptor Coactivator-4 and Ferritin

Presenter's Name: Nicholas Flint
Faculty Mentor: Dr. Fadi Bou-Abdallah
Co-author: Ayush Srivastava
SUNY Potsdam

To prevent free iron from generating harmful reactive oxygen species, cells use ferritin, a ubiquitous iron storage and detoxification protein. In mammals, ferritin is expressed as two different subunits, Heavy or (H) and Light or (L), which co-assemble to form a spherical protein shell of 24-subunits. Ferritin is able to accommodate up to 4000 Fe atoms per molecules inside its hollow cavity. The process of releasing iron from ferritin to maintain cellular iron homeostasis is largely unknown. It has been proposed that the C-terminus of a 70-kDa protein called the cargo receptor Nuclear Coactivator-4 (NCOA4) binds to ferritin and induces its autophagic degradation through a process known as ferritinophagy. However, the exact mechanism of this interaction has not yet been determined. To determine the thermodynamics of this binding interaction and understand the process of ferritinophagy, we used isothermal titration calorimetry, fluorescence quenching, and absorption spectroscopy. Our results show a binding stoichiometry of 8 NCOA4 molecule per ferritin shell suggesting that the binding occurs at the intersection of the 8 ferritin three-fold channels. The interaction of NCOA4 with ferritin is shown to proceed via an exothermic process with an average association constant about 105 M-1. In-vitro iron release kinetics using the ferritin-NCOA4 complex demonstrated about 50% reduction of iron released, suggesting inhibition of the pathways through which the electrons generated by reducing agents can access and reduce the ferritin iron core.

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation # 3**********

Synthesis of poly(diallyldimethyl ammonium chloride) coated cellulose nanocrystals as a sustainable and biocompatible antimicrobial agent

Presenter's Name: Beza Tuga
Faculty Mentor: Dr. Rajesh Sunasee
Co-authors: Yusha Imtiaz, José de Ondarza
SUNY Plattsburgh

As a result of their bioavailability, sustainability, biocompatibility, low cost and large surface area to volume ratio, CNCs could be used to design effective antimicrobial agents. In this study, our main goal is to investigate the effect of physical immobilization of the antimicrobial polymer, poly(diallyldimethyl ammonium chloride) (PDDA) on biocompatible CNCs surface. Cationic PDDA with two different molecular weights (MW~8000 and 240,000) were coated on the negative surface of carboxylated CNCs via electrostatic interactions in the presence of sodium chloride at room temperature. The resulting CNCs-PDDA complexes were purified by centrifugation and isolated by freeze-drying. CNCs-PPDA complexes were characterized by FT-IR spectroscopy, and their apparent hydrodynamic sizes were analyzed by dynamic light scattering (DLS). An increase in the hydrodynamic size was obtained which indicated the successful coating of PPDA on the CNCs surface. The nature of the surface charges on carboxylated CNCs and CNCs-PDDA complexes were characterized by measuring the zeta potential of the particles in Milli-Q water. The antimicrobial activity of the CNCs-PDDA complexes, currently under investigation, shows inhibition of bacterial growth in disk-diffusion assays by high molecular weight CNCs-PDDA but not by CNC alone or low molecular weight conjugates.

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation # 4**********

Isolation and Identification of Amyloid Fibers from Archaeon Haloferax volcanii

Presenter's Name: Lisa Kozodoy
Faculty Mentor: Dr. Nadia Marano
St. Lawrence University

Amyloids are proteins that when aggregated form large insoluble fibers characterized by their cross beta sheet structure. While these proteins are often implicated in human neurodegenerative diseases, such as Alzheimer's, many organisms make functional amyloids. These have been studied in bacterial biofilms and are known to aid in stability and structure. Archaea also form biofilms; however, they have not been researched as extensively. Functional amyloids have been identified in the archaeon Haloferax volcanii. The aim of this study is to isolate and purify amyloid fibers from H. volcanii to elucidate more about their composition and structure. Isolation is done through differential centrifugation and sonication, following previous research by Heather Raimer '17. Sonicating the cells releases the amyloid fibers from the cells, which are detected using Thioflavin T (ThT) assays. Low speed centrifugation allows for the removal of cellular debris. Ultracentrifugation then isolates the larger fibers from suspension. Lastly, tube SDS-PAGE is used to purify the amyloids from contaminating proteins because they do not enter the gel. This isolated fibers are deaggregated into monomers using formic acid. The monomers are resuspended for further study.

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation #5**********

Is nanotechnology the solution to the vaccine adjuvant shortage?

Presenter's Name: Hannah Despres
Faculty Mentor: Dr. Karina Ckless
Co-authors: Jennifer Crain, Saejuti Kanungo, Jason Nguyen, Barrett Waling, Beza Tuga, Rajesh Sunasee
SUNY Plattsburgh

Vaccine adjuvants are component of vaccines that prime the immune system to recognize the antigen. Only two adjuvants—alum and AS04—are used in commercially available vaccines in the United States, according to NIAID website. Therefore, it is urgent to develop effective, economically viable and safety materials that can act as vaccine adjuvants. Crystalline nanomaterials such as cellulose nanocrystals (CNCs) have similar structure to alum and might elicit comparable immune response. **The goal of this study is to assess the immune response in vitro of chemically related CNCs derivatives to further develop as vaccine adjuvant, using cell-based assays**. This study examined the immune response induced by CNCs grafted with cationic moieties in human monocyte cell line (THP-1) and mouse macrophage-like cell line (J774A.1). Our results indicated that none of the cationic CNCs induced a dramatic increase in the secretion of pro-inflammatory cytokines interleukin 1β and tumor necrosis factor α (TNFα) in human cell lines. However, a notable increase in TNFα secretion by mouse cells was detected in all tested conditions. We will continue to investigate the immune response of cationic CNCs in primary human cells because the extent of their immunomodulatory activity can determine the potential applicability as vaccine adjuvants.

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation # 6**********

Detection of Pharmaceutical and Personal Care Products in Water Systems Using Capillary Electrophoresis

Presenter's Name: John Paliakkara
Faculty Mentor: Dr. Fadi Bou-Abdallah
SUNY Potsdam

Humans have flooded water systems with active pharmaceuticals, personal care products, and toxic metals that have been detected globally in many natural water systems including rivers, lakes, and drinking water. While waste water treatment plants can remove some pharmaceuticals, many drugs can still pass through in small quantities over a long period of time. This represents a major threat to human health and the environment. Here, we use Capillary Electrophoresis (CE), an efficient and relatively rapid separation technique to detect and quantify these chemicals in water samples collected along the Raquette River (from Tupper Lake to Potsdam) and from different wastewater treatment plants. The overall goal of this study is to examine how widespread the presence of pharmaceutical pollutants is, and to bring to light a potential contamination and health issue to the population of Northern New York.

==========

Undergraduate Oral Presentations

==========

********** **Oral Presentation # 7**********

Nanotechnology-Enabled Paper-Based Biosensor for Ethanol Detection

Presenter's Name: Megan Carhart
Faculty Mentor: Dr. Silvana Andreescu
Clarkson University

Paper-based biosensors are a cheap, simple, portable, and disposable option for chemicals monitoring. Alcohol content needs to be monitored in industries like; farming, food, beverages, and law enforcement. In this presentation, a new method is developed to incorporate nanotechnology into paper-based biosensing for ethanol. Nanoparticles have been used on cellulose filter paper with alcohol oxidase to detect trace amounts of ethanol. Chromogenic indicators generate a colorimetric response dependent on ethanol concentration. The response is quantified using online software. The method demonstrated high sensitivity, and the linear working range was found to 0.05-1% ethanol.

==========

Undergraduate Poster Presentations

– SUNY Plattsburgh –

==========

********** **Poster # 1**********

A mild and green esterification method of carboxylated cellulose nanocrystals

Hafsa Abid, Caitrin Bodmer, Michael Keating, Rajesh Sunasee
Department of Chemistry, State University of New York at Plattsburgh

Over the past decades, there has been extensive research in esterification of native cellulose and recently, it has been extended to nanocelluloses, particularly, cellulose nanocrystals (CNCs). The design of simple esterification techniques will lead to a wide range of structural and functional moieties covalently grafted on the surface of nanocelluloses for various applications. Previous typical methods involved reaction between the hydroxyl groups of cellulose and carboxylic acids in the presence of acid as catalyst. In this work, we have reversed the chemical method by starting with a carboxylated CNCs and studied their esterification reactions with simple alcohols. Instead of the typical inorganic acids, we use bismuth (III) salts (bismuth triflate or bismuth trichloride) as an inexpensive, mild, easily handled, and green catalysts. The esterification reaction was performed in water at room temperature for 24 hr. The resulting surface esterified CNCs products were purified by centrifugation, dialysis and isolated by freeze-drying. Proof of covalent ester linkages were obtained by FT-IR spectroscopy, and their hydrodynamic size and surface charge were analyzed by dynamic light scattering and zeta potential measurements respectively. The application of this mild and green esterification protocol was extended for the conjugation of a modified 5-Fluorouracil drug on the surface of carboxylated CNCs to further study their anti-cancer properties.

==========

==========
********** **Poster # 2**********

Bioassays to Reveal the Effects of Glyphosate on Daphnia magna using Biochemical Biomarkers

Yusha Imtiaz, Amy Ryan.
Department of Biological Sciences, State University of New York at Plattsburgh

Daphnia, more commonly known as water fleas, are important organisms in freshwater ecosystems due to their role as primary consumers. These minute crustaceans are highly sensitive to their surrounding environment and can even undergo phenotypic plasticity in response to predators. Due to these characteristics, daphnia have been used extensively for ecotoxicology research. However, glyphosate, a potential threat to the health of Lake Champlain, has yet to be screened on the organisms. Glyphosate is the core active ingredient in Roundup, a highly popular non-selective herbicide. Though pure glyphosate is generally low in toxicity, the excessive amount found nationally in streams and lakes may have severely detrimental effects on organisms lower in the food chain, such as daphnia. The objective of this project is to conduct bioassays on samples of Daphnia magna in order to understand the effect of glyphosate on the organisms. This includes determining fatal concentrations, analyzing immobilization, and measuring the level of biomarker activity for acetylcholinesterase and catalase.

==========
********** **Poster # 3**********

Cellulose nanocrystals as promising nanoplatform for the removal of toxic cationic dye, Auramine O

Richard Chandradat[a], Jeffrey K. Taylor[b], Alexandre H. Pinto[b], Rajesh Sunasee[a]
[a]Department of Chemistry, State University of New York at Plattsburgh
[b]Department of Chemistry, Ithaca College

The use of cellulose nanocrystals (CNCs) for waste water treatment and removal of toxic contaminants has recently generated attention due to CNCs high specific surface area, aspect ratio and capacity retention as well as their environmental inertness. In this work, we explore the use of unmodified CNCs and carboxylated CNCs as adsorbents for the removal of toxic water-soluble cationic dye, Auramine O (AO). Both the surfaces of CNCs and carboxylated CNCs are negatively charged which can non-covalently induce the adsorption of the cationic AO via electrostatic interaction. Batch adsorption experiments were carried out at 0 and 25 ^{o}C and the highest removal percentage (65 %) and adsorption capacity (7 mg/g) were obtained for unmodified CNCs (equilibrium

contact time of 30 mins). The kinetic data was fitted to the pseudo 2nd order adsorption model, with the highest rate constant (0.36 $g.mg^{-1}.min^{-1}$) related to the unmodified CNCs sample, for the adsorption at 25 ºC. The thermodynamics parameters indicated that the adsorption process is exothermic for all samples, and with a decrease in the entropy of the system throughout the process. Both Temkin and Dubinin-Radushkevich isotherms properly described the adsorption behavior for all samples, either at 0 or 25 ºC. Overall, unmodified CNCs displays promising adsorbent ability for removal of toxic AO dye.

==========
********** **Poster # 4**********

Docking of therapeutic compounds to FtsZ

Ty-niquia Jones, Kelly Theisen
Department of Chemistry, State University of New York at Plattsburgh

Bacterial cell division is accomplished mostly through the actions of the protein FtsZ. The FtsZ monomers form filaments that wrap around the cell circumference and then constrict to start the division process. This role in cell division makes FtsZ an attractive target for antibiotic agents, especially ones to combat MRSA and VRSA infections. Some compounds have been identified, but the effect of their binding has not been fully explored computationally yet. We used the SwissDock program to investigate the binding of an identified inhibitor to the S. aureus FtsZ protein. Preliminary results suggest multiple binding sites, including along the filament and at filament interfaces.

==========
********** **Poster # 5**********

The mechanical stability of FtsZ filaments.

Thomas Jennings, Kalyn Nguyen, Kelly Theisen
Department of Chemistry, State University of New York at Plattsburgh

Bacterial cell division is accomplished mostly through the actions of the protein FtsZ, making this protein an attractive antibiotic target to combat MRSA and VRSA infections. The FtsZ monomers form filaments that wrap around the cell circumference and then constrict to start the division process. These long filaments have not been studied computationally yet, due to the amount of processing power required. We used coarse-grained simulations run on graphics cards to overcome this barrier and performed stretching and bending simulations of an FtsZ filament. Preliminary results show that the species of FtsZ determines the strength of the filament interface.

==========
********** **Poster # 6**********

Impact of endotoxin contamination on the immune response caused by cellulose nanocrystal (CNCs) derivatives designed for potential vaccine adjuvants, in human and mouse cells

Jennifer Crain, Saejuti Kanungo, Barrett Waling, Jason Nguyen, Christopher Smith, Rajesh Sunasee, Karina Ckless
Department of Chemistry, State University of New York at Plattsburgh

Cellulose nanocrystals (CNCs) are cellulose-based nanomaterials that have fiber-like structure. They have emerged as a new class of nanomaterial for multiple biomedical applications, including potential vaccine adjuvants. Vaccine adjuvants are substances or molecules that activate complex signalling networks, necessary to develop antigen-specific adaptive immunity. We have demonstrated that cationic CNCs have immunogenic properties. More recently it has been discussed whether a robust immune response can be attributed at least in part to the presence of endotoxins. Endotoxins are small bacterially-derived hydrophobic lipopolysaccharide (LPS) molecules that can contaminate CNCs during synthesis and preparation of colloidal suspension, and ultimately can significantly impact both *in vitro* and *in vivo* experiments. **The goal of this study is to explore different sterilization methods of a series of cationic CNCs and access their immunogenicity and correlate with the respective endotoxin levels, using cell-based assays**. In summary, we found that non-sterile and autoclaved colloidal suspensions of cationic CNCs caused the greatest dose response immune response indicated by secreted IL-1β in both cell types, which corresponds with the greatest concentrations of endotoxin. These results suggest that the preparation methods of CNCs colloidal suspension affect the immunogenicity of CNCs and this may be associated with presence of endotoxins.

********** **Poster # 7**********

Synthesis of Beta-o-4 lignin compounds

Sneha Mohan, Vanshika Patel, Barret Waling, Napoleon, Devangi Patodiya, Dexter Criss
Department of Chemistry, State University of New York at Plattsburgh

The research was based on wood pulp, the source of which is trees. The research stemmed from the desire to investigate ways to increase the efficiency of the wood pulp, essentially to increase the hydrolysis rate. Chemical models were used in order to investigate the hydrolysis of ethers, since the major linkage in wood is ether linkage. In order to create the chemical models, a proper

understanding of how the polymer lignin polymer is broken down and detached from one moiety to another. The goal is to synthesize these lignin model compounds. We have previously determined that the ratio with the best separation was that of 25% Ethyl Acetate and 75% Hexane. This semester the research was further directed towards synthesis of the polymer β-O-4-lignin. TLC (Thin layer chromatography) and GC (Gas Chromatography) have been carried out in addition to GC results of multiple preliminary experiments suggest that the dimer was synthesized, with the best result showing 92% yield of the final product. The ratios of the GC were determined by area under the curve. We have hypothesized that the product obtained is coupled. However, Gas chromatography and mass spectrometry (GC/MS) will help to confirm if this is true or not. The expectation is the molecular weights that the GC/MS will give us, of the starting material and the final product, will be very different. We have made this final molecule and so now our focus is reducing it using sodium borohydride ($NaBH_4$).

********** **Poster # 8**********

Comparison of different methods of sterilization on the cytotoxicity of cellulose nanocrystal (CNCs) derivatives designed for biomedical applications

Barrett Waling, Jason Nguyen, Jennifer Crain, Saejuti Kanungo, Christopher Smith, Rajesh Sunasee, Karina Ckless
Department of Chemistry, State University of New York at Plattsburgh

Cellulose nanocrystals (CNCs) are utilized for a variety of applications from nanofillers to potential drug delivery. CNCs have a fiber-like structure that can be modified with different moieties to proper suit to biomedical applications. However, these modifications can potentially lead to drastic interactive changes of cell-material interactions. While a number of studies have focused mainly on the cytotoxicity of unmodified CNCs and/or fluorescently-labelled CNCs, there are still very limited data regarding the cytotoxicity assessment of surface-modified CNCs. Therefore, it is crucial to evaluate the risks associated with surface-modified CNCs before they can be fully exploited for biomedical application. The goal of this study is to assess the cytotoxicity of chemically related cationic CNCs prepared using different sterilization methods. The colloidal CNCs suspension were prepared at 1 mg/mL and were sterilized by filtration or autoclaving and cytotoxicity was evaluate using (4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) and neutral red assays in mouse macrophage-like cells (J774A.1) and human peripheral blood mononuclear cells (PBMCs). Overall, the results indicated cationic CNCs did not affect cell viability in both cell types, regardless the sterilization methods

utilized to prepare the colloidal suspension. However, we observed that some cationic CNCs formed aggregates in cell culture, as observed using live-cell imaging.

==========

Undergraduate Poster Presentations
– St. Lawrence University –

==========

********** **Poster # 9**********

Mercury Pollution in Church Pond

John Hoefler, Matthew Skeels
Department of Chemistry, St. Lawrence University

Fish, insect, plant, sediment and shell samples were taken from Church Pond in Paul Smiths, NY over the course of 6 weeks during June and July of 2018. These samples were tested for total mercury (THg) concentrations using the LECO AMA254 Mercury Analyzer. Mercury is a neurotoxin posing serious health threats to humans, primarily through consumption of contaminated fish. Church pond was selected due to its lack of previous research surrounding mercury contamination and its frequent use as a recreational site. THg results were used to assess New York State's current advisories for consuming fish from the Adirondack region and identify other Hg sinks in this ecosystem. New York State's standards for fish consumption were found to be adequate based on Hg levels for 4 species of fish (L. gibbosus, M. salmoides, M, dolomieu and P. flavescens). Insects, plants and sediment were also found to have significant levels of mercury while the majority of mussel shells had concentrations below detection levels. Higher concentrations of Hg were generally found in species occupying higher trophic levels. Within trophic levels, piscivorous fish, plant leaves and fully aquatic insects showed the highest THg concentrations.

==========

Graduate Poster Presentations

==========

********** **Poster # 10**********

Paper-based colorimetric biosensor and application in food freshness and smart packaging

Fatima Mustafa, Ali Othman, Silvana Andreescu
Department of Chemistry and Biomolecular Science, Clarkson University

Food safety monitoring has become necessary as foodborne diseases are increasing. Work to develop smart sensors and labels to indicate food spoilage or presence of harmful toxins is growing. This presentation will discuss design, development and application of a portable biosensor platform that integrates functional nanoparticles and biomolecules on paper for monitoring food quality and safety. To fabricate the biosensors, we use nanoparticles that have tunable redox activity, optical and catalytic properties and can transduce and catalytically amplify signals in chemical and biological detection schemes involving biomolecules. The presentation will discuss the assembly of nanoparticles and target-specific biomolecules in portable sensing platforms and provide examples of applications for food quality monitoring.

==========

********** **Poster # 11**********

Electrochemical release of His-tagged proteins by destruction of NTA-Cu(II)-protein complex

Madhura Bellare, Vasantha K Kadambar, Maria Gamella, Artem Melman, Evgany Katz
Department of Chemistry and Biomolecular Science, Clarkson University

Stimuli responsive release of biomolecules from surfaces such as gold and carbon is gaining importance for past couple of decades due to its application in biomedical field. Electrochemically induced release of biomolecules from the surfaces is one of such techniques. The simplicity of the electrochemical techniques brings-in wide opportunity for loading and releasing biomolecules from the electrode surfaces. Here-in we report the loading and electrochemical release of His-tagged proteins from the electrode surfaces such as gold and graphite. Reversible chelation of His-tagged proteins on Ni-NTA surfaces is studied for decades. Competing ligands such as imidazole and EDTA are used for releasing the His-tagged proteins from the Ni-NTA surfaces. However,

switching the metal to Cu(II) instead of Ni(II) brings an opportunity for releasing the His-tagged proteins by the reduction of Cu(II) to Cu(I) or metallic copper. The affinity of Cu(I) towards complexation with NTA and His-tag is substantially lower than Cu(II) which facilitates the release of the protein. Also, Cu(II) can electrochemically be reduced. We use Cu-NTA crafted graphite and gold electrode for the coordinative loading of His-tagged proteins and electrochemical reduction of metal ion for the release of the proteins from the surface. In this study we used a redox mediator coupled model peptide (ferrocene-hexahistidine) and a model recombinant protein called "Protein A" as examples for loading and electrochemical release.

==========
********** **Poster # 12**********

Derivatization of Proteins Containing Oligohistidine Tags

Vasantha K Kadambar , Artem Melman
Department of Chemistry and Biomolecular Science, Clarkson University

Chemical modification of proteins and other biomolecules is of major interest in chemical biology for various purposes. However, the presence of various reactive functional groups in these biomolecules makes it challenging to achieve a chemo- and site-specific derivatization. The commonly used methods for chemical modification of proteins are based on labeling of cysteine or lysine residues. Hexahistidine tag is one of the most widely used protein tags for separation of recombinant proteins by affinity chromatography. The ubiquity of this tag suggests is utilization for other purposes such as covalent derivatization of recombinant proteins. We are developing a novel methodology for the covalent derivatization of such proteins by using chelation followed by addition-elimination reaction at the histidine tags with our reagent. It is based on interaction of the hexahistidine tag with Ni2+ and a chelate ligand bearing a reactive electrophilic group to form a stable ternary complex, which subsequently promotes chemoselective intramolecular reaction of the electrophilic group with a histidine residue of the hexahistidine sequence. Our approach features a Nitrilotriacetic acid (NTA) or Imino Diacetic acid (IDA) as the chelate functions for binding hexahistidine tag through Ni2+or another bivalent metal cation, and a Baylis-Hillman (BH) ester group as reactive electrophilic group. The reaction involves alkylation of an imidazole residue from hexahistidine tag accompanied by detachment of the chelate function. The present talk involves development and selective derivatization study of his-tagged proteins in presence of other proteins like BSA.

==========
********** **Poster # 13**********

Kinetics of Fe^{2+} oxidation by oxygen in ferritin

Tyler Wilkinson[a], Fadi Bou-Abdallah[b], Nicholas Flint[b], Samantha Smith, Artem Melman[a]
[a]Department of Chemistry and Biomolecular Science, Clarkson University
[b]Department of Chemistry, SUNY Potsdam

The excessively high and inconsistent literature values for Km, Fe and Km, O_2 prompted us to examine the iron oxidation kinetics in ferritin, the major iron storage protein in mammals, and to determine whether a traditional Michaelis-Menten enzymatic behavior is obeyed. The observed iron oxidation kinetics exhibited two distinct phases (Phase I and Phase II), neither of which obeyed Michaelis-Menten kinetics. While Phase I was very rapid and corresponded to the oxidation of approximately 2 Fe(II) ions per H-subunit, Phase II was much slower and varied linearly with the concentration of iron(II) cations in solution, independent of the size of the iron core. Under low oxygen concentration close to physiological, the iron oxidation kinetics revealed a Michaelis-Menten behavior with Km, O_2 values in the low μM range (i.e. ~ 1 – 2 μM range). Our experimental Km, O_2 values are significantly lower than typical cellular oxygen, indicating that iron oxidation and mineralization in ferritin should not affected by the oxygenation levels of cells, and should proceed even under hypoxic events.

==========
********** **Poster # 14**********

Mass Spectrometry based Proteomics to Investigate and Characterize the Jumping Translocation Breakpoint (JTB) Protein using Cancer Cell Lines

Madhuri Jayathirtha, Devika Channaveerappa, Kangning Li, Costel C. Darie
Department of Chemistry and Biomolecular Science, Clarkson University

Human JTB (hJTB) is a gene located on the human chromosome 1 at q21 which is involved in the unbalanced translocation in various types of cancer. JTB protein is ubiquitously present in normal cells and is overexpressed in various types of cancer including prostate and breast cancer. Hence this protein could be a biomarker for tumor malignancies and a potential target for their treatment. However, the pathway through which this protein causes increased cell growth and differentiation is not clear. Investigation and comparison of the proteomes of cells with upregulated and downregulated JTB can be a good approach to understand the function of the protein and its contribution to tumorigenesis.

Here, the MCF7 breast cancer cell lines were transfected with the sense and antisense orientation of the JTB cDNA in HA, His and FLAG tagged CMV expression vector. The expression of JTB was confirmed by western blotting. Proteins extracted from the transfected cells were separated using SDS-PAGE and the peptides were analyzed by a Nano Acquity UPLC coupled with Xevo G2 Mass Spectrometer. Data analysis was done using Mascot server and Scaffold 4.1 software. In addition, two other JTB isoforms will be investigated and their possible cellular function(s) will be compared with the functions of the wild type JTB. These studies could help us elucidate the mechanism through which JTB induces cell proliferation and test the JTB protein as a potential drug target for malignancies with overexpression of the protein.

==========
********** **Poster # 15**********

Magneto-Controlled Biocatalytic Cascades with Logically Processed Input Signals – Substrate Channeling versus Free Diffusion

Yaroslav Filipov[1], Andrey Zakharchenko[2], Sergiy Minko[2], Evgeny Katz[1]
[1]Department of Chemistry and Biomolecular Science, Clarkson University
[2]Nanostructured Materials Lab, University of Georgia

Magnetic nanoparticles (MNPs) functionalized with various enzymes (amyloglucosidase, glucose oxidase and horseradish peroxidase) were used to perform biocatalytic cascades in two different states, solute suspension or aggregated, produced in the absence or presence of an external magnetic field. The biocatalytic reactions proceeded through bulk solution diffusion of intermediate substrates or substrate channeling, when the systems were dispersed or aggregated, respectively. The both pathways have shown very similar kinetics, unless the intermediate substrate was consumed by an additional biocatalytic process called "filter" for brevity. In the presence of the "filter" process, the diffusional process in the bulk solution was significantly inhibited, while the process based on the substrate channeling was still active. The systems were switched reversibly between the inhibited dispersed state and the active aggregated state by removing and applying the external magnetic field, respectively. The signal-controlled biocatalytic cascades were considered as Boolean logic circuits with the inputs consisting of biomolecules and the magnetic filed on-off.

==========

==========
********** **Poster # 16**********

Fundamental Characterization of Arsenic Adsorption on Metal Oxide Nanoparticles by Nanoimpact Electrochemistry

Farideh Hosseini Narouei, Daniel Andreescu, Silvana Andreescu
Department of Chemistry and Biomolecular Science, Clarkson University

Metal oxide nanoparticles (MONP) such as Titania (TiO_2), Ceria (CeO_2) and Iron Oxide (Fe_3O_4) are heavily used in consumer products and discarded in the environment with little regulation. Although these NPs are found to be relatively non-toxic, when released in the environment they can undergo transformation and interact with existing contaminants such as heavy metals which can drastically change their properties and toxicity profile. This presentation will discuss electrochemical studies to investigate the interaction of MONPs with inorganic arsenic species and characterize surface processes (e.g. oxidation, adsorption) at the level of individual particles. Examples of NP systems and studies to assess the effect of particle type, surface coatings and environmental composition will be provided along with the parameters controlling adsorption/desorption of toxicants, using electrochemical methods and a suite of spectroscopic procedures. We demonstrate the use of electrochemistry as a powerful tool to quantifying heavy metal adsorption and determining mechanisms that can be used to predict the interaction of NPs in the environment.

==========
********** **Poster # 17**********

Development of Selective Sensor for On-Site Detection of Arsenic (V) in Environmental samples

Zahid Wajdan, Farideh Hosseini Narouei, Najma Memon, Silvana Andreescu
Department of Chemistry and Biomolecular Science, Clarkson University

There are several researches have been done for the detection of As (III) in neutral pH by electrochemical methods. As (V) is not electroactive in nonacidic media there is a need for its direct detection in natural waters. Current work demonstrates the direct detection of As (V) for its on-site determination by modified glassy carbon electrode. Glassy Carbon Electrode (GCE) was electrochemically modified with poly (aniline-co-o aminophenol) and decorated with Nano-Au particles (Nano-Au/PANOA/GC) electrode. Conditions were optimized for sample; Modification of GCE with PANoAP was performed using cyclic voltammetry at 0.05 V/s under the potential window -0.2 to 0.6, followed by the amperometry deposition of Nano-Au particles at -0.5 potential for 45s. As

(V) was later determined by anodic stripping voltammetry under optimized conditions. The SWASV parameters used were as follows: preconcentration potential of -1.6 V; preconcentration times for 4 min, for As (V) concentrations; 10 s equilibration time; 40-100 Hz frequency; 25 mV potential pulse amplitude; 5 mV potential step height; and a potential stripping ramp from -0.2 V to 0.6 V. This step was preceded by a conditioning step at +500 mV for 30 s. The calibration curves show linearity range of 50 to 250 µM ($r2 \geq 0.99$). The methodology can be applied onto the surface of low-cost screen-printed electrodes and detected.

==========
********** **Poster # 18**********

A versatile 3D printing platform for manufacturing hydrogel-based biosensors for different applications

Abraham Samuel Finny, Ali Othman, Silvana Andreescu
Department of Chemistry & Biomolecular Science, Clarkson University

3D printed bioanalytical sensors offer tremendous possibilities towards creating inexpensive clinical diagnostic devices for molecular measurements that are simple and quick. This presentation will describe the development and optimization of 3D printed hydrogel-based biosensors prototypes with incorporated receptor molecules and transduction interfaces. The sensors display target specific detection capabilities with improved sensitivity, stability and disposability as compared to existing sensors. To 3D print these biosensors, a conventional 3d printer, an extrusion-based 3D bioprinter, and computer-aided designing software were used along with a novel bio-ink formulation that contains nanoparticles having tunable redox, optical and catalytic properties. The optimum hydrogel composite provides good mechanical properties to the printed biosensors enabling them for use in a wide range of applications. Further, the proposed biosensors can analyze low analyte concentrations, are reagent-less and are highly portable making them appealing in the area of wearable devices, flexible and portable bioelectronics and lab on chip technology. In this approach, we have combined traditional 3D printing techniques with 3D bioprinting techniques to fabricate our final wearable biosensors.

2019 NNY ACS Research Symposium
Plenary Speaker
Prof. Silvana Andreescu

"Biosensors in Everyday Life"

The demand for inexpensive field portable devices that could respond to the today's needs for low cost and rapid detection with on-site measurement capabilities is growing. This presentation will discuss the status of chemical and biological sensors and the development of technologies with advanced capabilities designed to address emerging health and environmental challenges. Examples of sensors that utilize advanced nanomaterials possessing interesting optical, catalytic and oxygen storage/release properties and applications of these devices for the detection of food, clinical and environmental analytes will be presented. A unique feature of these devices is the built-in detection mechanism with all the sensing components needed for analysis fixed onto the sensing platform. The sensors have been interfaced with portable databases and user-friendly signal transduction methods such as portable electronics and have demonstrated excellent analytical performance when used for on-site analysis. Recent work focusing on the development of field deployable tests for environmental monitoring, as well as wearables and consumer healthcare devices will be discussed, with examples of applications.

Short Biography: Prof. Silvana Andreescu is the Egon Matijević Chair in Chemistry and Professor of Bioanalytical Chemistry in the Department of Chemistry and Biomolecular Science at Clarkson University in Potsdam, NY. She has received a PhD in Chemistry, specializing in biosensors from the University of Perpignan, France, and University of Bucharest, Romania in 2002, and has been a member of the Clarkson faculty since 2005. Between 2003 and 2005 she was a NSF-NATO postdoctoral fellow at the State University of New York at Binghamton. Her research interests are in biomaterials, analytical and bioanalytical chemistry, bio-nanotechnology, device manufacturing, environmental nanotechnology and development of practical biosensors for clinical and environmental monitoring. Recent work involves the use of electrochemistry to characterize surface properties and reactivity of inorganic materials and the advanced manufacturing of portable sensing platforms for consumer applications. She is the recipient of a French Government Graduate Fellowship, a NATO-NSF Postdoctoral Fellowship, and the NSF-CAREER award, the John W. Graham Faculty Research Award, the Research Excellence Award and a Member of the Million Dollars Club at Clarkson University. She has published over 110 peer-reviewed publications, co-edited three books, has three patents awarded for her technology and has delivered over 100 presentations worldwide. Her research on portable sensors has sparked the interest of major science and media publications from all over the world. She has managed over 3 million dollars in research funding from federal, primarily NSF and NIH, and New York State agencies.

2019 NNY ACS SYMPOSIUM
* AWARDS AND PRIZES *

The 10th Annual Undergraduate and Graduate Chemistry and Biology Research Symposium is a one one-day event featuring undergraduate oral and poster presentations, a keynote speaker (Dr. Silvana Andreescu, Clarkson University) and an award ceremony that includes:

1- Six student ACS memberships (4 undergraduates and 2 graduates) to encourage chemistry and/or biochemistry students to join ACS and become regular members.

2- Award certificates and monetary prizes to winners of poster and podium presentations:

- *Best undergraduate oral presentation: (Certificate + $100 prize)*
- *2nd best undergraduate oral presentation: (Certificate + $100 prize)*

- *Best undergraduate poster presentation: (Certificate + $100 prize)*
- *2nd best undergraduate poster presentation: (Certificate + $100 prize)*

- *Best graduate poster presentation (Certificate + $100 prize)*

3- Two 50"× 60" periodic table of the elements blankets (100% cotton).

Notes: