THE FOURTH ANNUAL NEW YORK CAPITAL REGION APPLIED SPECTROSCOPY SYMPOSIUM

FRIDAY, JUNE 20TH
TIME: 10:00 AM-4:00 PM
UNIVERSITY AT ALBANY
EMERGING TECHNOLOGY AND ENTREPRENEURSHIP COMPLEX (ETEC)
1220 WASHINGTON AVE, ALBANY, NY

Symposium Schedule
Keynote speaker
Abstracts
Symposium committee
Sponsors

June 20th 2025

KEYNOTE SPEAKER

DIANA S. AGA
SUNY DISTINGUISHED PROFESSOR AND RENEW DIRECTOR
UNIVERSITY OF BUFFALO

“Free Drugs”, “Superbugs”, and “Forever Chemicals” in the Environment: Occurrence and Implications

Diana Aga, PhD, is the Henry Woodburn Professor of Chemistry and a SUNY Distinguished Professor at UB, where she also serves as the Director of RENEW (Research and Education in eNergy, Environment and Water) Institute. An analytical chemist, her research involves studying the fate, transport, effects, and treatment of chemicals of emerging concern and persistent organic pollutants in the environment. Recipient of numerous awards and honors, Dr. Aga has received the National Science Foundation CAREER award; the Alexander von Humboldt Foundation Research Fellowship; 2 Fulbright Fellowships; and, the Menzie Environmental Education Award from the Society of Environmental Toxicology and Chemistry. She is a Fellow of the American Chemical Society (ACS), and the recipient of the Jacob F. Schoellkopf Medal by the Western New York Section of the ACS.

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TIME: 10:00 AM-4:00 PM
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EMERGING TECHNOLOGY AND ENTREPRENEURSHIP COMPLEX (ETEC)

REGISTRATION (9:30 - 10:00)

Pickup name badges and symposium materials	**REGISTRATION DESK**

OPENING REMARKS (10:00 - 10:15)

KEYNOTE PRESENTATION (10:15 - 11:15)

“Free Drugs”, “Superbugs”, and “Forever Chemicals” in the Environment: Occurrence and Implications	**DIANA S. AGA**	University at Buffalo

COFFEE BREAK (11:15 - 11:30)

ORAL PRESENTATIONS SESSION (11:30 - 12:30)

Solution-cathode Glow Discharge for Isotopic Analysis in Geochronological Dating	**JARED VIGGERS**	Renssealer Polytechnic Institute
Spectroscopic Investigation of the Energetics of Electron Transer in the menB Variant of Photosystem I	**BRANDON RUSSELL**	Rensselaer Polytechnic Institute
Two-dimensional correlation mass spectrometry for complex mixtures and Martian organics	**ELLY BREVES**	Renssealer Polytechnic Institute
Creating a Literature Database to Constrain Peptide Synthesis Parameter Space	**MICKEY MUSCALLI**	Renssealer Polytechnic Institute

LUNCH BREAK (12:30 - 1:30)

ORAL PRESENTATIONS SESSION (1:30 - 2:30)

ATR-FTIR Spectroscopy and Chemometrics for Forensic Differentiation of Smokers and Non-Smokers from Fingermarks	**MOHAMED O. AMIN**	University at Albany
Fluorescence and Raman Spectroscopy for Forensic Skin Cell Analysis	**RILEY ALPUCHÉ CARTER**	University at Albany
Enhancing Crime Scene Analysis with Raman Spectroscopy for Gunshot Residue	**CODY SILVERMAN**	University at Albany

COFFEE BREAK (2:15 - 2:45)

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THE FOURTH ANNUAL NEW YORK CAPITAL REGION APPLIED SPECTROSCOPY SYMPOSIUM

POSTER PRESENTATIONS (2:45 - 3:30)

Metal artifact reduction and contrast agent performance as a function of source spectral shape	**JACOB AUBREY**	Rensselaer Polytechnic Institute
Investigation of Benchtop Nanoparticle Syntheses for Surface Enhanced Raman Spectroscopy	**ABDULSOBUR FAGBENRO**	Rensselaer Polytechnic Institute
2D-COS Analysis of Blood Fluorescence Spectra During ex vivo aging	**SILA JIN**	University at Albany
Using EPR and DFT methods to understand the heterodimer BChlg'/Chla' generated by exposure of Heliomicrobium modesticaldum primary donor P800 to dioxygen	**PATRICK LANDRY**	Rensselaer Polytechnic Institute
Structural Biology of DIAPH1-Actin Interaction	**PARASTOU NAZARIAN**	University at Albany
A novel approach for the detection of gunshot residue for forensics purposes using Raman spectroscopy: Optimizing the laser excitation.	**DOMINIQUE PLATT**	University at Albany
Pulse chase fingerprints of neuronal cell maturation using In cell NMR technique	**SPOORTHY SANDRAS**	University at Albany
An Open-Chamber System for Live Cell Raman Spectroscopy	**RUI ZHENG**	University at Albany

NETWORKING (3:30 - 3:45)

STUDENT AWARDS AND CONCLUDING REMARKS (3:45 - 4:00)

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ABSTRACTS

TITLE

SOLUTION-CATHODE GLOW DISCHARGE FOR ISOTOPIC ANALYSIS IN GEOCHRONOLOGICAL DATING

Authors and Affiliations

Jared Viggers, Jacob T. Shelley
PhD Student
Rensselaer Polytechnic Institute

Mass Spectrometry (MS) is a highly sensitive and selective technique for trace element analysis. However, common ionization sources like inductively coupled plasma (ICP) require high power, extensive cooling and large amounts of argon gas. In contrast, the solution-cathode glow discharge (SCGD) is a low-cost, simple microplasma that has demonstrated performance comparable to ICP-MS for atomic MS. The SCGD operates at atmospheric pressure and the plasma is sustained between a tungsten anode and flowing solution cathode. The atoms within the sample are sputtered from the solution and may form adduct or cluster ions with species present in the surrounding environment, such as oxygen. Occasionally, the atom may also be measured in its bare ion form. This study explores the use of SCGD for the detection and isotopic analysis of rubidium and strontium. Elements with higher oxidation states tend to form oxide adducts, whereas lower oxidation states lead to adducts of hydroxides and water. Rubidium was detected as bare ions, while strontium was detected as both elemental ions and molecular ion in the form of $(SrOH)^+$. Rubidium and strontium isotope-ratio measurements were used to obtain greater measurement precision for the detected ions. Precision improvements were also made by investigating the operational parameters of the mass spectrometer. These results are potentially useful measurements for geochronological dating and demonstrate that SCGD is an effective tool in trace metal analysis when coupled with a mass spectrometer and demonstrates the successful use of a cost effective ion source.

ABSTRACTS

TITLE

SPECTROSCOPIC INVESTIGATION OF THE ENERGETICS OF ELECTRON TRANSFER IN THE MENB VARIANT OF PHOTOSYSTEM I

Authors and Affiliations

Brandon Russell, K.V. Lakshmi
Post-Doc
Rensselaer Polytechnic Institute

Photosynthetic electron transport depends on quinone derivatives that serve as important photochemical intermediates. Phylloquinone (PhQ) is a naphthoquinone derivative that binds at the A1A and A1B sites of Photosystem I (PSI). Previous work showed that the disruption of PhQ biosynthesis in the menB variant of the cyanobacterium Synechocystis sp. PCC 6803 results in the binding of the benzoquinone derivative plastoquinone-9 (PQ-9) in the A1A and A1B sites instead of PhQ. The construction of the menB variant was an elegant demonstration that a simple interruption of the biosynthetic pathway for PhQ allows for the incorporation of PQ-9 in the quinone sites. Recently, we determined the cryo-electron microscopy structure of PSI from a recent strain of the original menB deletion variant (referred to as menB(2023)), which revealed an unusual quinone in the A1A and A1B sites. Through mass spectrometry, we found that the unusual quinone contains a benzoquinone head group similar to PQ-9 and a phytyl tail similar to PhQ. We performed whole genome and Sanger sequencing combined with transient optical and time-resolved electron paramagnetic resonance (EPR) spectroscopy to investigate the kinetics and thermodynamics of electron transfer in PSI from the menB(2023) variant. We found that secondary mutations in the original menB variant resulted in the binding of the alternative quinone, 2,3-dimethyl-5-phytyl-1,4-benzoquinone (DMPBQ), in menB(2023). Moreover, transient optical and time-resolved EPR spectroscopy reveal that the incorporation of DMPBQ leads to markedly different energetics of electron transfer in menB PSI.

This work is supported by the U.S. Department of Energy, Photosynthetic Systems Program.

ABSTRACTS

TITLE

TWO-DIMENSIONAL CORRELATION MASS SPECTROMETRY FOR COMPLEX MIXTURES AND MARTIAN ORGANICS

Authors and Affiliations

Elly Breves, Jacob T. Shelley
PhD Student
Rensselaer Polytechnic Institute

Identification of analytes in complex mixtures with mass spectrometry (MS) is often complicated by isotopic distributions, adduct/fragment formation, and isobaric overlap. Common methods of analysis such as gas chromatography-MS (GC-MS) and tandem-MS require physical separation of analytes prior to mass analysis. This work adapts a two-dimensional correlation technique used widely in optical spectroscopy, 2D-COS, to mass-spectral analyses of mixtures to identify spectral features that arise from a common molecular origin using computational means rather than isolation of analytes. This adapted technique, two-dimensional correlation mass spectrometry (2D-CMS), was used to correlate fragment ions to their precursors from a rapid, direct mass-spectral analysis of a mixture of pharmaceuticals. This correlation was achieved using synchronous fragmentation of all species followed by a single mass analysis step rather than sequential isolation, fragmentation, and mass-spectral analysis of each analyte as in tandem-MS. This novel approach extracts spectral features arising from a single analyte computationally while circumventing the need for physical separation, reducing analysis time and sample consumption.

The versatility of 2D-CMS was extended to a conventional pyrolysis GC-MS analysis of a complex Martian meteorite to characterize the diverse inventory of organic molecules in the sample, a high priority objective for NASA planetary missions. 2D-CMS enabled the correlation of fragments formed during the electron ionization process to their intact precursors. Network analysis of 2D-CMS results indicates that several clusters of structurally-similar fragments each arise from a different isomer of the precursor molecule. This isomer-specific precursor/fragment correlation aids in the structural identification of analytes in complex samples.

ABSTRACTS

TITLE

CREATING A LITERATURE DATABASE TO CONSTRAIN PEPTIDE SYNTHESIS PARAMETER SPACE

Authors and Affiliations

Mickey Muscalli, Jacob T. Shelley
PhD Student
Renssalaer Polytechnic Institute

The fundamental role of peptides in life on modern Earth implies that peptide synthesis was a critical step in the development of prebiotic chemistry necessary for the emergence of the first life-like entity. However, polymerization of amino acids to form simple peptides is unfavorable in aqueous solutions under a wide range of temperature and pressure conditions because these reactions require the loss of a water molecule into solution. Previous studies have focused on how polymerization yields differ across ranges of temperature, pressure, pH, and fluid composition; however, an inclusive assessment of these experiments has not been undertaken. This work surveys an existing body of experiment-based peptide-synthesis literature to investigate how environmental conditions impact abiotic amino acid polymerization, and to identify key patterns or gaps in the parameter space of prebiotic peptide formation. Following the collation of this dataset, we plan to utilize various data science approaches, including clustering and comparative analysis, in order to identify correlations between experimental conditions (temperature, pressure, pH, fluid composition, mineral surface) and peptide yields. We can also compare experimental outcomes to thermodynamic predictions under the same conditions. Expanding on these geochemical models, we expect to be able to identify regions of thermodynamic space in which oligomerization occurs most readily.

ABSTRACTS

TITLE

ATR-FTIR SPECTROSCOPY AND CHEMOMETRICS FOR FORENSIC DIFFERENTIATION OF SMOKERS AND NON-SMOKERS FROM FINGERMARKS

Authors and Affiliations

Mohamed O. Amin, Igor K. Lednev
Post-Doc
University at Albany, SUNY

Chemical analysis of latent fingermark (LFM), with particular reference to “touch chemistry,” offers additional intelligence for forensic examination. Continuous improvements in the versatility and sensitivity of detection of the molecular makeup of fingermark (FM) is of considerable importance. This presentation aims to provide further knowledge on the chemical analysis of FM using vibrational spectroscopy; Raman spectroscopy (RS) and attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), to understand individuals’ lifestyles and traits. Raman spectroscopy was employed to analyze nonsteroidal anti-inflammatory drugs (NSAIDs)-contaminated FMs produced after gentle contact with the drug tablets. Utilizing advanced chemometrics for data analysis, partial least squares discriminant analysis (PLS-DA), in particular, resulted in 100% accuracy on a FM level according to external validation. Furthermore, the effect of environmental conditions showed that the Raman signals of aspirin, diclofenac, and ibuprofen in contaminated FMs decreased significantly at high temperatures, whereas naproxen and ketoprofen were relatively stable. Additionally, the characteristic decay time of each drug was investigated, which showed a significant variation between 5 and 600 h. In another study, ATR-FTIR spectroscopy combined with PLS-DA modeling was employed to differentiate between smokers and non-smokers based on their FMs. External validation of the model resulted in 100% accuracy at the donor level using a 50% threshold for individual spectra. This preliminary study shows a great promise for understanding human lifestyle based on chemical analysis of FM residues.

ABSTRACTS

TITLE

Authors and Affiliations

FLUORESCENCE AND RAMAN SPECTROSCOPY FOR FORENSIC SKIN CELL ANALYSIS

Riley Alpuché Carter, Igor K. Lednev
PhD Student
University at Albany, SUNY

Skin is the largest organ of the human body; it is the barrier between our organs and any outside interferences. Because it is accosted daily by things like chemicals and sunlight, it is constantly replenishing itself, forcing new skin to the surface, and shedding the old cells on top. By shedding skin cells every second of the day, we as people are leaving an undeniable footprint of genetic material everywhere we go. Applying this to a forensic setting means that there is a plethora of trace DNA evidence that criminals may forget to think about cleaning up. By developing a method to identify and characterize skin cells in a non-destructive manner, a new avenue for DNA profiling is opened up. By using fluorescence spectroscopy to identify the presence of skin cells, and Raman spectroscopy as a confirmatory test, we can quickly and safely identify skin cells that may be used to generate a DNA profile. The ultimate goal here is to develop a method of identification for the origin site of skin cells, which may be used to corroborate claims for crimes in the future.

ABSTRACTS

TITLE

ENHANCING CRIME SCENE ANALYSIS WITH RAMAN SPECTROSCOPY FOR GUNSHOT RESIDUE

Authors and Affiliations

Cody Silverman, Igor K. Lednev
PhD Student
University at Albany, SUNY

Gunshot residue (GSR) refers to the particles or debris left on hands, clothing, or surfaces after a firearm is discharged. As a common type of trace evidence, GSR consists of a complex mixture of organic and inorganic compounds, including materials from the propellant, primer, and cartridge case. Forensic scientists analyze GSR because it provides critical evidence that can help establish the involvement of a suspect in shooting-related crimes. The most common tool used for GSR analysis is scanning electron microscope energy-dispersive X-ray spectroscopy (SEM/EDS), which is primarily effective for detecting inorganic gunshot residue (IGSR). However, as lead-free ammunition becomes more prevalent, SEM/EDS alone may not yield conclusive results. This has led to a growing interest in developing methods for detecting organic gunshot residue (OGSR). In current forensic science, there is no single validated instrument for determining the chemical composition of OGSR, while also providing differentiation on the type of ammunition used. Forensic scientists strive to collect GSR efficiently at crime scenes, analyze it quickly, and accurately identify its components. Raman spectroscopy shows great potential in achieving this goal. This technique is increasingly utilized in the analysis of OGSR due to its ability to offer detailed information for identification and classification purposes. This research focuses on advancing our lab's two-step method for differentiating ammunition types using a benchtop Raman microscope.

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ABSTRACTS

TITLE

Authors and Affiliations

METAL ARTIFACT REDUCTION AND CONTRAST AGENT PERFORMANCE AS A FUNCTION OF SOURCE SPECTRAL SHAPE

Jacob Aubrey, Peter Bonitatibus
PhD Student
Rensselaer Polytechnic Institute

This study empirically mapped the x-ray source spectrum of a Medipix All Resolution Scanner (MARS) photon counting CT (PCCT) system across multiple copper (Cu) and tin (Sn) pre-filtration conditions, evaluated the metal artifact reduction (MAR) potential of these filters, and assessed their impact on contrast performance (CP) for both FDA-approved iopromide and experimental tantalum oxide nanoparticles (TaOx NPs). Mapping was performed using no filter, seven Cu filters (0.3–2.1 mm), and seven Sn filters (0.15–1.05 mm). A multi-insert phantom containing water, lipid, iopromide, TaOx, and metal was scanned under each condition. Insert signal, noise, and contrast-to-pooled-noise ratio (CPNR) were calculated to evaluate MAR and CP. Thick Cu and Sn filters shifted the mean x-ray energy by 19.2 and 23.4 keV, respectively, relative to the unfiltered source (47.9 keV), and reduced noise by up to 74%. Even thin filtration reduced noise by up to 47%. However, contrast was variably affected: iopromide showed up to 50% contrast loss with thick filtration, particularly in the k-edge bin, while TaOx NPs exhibited smaller losses (up to 38%). Both iopromide and TaOx NPs exhibited CPNR gains with filtration, though improvements were more pronounced for TaOx, with increases up to 61%, suggesting greater compatibility with spectral shaping. Overall, empirical source mapping revealed how photon flux distribution varies with pre-filter material and thickness, and also enabled identification of detector-specific artifacts. These insights, together with the demonstrated MAR benefits of filtration may help guide protocol development for emerging clinical PCCT systems such as the MARS Microlab 5X120.

The ultimate goal of applied research is to bring the developed novel technology to the market. We approach this goal through the start-up company SupreMEtric LLC. SupreMEtric's mission is to streamline the forensic analysis of biological stains by creating a universal nondestructive method for the identification of all main body fluids. This presentation will discuss the process from researching the problem in an academic laboratory to commercialization process of this technology.

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ABSTRACTS

TITLE

INVESTIGATION OF BENCHTOP NANOPARTICLE SYNTHESES FOR SURFACE ENHANCED RAMAN SPECTROSCOPY

Authors and Affiliations

Abdulsobar Fagbenro, Jacob T. Shelley
High School Student
Rensselaer Polytechnic Institute

Surface-enhanced Raman spectroscopy (SERS) is a powerful technique for the detection of trace-level analytes via the enhancement of Raman scattering signals with metallic nanoparticles. In this study, two silver nanoparticle syntheses were evaluated for their effectiveness as SERS substrates using methylene blue as a model analyte. The first synthesis involved reduction with hydroxylamine hydrochloride, while the second used a mixture of ascorbic acid and sodium borohydride. Both methods were simple benchtop procedures designed to be safe and accessible for educational settings. The synthesized nanoparticles were characterized via UV-Vis spectroscopy before and after aggregation with sodium chloride. Aggregation led to spectral shifts and decreased absorbance, indicating changes in particle size and interaction. Raman spectroscopy showed significant signal enhancement for methylene blue when combined with particles from the first synthesis, particularly after aggregation. Key vibrational peaks were clearly observed, and signal intensity increased with analyte concentration and integration time. These results demonstrate that the nanoparticles synthesized yield effective SERS enhancements and that benchtop nanoparticle methods can be successfully applied to educational and analytical applications.

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TITLE

2D-COS ANALYSIS OF BLOOD FLUORESCENCE SPECTRA DURING EX VIVO AGING

Authors and Affiliations

Sila Jin, Igor K. Lednev
Post-Doc
University at Albany, SUNY

Blood is one of the most commonly found body fluids at crime scenes. It is one of the most important types of forensic evidence because it can confirm an individual's identity if it matches a known DNA profile. Determining the time since deposition (TSD) can help investigators determine when a crime occurred. Developing a forensically sound method for determining TSD from bloodstains requires an understanding of the fundamental biochemical mechanisms that occur during aging process. The biochemical processes that occur in blood are an important topic in human biology and biomedicine and are well understood because they are necessary for the continued survival of living organisms. However, the biochemistry of ex vivo blood stain aging is of major interest for forensic scientists and has not yet been thoroughly studied.

In this study, we investigated changes in the fluorescence properties of blood exposed to air. Blood contains fluorophores such as tryptophan, NADH, and flavins. We found that the fluorescence of flavins was less reproducible and showed more complex behavior than tryptophan and NADH. The changes in tryptophan and NADH fluorescence intensity showed different characteristic times, indicating the complex biochemical mechanism of blood aging.

2D hetero-correlation analysis is a unique and powerful feature of the generalized 2D correlation spectroscopy (2D-COS) that has great potential in a variety of scientific applications. In 2D-hetero correlation studies, 2D correlation spectra are obtained from two different spectral data sets occurring under different conditions. Hetero-sample correlation is one form of hetero-correlation analysis, where the existence or lack of correlation is examined among spectral intensity variations of different samples by using the same analytical probe and perturbation condition. The emission spectra of tryptophan, NADH, and flavin were collected after the excitation at 285, 350, and 465 nm, respectively. The perturbation condition was the post-deposition aging time. We revealed hidden bands of flavin using 2D-COS that were difficult to identify in one-dimensional fluorescence spectra, shedding light on the complex biochemical mechanism of blood aging.

ABSTRACTS

TITLE

USING EPR AND DFT METHODS TO UNDERSTAND THE HETERODIMER BCHLG’/CHLA’ GENERATED BY EXPOSURE OF HELIOMICROBIUM MODESTICALDUM PRIMARY DONOR P800 TO DIOXYGEN

Authors and Affiliations

Patrick Landry, K.V. Lakshmi
PhD Student
Rensselaer Polytechnic Institute

Heliobacteria are anaerobic phototrophic bacteria with a Type I homodimeric reaction center (RC) using bacteriochlorophyll g (BChl g). H. modesticaldum, the model organism used for heliobacteria, has been well studied and is understood to convert BChl g into 81-OH-chlorophyll aF (BChl aF) in the presence of light and dioxygen. Conversion of BChl g results in the loss of the light-driven charge separation. Previous work work shows that once both of the BChl g’ molecules of the primary donor P800 have been converted to BChl aF’, the RC can no longer perform electron transfer. We show that a partially converted P800 can exist by exposing the RC to dioxygen and demonstrate the presence of a BChl g’/ BChl aF’ heterodimer by Q-band 1H ENDOR, 14N HYSCORE spectroscopy and DFT methods. The DFT calculations of a BChl g’/ BChl g’ homodimeric primary donor predict that the unpaired electron spin of P800+ will be evenly delocalized across both of the BChl g’ molecules, which is in excellent agreement with experimental hyperfine couplings of the anaerobic samples. Exposure to dioxygen drastically changes the experimental hyperfine interactions of the RC, which displays greater localization of the unpaired electron spin in P800+. In agreement with the experimental hyperfine couplings, DFT calculations using a computational model of the heterodimeric primary donor P800 obtained by replacing one of the BChl g’ with BChl aF’ shows significant localization of the electron spin density on the BChl g’ molecule in the heterodimer.

*This work was supported by the U.S. DOE under the contracts DE-FG02-07ER15903(KVL) and DE-SC0010575(JHG). NSF GRFP grant (PL), NSERC Discovery grant 2015-04021 (AvdE) and Brock university New Faculty start-up funds (DK).

ABSTRACTS

TITLE

STRUCTURAL BIOLOGY OF DIAPH1-ACTIN INTERACTION

Authors and Affiliations

Parastou Nazarian, Advisor
PhD Student
University at Albany, SUNY

Human Diaphanous Homologue 1 (DIAPH1) belongs to the Formin family of proteins that play crucial roles in regulating the actin cytoskeleton and contribute to various cellular processes such as filopodia formation, stress fiber assembly, vesicle transport, and cell motility. However, the precise mechanisms by which formins regulate actin assembly remain unclear.

In its inactive state, DIAPH1 exists as an autoinhibited complex, where the DID domain interacts with the DAD domain, preventing actin filament nucleation and polymerization by blocking the actin-binding sites on FH2 domain (1). Activation of DIAPH1 occurs upon binding of Rho-GTPases to the GBD domain, which induces conformational changes that disrupt the DID-DAD interaction and release the FH1 and FH2 domains from autoinhibition(2).

DIAPH1 in its active state can promote polymerization of actin from the C-terminal region through at least three mechanisms: initiating new filament nucleation, controlling the rate of filament elongation, and determining how long filaments grow before being capped. It has been shown that FH2-DAD, enhances the nucleation of actin through the interaction between DAD and G-actin monomers directly. Additionally, FH1-FH2 fragments of the C-terminus DIAPH1 (ct-DIAPH1), increase both the rate of filament barbed end elongation and duration of filament growth before capping happens. (3) To study the interaction between ct-DIAPH1 and actin, we employed reverse-phase and size exclusion chromatography to purify proteins to high purity, followed by mass spectrometry to validate protein identity. Furthermore, we utilize fluorescence spectroscopy to determine the binding affinity of the ctDIAPH1-actin interaction, and nuclear magnetic resonance (NMR) spectroscopy to characterize the structure of the complex and gain insight into how ct-DIAPH1 influences actin polymerization or depolymerization.

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ABSTRACTS

TITLE

A NOVEL APPROACH FOR THE DETECTION OF GUNSHOT RESIDUE FOR FORENSICS PURPOSES USING RAMAN SPECTROSCOPY: OPTIMIZING THE LASER EXCITATION.

Authors and Affiliations

Dominque Platt, Igor K. Lednev
Undergraduate Student
University at Albany, SUNY

Forensic investigators often rely on trace evidence, such as gunshot residue (GSR) found at crime scenes for shooting-related crimes. GSR can help identify the type of ammunition used in the offenses, providing investigative leads and narrowing the search. There are two types of GSR: Inorganic GSR (IGSR) and Organic GSR (OGSR). IGSR are metallic particles formed after the vaporization and condensation of inorganic elements, while OGSR are organic compounds originating from incomplete ignition, vaporization, and condensation of propellant powder.

In typical forensic casework, IGSR is analyzed using Scanning Electron Microscopy/Energy Dispersive X-Ray Spectroscopy (SEM/EDS), while OGSR is analyzed using Gas Chromatography (GC) or Liquid Chromatography (LC) coupled with Mass Spectroscopy (MS). These techniques require high training, are expensive, potentially destructive, and lack applicability for onsite crime scene analysis. However, new techniques in the field of Raman Spectroscopy offer an alternative pathway that does not require heavy training, is relatively inexpensive, less destructive, and has potential for application on crime scenes.

The lab's objective is to develop a system that can take Raman spectra from any GSR particle in the field and identify the ammunition of the GSR. This goal starts with optimizing various parameters that may affect analysis. Preliminary results show a difference between the raw spectra collected at 785 nm and 514 nm for the same particle. The next steps involve testing the effect of excitation wavelength on particles of differing morphologies to determine if there are differences between the spectra. Understanding these differences is crucial for achieving one of the lab's major goals.

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ABSTRACTS

TITLE

PULSE CHASE FINGERPRINTS OF NEURONAL CELL MATURATION USING IN CELL NMR TECHNIQUE

Authors and Affiliations

Spoorthy Sandras, Alex Shekhtman
PhD Student
University at Albany, SUNY

Cellular metabolism is pivotal to neuronal function and survival, and its dysregulation is implicated in various neurodegenerative disorders. To explore metabolic transitions during neuronal maturation, we developed an integrated platform combining in-cell ^{13}C NMR spectroscopy with bioreactor-based long-term culture. Using the SH-SY5Y neuroblastoma cell line as a model, we applied a pulse-chase isotope labeling strategy to monitor real-time metabolic changes during differentiation induced by retinoic acid (RA) and TPA. Encapsulation of cells in alginate beads within an oxygenated bioreactor enabled stable culture conditions and continuous delivery of ^{13}C-labeled substrates.

NMR spectral analysis revealed a striking metabolic reprogramming: undifferentiated cells exhibited high levels of glycolytic intermediates such as fructose-1,6-bisphosphate, whereas differentiated cells showed complete loss of these signals and increased activity of the tricarboxylic acid (TCA) cycle. Notably, differentiated cells retained glutamate and alanine, with glutamate accumulation suggesting vesicular neurotransmitter storage. A competitive ELISA further confirmed elevated dopamine production, validating functional neuronal characteristics. These observations support a metabolic shift from aerobic glycolysis to oxidative phosphorylation, mirroring the bioenergetic profile of mature neurons.

Our approach provides a high-resolution, physiologically relevant window into the metabolic transformations underpinning neuronal differentiation. This work not only enhances our understanding of neural development but also establishes a versatile platform for studying neurodegenerative disease mechanisms and identifying potential therapeutic targets.

ABSTRACTS

TITLE

AN OPEN-CHAMBER SYSTEM FOR LIVE CELL RAMAN SPECTROSCOPY

Authors and Affiliations

Rui Zheng, Alexander Khmaladze
High School Student
University at Albany, SUNY

Raman spectroscopy is a non-destructive technique in physical chemistry that uses Raman scattering to produce a chemical spectrum. It can be coupled with microscopy to produce images and has diverse applications in medicine. Raman spectra of live cells are especially useful indicators of life stage and pathology, but are difficult to collect data for due to their lifespan and need for continuous change of medium. In the present study, an open-chamber system was designed and calibrated to work with a HORIBA Raman microscope, which was used to collect Raman signals of C6 glioma cells. The data was collected and analyzed, identifying characteristic peaks of the cells at various stages of development. Results demonstrate the plausibility of a simple setup for the collection of long-term continuous Raman measurements on live cells, and will be used as a principle component in future studies in investigating the coupling of wide-scanning Raman spectroscopy and a transport-of-Intensity Equation (TIE) system.

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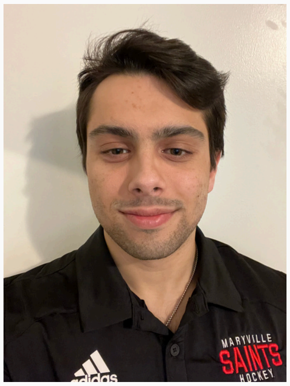

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VIGGEJ@RPI.EDU

CODY SILVERMAN
UNIVERSITY AT ALBANY, SUNY
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