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McMaster Undergraduate Society for the Chemical Sciences Summer Research Symposium 2024

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Abstract
The MUSCS (McMaster Undergraduate Society for the Chemical Sciences) Summer Research Symposium is a one-day, student run, undergraduate research symposium. In McMaster University's Department of Chemistry & Chemical Biology, many undergraduate students participate in research during the Spring and Summer terms. Undergraduate students hold positions in research groups as scholarship recipients, research assistants, cooperative education students, and project course students. Despite the vast amounts of undergraduate research occurring annually, undergraduate students rarely have opportunities to communicate their work. The MUSCS Summer Research Symposium aims to give undergraduate students from McMaster's Department of Chemistry & Chemical Biology a platform to share the research they conducted over the previous summer. The 2024 symposium was held on September 29th, 2024, with over 60 attendees. In this event, 12 students presented work from many fields of chemistry (e.g., organic chemistry, chemical biology, theoretical chemistry). The symposium also featured two keynote presentations from professors in the department. A judging panel, comprised of graduate students, provided feedback to student presenters and awarded prizes to the top three presentations. This symposium will become an annual event in the department, and operate next year to include feedback from presenters, attendees, judges and professors.

Keywords: chemistry conference; undergraduate research; organic chemistry; inorganic chemistry; chemical education

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Conference Abstracts
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Presentation in Chemical Education

Chem-FAST: The Chemistry Formative Assessment Study Tool

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An important yet difficult part of the transition to first-year university is the development of proper study skills and habits to achieve academic success. To support students in developing their study skills and habits, our team has developed a digital instructional tool that applies principles of cognitive psychology and computer-adaptive testing can support students facing these challenges. Our tool for first-year chemistry students is called the chemistry formative assessment study tool (Chem-FAST), which provides students with extensive practice based on a database of questions from the past decade of assessments. In our first-year chemistry courses, multiple-choice practice tests from prior assessments are students' primary study resources. Chem-FAST incorporates cognitive psychology principles such as spaced practice, active retrieval, and formative assessment to promote effective learning. A computer-adaptive testing model uses statistical data to deliver individualized questions to challenges students at a level tailored to their abilities, allowing them to obtain a realistic picture of their progress. With Chem-FAST, students are ultimately guided through effective studying strategies to facilitate long-term academic learning.

In this presentation, we will discuss how we have built Chem-FAST, including: (1) collecting and appropriately formatting past assessments; (2) writing solutions for each question compiled; (3) ensuring equations, images, and special symbols are compatible with the user interface and accessibility standards; (4) designing software that maximizes the student experience; (5) extending Chem-FAST to another first-year chemistry course; (6) conducting a research study on the effectiveness of Chem-FAST for our first-year students. Our hope is that Chem-FAST will improve the undergraduate student experience and can be expanded to other courses.

Presentations in Physical, Inorganic, Computational & Theoretical Chemistry

Computing Binary Operations with Photopolymerization-based Waveguide Formation

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Materials capable of processing, sensing, and interacting reciprocally with their external stimuli possess the potential of local computational ability for the next generation of stimuli-responsive materials. Hudson et al. demonstrated a photopolymer cuboid capable of performing binary addition and subtraction by patterning incoming incandescent beams of light. The photopolymer's nonlinear response to three orthogonal incident light beams leads to the formation of white light filaments in either a disordered, 1-D, or 2-D periodic geometry. The beam along the x-axis, or imaging beam, forms a large population of self-trapped beams due to modulation instability. Simultaneously, the y-axis and z-axis light beams (encoding beams) are also forming self-trapped beams along their respective axis, influencing the propagation of self-trapped beams along the x-axis. By patterning the encoding light beams using bright and dark regions, we can control the geometry of self-trapped beams along the imaging beam, or the output. Here, by incorporating three orthogonal white LEDs instead of three quartz-tungsten halogen lamps, we develop a miniaturized system of the Hudson et. al. work. Following the optimization of the miniaturized system, we aim to expand on the binary arithmetic performed in the original work, performing binary multiplication.

Quadratically Convergent Self-Consistent Field (QC-SCF) Orbital Optimization

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In quantum chemistry, the electronic structure of molecules is analyzed using quantum mechanics, typically through the solution of the N-electron Schrödinger equation. Due to the lack of an analytical solution for this equation, numerical methods are required for approximation. Various quantum chemistry methods have been developed to improve the accuracy of these approximations for different systems. In this work, we implemented the quadratically convergent self-consistent field (QC-SCF) algorithm to numerically solve the N-electron Schrödinger equation and adapted the results for orbital optimization, leading to more accurate solutions. The QC-SCF algorithm employs an exponential parametrization of the wave function through a local unitary transformation, which allows the energy to be expanded using the Baker–Campbell–Hausdorff (BCH) series truncated at the second order. This approach facilitates gradient descent optimization to minimize the energy function and achieve optimized orbitals. During orbital optimization, configuration interaction (CI) wave functions are constructed based on the QC-SCF optimized orbitals using PyCI, with initial guesses iteratively refined for further optimization. A key advantage of this method is its use of second quantization formalism, a standard in modern quantum theory, along with a guaranteed convergence to tackle the challenging problem of orbital optimization.

Developing a Framework for the Synthesis of Atomically Dispersed Polymerized FeTPP Catalysts with Precise Active Site Structures for NO_3R

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Ammonia (NH_3) is an essential product for the agricultural, pharmaceutical, and the chemical industries. It is also emerging as a chemical of interest for the clean energy sector as a hydrogen carrier, and transportation fuel alternative due to its high gravimetric energy density. Presently, the Haber-Bosch process is the dominant way that NH_3 is produced globally. Using high heat and pressure, Haber-Bosch consumes 1-2% of global energy supplies and contributes roughly 1-2% of global CO_2 emissions. Electrochemical nitrate reduction to ammonia (NO_3R) has become an interesting topic of research as it stands to remedy two issues through the recycling of nitrates (NO_3^-). It would supplement some of the need for the energy intensive Haber-Bosch process, and it would also remove a harmful pollutant from the environment, helping to restore balance to the global nitrogen cycle. This work sets out to develop a framework for the synthesis of atomically dispersed iron tetraphenyl porphyrin (FeTPP) catalysts with precise active site structures for nitrate reduction. Aiming to improve the controlled dispersion of active sites through Scholl reaction polymerization and improve the porosity and conductivity of these materials through the addition of CNTs and/or pyrolysis.

Spectro - Spectroscopic Characterization of Molecules with AI

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Molecular structure elucidation is a crucial but fundamentally challenging step in the characterization of materials given the large number of possible structures. Here, we introduce Spectro, an innovative multi-modal approach for molecular elucidation that combines 13C-NMR and 1H NMR data with IR. Spectro translates the embedded representations of the spectra into molecular structures using the SELFIES notation. We employed a vision model for the embedded representation of the IR data, which was pretrained to detect relevant functional group peaks in the IR spectra achieving an F1 score of 91%. For NMR data, we utilized LLM2Vec, treating the NMR spectra as text. This integration of multiple spectroscopic techniques allows Spectro to achieve an overall test accuracy of 93% when trained jointly with the vision model for the IR spectra, and 82% when trained with fixed embeddings. Our approach demonstrates the potential of multi-modal learning in tackling complex molecular characterization tasks.

Development and Integration of a Black Box Preprocessor Transition State Guesser for the Geometry Optimization Package GOpt

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A transition state contains vital information about the thermodynamic and kinetic properties of a reaction. Current geometry optimizers struggle to converge to a transition state; a simple gradient ascent cannot be employed as the transition state exists as a saddle point along the pathway. We are developing a black box transition state guesser to use as a preprocessor in the GOpt geometry optimization package. If one were to ask for the relative location of a transition state, the simplest answer would be midway between the reactant and product. This philosophy gives rise to the first and most basic model; the structure of the transition state is estimated from the arithmetic mean of the internal coordinates from the reactant and product. However, we can expand this idea by considering weighted averages of the reactant and product; the weight that leads to the highest energy gives a guess for the transition state structure. This extension results in our second, more robust, model. The second model works well in theory, but in practice it is computationally expensive as the Schrödinger equation must be repeatedly solved. Our third model retains the second model's method yet is more efficient: by augmenting the internal coordinates of the reactant and product with their respective density matrices, we can estimate the energy of intermediate structures without resolving the Schrödinger equation. The fourth and final model expresses the energy of the reaction pathway as a polynomial function with the transition state existing at the function's maximum, thereby saving even the need to manipulate the density matrix. With these four models, we can have a variety of transition-state guesses, from high-accuracy and high cost (model 2) to low accuracy and low cost (model 1). Models 3 and 4 are relatively less expensive and less accurate. By developing better initial guesses, this research leads to quicker, more efficient, geometry optimization and decreases the likelihood of convergence failures.

Presentations in Organic & Medicinal Chemistry, & Chemical Biology

Development of a Pseudomonas Aeruginosa Biofilm Model for Evaluating Antimicrobial Photodynamic Therapy Efficacy

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Biofilms are known for their persistent nature and increased tolerance to antimicrobial treatments, contributing significantly to chronic infections and infections associated with medical devices. Recent studies have highlighted the need for more complex infection models to better predict clinical outcomes of antimicrobial therapies. Herein, we developed and optimized an *in vitro* biofilm model of *Pseudomonas aeruginosa* strain Xen 41 specifically for testing and imaging antimicrobial treatment. Biomass quantification using crystal violet revealed that continuous orbital motion at lower speeds was more effective in promoting biofilm growth compared to continuous rocking motion. Moreover, LB-Miller broth was found most effective in supporting biofilm growth against other mediums and supplementations. Confocal imaging further showed that biofilms grown under these conditions for 72 hours achieved a thickness of 30 μm. Furthermore, the spatial organization of cells within the biofilm was consistent with clinical observations, where dead cells accumulated at the surface attached to the substrate, while live cells localized towards the nutrient-rich medium. Using the *P. aeruginosa* biofilm model, we conducted a comparative antimicrobial study and demonstrated that antimicrobial photodynamic therapy (aPDT) with a novel photosensitizer nanoemulsion (100 μM) was more effective at eradicating biofilms than the classic antibiotic levofloxacin (138.5 μM). Importantly, no dark toxicity was observed with the nanoemulsion at concentrations up to 500 μM, highlighting the light-selectivity of aPDT. These findings suggest that this *P. aeruginosa* biofilm model is a valuable tool for investigating new antimicrobial therapies. Further research is ongoing to demonstrate if this model accurately reflects the efficacy of aPDT *in vivo*.

Stability Testing for Oral Thin Films, A Novel Platform for Vaccine Delivery

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Several vaccines require ultracold temperatures during transport and storage, reducing their accessibility in developing countries that lack refrigeration equipment. This dampens the progress of global immunization programs. To increase vaccines' thermostability, research has been directed towards stabilizing vaccines by solvent casting (SC), a gentle method of drying biologics into a solid, oral thin film (OTF). This work is focused on preserving adenovirus serotype 5 (Ad5)-based viral vector vaccines and uses Ad5 encoding green fluorescent protein (Ad5GFP) as a model. The pullulan-based film formulation contains trehalose, poly (maleic anhydride-alt-1-octadecene) substituted with 3-(dimethylamino) propylamine (PMAL), and PEG-8000, which immobilize the viral protein capsid and could prevent chemical interactions that cause denaturation within the dried film. Alongside imparting thermostability, the film is easier to dose and transport and can be administered orally. Currently, Ad5GFP-loaded OTFs have been optimized to retain 40 % ± 4 % infectious titer after 7 days at 25ºC. However, characterization beyond this temperature had not been performed. Stability testing at 37ºC was conducted to be representative of extreme environmental conditions. An *in vitro* flow cytometry assay was used to quantify the recovery of Ad5GFP-loaded OTFs and compare it to the recovery of a liquid Ad5GFP formulation. Duplicate studies determined that after 7 days, the OTF has statistically significant higher recoveries than the liquid formulation, retaining three-fold more infectious titer. Despite some infectious titer being lost during SC, the remaining titer is retained for a longer period. At 37ºC, Ad5GFP-loaded OTFs retain infectious titer within two orders of magnitude as other film formulations in the literature. The results can also be interpreted as an accelerated stability study, demonstrating that Ad5GFP-loaded OTFs are more stable at 25ºC than previously characterized. These stability studies provide rationale that OTFs can be loaded with an adequate dose, and inform experimental protocols as research progresses to *in vivo* studies.

Examining the Role of Microsatellite Stability in the Disparities of Colon Cancer Outcomes in People of African Ancestry

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Colorectal cancer (CRC) is the 4th most common cancer and a leading cause of cancer death in men and women. Polyp formation is common in the beginning of CRC development and is characterised as abnormal tissue growth on the inner lining in the colorectal area creating an environment for mutations to transpire. CRC has been attributed to dysfunction of several molecular pathways, proteins or genes that play roles in cell proliferation, migration and apoptosis; intriguingly, there are disparities in incidence in people of African ancestry. One disparity is the difference in microsatellite stability (MSS) in people of African ancestry compared to people of European ancestry. MSS is a CRC subtype and phenomenon where increases or decreases in gene copy number and alterations to chromosomes create mutations that enhance polyp formation and CRC. The disparity has been linked to overall worsened prognosis, earlier tumor onset CRC and more advanced stages of disease for African ancestry patients. The main mechanisms impacting MSS tumors and contributing to its worsened survival are inflammation, differential mutations of tumor-related genes, and weakened immune responses. Recently, the POZ-ZF transcription factor Kaiso was shown to play a role in tumorigenic processes such as inflammation, enhanced proliferation, and metastasis. Given that Kaiso is linked to racial disparities in outcomes in women of African ancestry diagnosed with breast cancer, we hypothesize that Kaiso may also play a role in CRC racial disparities. Thus, this research will investigate MSS characteristics in colorectal tumors and the role Kaiso may play in this disparity using immunohistochemical (IHC) and immunofluorescence (IF) staining and analyses. While both IHC and IF allow for analysis at the expression of a protein of interest and its subcellular localization, IHC can only stain for one protein while IF can stain for multiple proteins allowing for comparison of their expressions and sub-cellular localizations in the same cells. The usage of IHC will be for detecting CRC subtypes, while IF will detect for colocalization of Kaiso with proteins more commonly associated in the MSS CRC pathway such as K-Ras and Tp53. Results from this study will determine what role Kaiso plays, if any, in MSS CRCs and what role of MSS in the racial disparities for African ancestry CRC patients.

Cationic Spherical Nucleic Acids: Overcoming Delivery Barriers in Oligonucleotide Therapeutics

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Oligonucleotides have emerged as a promising avenue in precision medicine therapeutics due to their high versatility and specificity. However, their delivery still proves challenging due to poor cellular uptake. Cationic backbone modified oligonucleotides have consistently been shown to exhibit increased uptake compared to their unmodified counterparts, however, they lack real-world functionality for gene therapy. Spherical nucleic acids (SNA) are nanostructures consisting of radially orienting single-stranded DNA covalently attached to the surface of a variable nanoparticle core. Unlike linear oligonucleotides, SNAs readily enter cells due to their 3-dimensional architecture and can achieve their designed therapeutic effects. However, SNAs fail to localize into intended intracellular sites such as the cytoplasm, limiting their therapeutic potential. The Bujold Group specializes in developing cationic modifications at the nanoscale level to modulate interactions for therapeutic applications. We hypothesize that by combining cationic backbone modified oligonucleotides with SNA architectures, we can facilitate uptake and access to specific cellular compartments. Towards this, we synthesized oligonucleotides containing a variable number of cationic linkages in the form of diamine (DA) and guanidinium (GUA) internucleotide linkages (3DA, 7DA, 3GUA, 7GUA) using standard phosphoramidite (P-O backbone) and phosphoramidate (P-N backbone) chemistry. Using these modified oligonucleotides, 13 nm gold nanoparticles were functionalized as dual-layer SNAs with a low-density Cyanine5 fluorophore labelled monolayer and dense second layer of oligonucleotides bearing cationic linkages. Flow cytometry following a 4-hour incubation with SNAs showed significantly increased uptake of cationic SNAs by triple-negative breast cancer cells (MDA-MB-231) in comparison to polythymine controls. However, shorter 1-hour incubations revealed only marginal improvements in uptake. We are currently conducting more flow cytometry studies to assess cellular uptake at multiple time intervals and will employ confocal microscopy to further validate intracellular localization. These insights will work to guide future designs and applications in therapeutics, with future work examining the application of cationic SNAs as tools for immunotherapy and gene therapy.

Conflicts of Interest

The authors declare no conflict of interests.

Authors' Contributions

AE: Conceptualized, planned, acquired funding, drafted the conference abstract booklet, and gave final approval the version to be published.
SL: Conceptualized, planned, acquired funding, drafted the conference abstract booklet, and gave final approval the version to be published.
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