MACTLAC 2023 Poster Abstracts

Integrating Open-Access Computation into the Sophomore-Level Organic Chemistry Curriculum

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Quantum calculations for molecules have advanced quickly over the past 30 years as computing power has grown. Calculations that used to take days or a supercomputer can now be done using the processing power of a commercially available desktop computer. Moreover, computational chemistry has expanded from proprietary technology that was highly guarded and costly to open-access software that is available free of charge for academic purposes. Over the past two years we have implemented a series of exercises within our sophomore-level organic chemistry class that incorporate basic principles of computational chemistry. In these exercises, students learn to calculate the energies and geometries of molecular orbitals, compute the position of a conformational equilibrium, and predict the structure of a transition state. Students report they appreciate the visual aspect of seeing chemical reactions in three dimensions as well as learning a marketable skill. Exercises described within this work have been adapted into an open-source textbook that is currently being published via LibreTexts.

Partnering with Industry: Developing Glowing Soap for Enhanced Hand Hygiene

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Hand hygiene is critical in many sectors of society and particularly in medical settings. Abluo is a startup company that designed an automated faucet with a black light and glowing soap. This allows users to visualize soap coverage during lathering and soap removal during rinsing. A study run at Bethel University (St. Paul, MN) found that users had 2.7x fewer bacteria on their hands after using an Abluo glow soap faucet system compared to a standard handwash. A glow soap faucet system was also installed a local hospital near campus. The response from medical professionals was overwhelmingly positive, with 95% agreeing with the statement that occasional use of a glow soap faucet system would reduce healthcare associated infections (HAIs).

Teaching Scientific Ethics to Junior-Year Chemistry Students

Christina Edwards, Loras College

Students are taught about scientific ethics as a unit within a 1-credit fall semester seminar course taken their junior year. They explore topics such as ethical frameworks, data ownership, and data representation. They learn about a specific strategy to evaluate ethical dilemmas which includes: identifying stakeholders, considering stakeholder obligations, noting points of conflict, and exploring possible points of action with associated potential consequences. This strategy is applied to case studies which are discussed between students and the instructor. Students participate in a role-play where each student group is assigned a specific stakeholder within a shared ethical dilemma, and the groups come together in a discussion setting which must result in a compromise between all the stakeholders as part of the assignment grade. Mastery of applying this strategy is assessed with students completing an argumentative essay at the end of the semester evaluating, proposing a solution, and presenting possible counterarguments with appropriate resolutions to an assigned ethical dilemma.

Advanced Organic Chemistry Laboratory Experiment: Synthesis of Biaryl Compounds via ipso-Borylation and Suzuki-Miyaura Coupling

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In this 8-week long advanced laboratory course, students design a synthetic method to synthesize a biaryl compound of their choosing. Their syntheses are guided to include an ipso-borylation and a Suzuki-Miyaura Coupling reaction sequence. Students designed their multiple-step syntheses, which included learning how to find procedures for synthesizing silyl ethers of their choice, which would then be ipso-borylated, and designing a Suzuki reaction with an electrophile of their choice. Students learned new synthetic techniques beyond the standard introductory organic lab sequence, designed their reactions based on literature precedent, and redesigned their syntheses when reactions did not proceed as intended. Students learned how to think and write like chemists in a more advanced way. They wrote a paper about their research to match a journal article, including a supporting information section. Students completed survey instruments at the beginning and end of the module, to gain their feedback on what they learned throughout their experience. At the end of the module, students reported increased practice with designing experiments and finding procedures, increased practice with scientific writing, increased self-confidence in the lab and increased understanding of chemistry literature. Students also reported learning resilience, and one reported learning "how to think on the spot". Students were excited to finish their experiment and wished they had more time to run their last reactions. Overall, this was a successful advanced organic laboratory experiment. Students were able to use their foundational knowledge from introductory organic chemistry lab courses and grow their skills and identity as chemists.

Tiny Earth Chemistry: An Antibiotic Discovery CURE

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Tiny Earth is a community of scientists, including instructors and students, working to fight the global health crisis of antibiotic resistance and improve diversity in science. The classic Tiny Earth microbiology course-based undergraduate research experience (CURE) involves student-sourced discovery of soil bacteria with antibiotic properties. A new course furthers this antibiotic discovery pipeline within the classroom; this Tiny Earth Chemistry Course covers concepts typically found in chemistry courses: chemical extractions, chromatography, and natural product chemistry. Versions of this course have been offered at Beloit College, within an elective, biochemistry capstone course and at Point Loma Nazarene University within the laboratory component of a general-organic-biochemistry course. The Tiny Earth Chemistry Research Guide is currently under development, and in the future instructor training workshops will be available to expand the Tiny Earth network and implement this natural products chemistry CURE.

Utilizing Entos Envision in the Undergraduate Chemistry Curriculum

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Our department has shifted from licensing expensive molecular modeling tools to utilizing the Entos Envision cloud-based platform. Currently free to academic users, Envision allows students to explore molecular structures from any computer with internet access. First year students begin by exploring molecular geometry, molecular orbitals, bond orders and charge distribution in molecules. Later, they move on to experiments combining experimental infrared spectra with computationally derived vibrational frequencies. In organic chemistry, Envision is used to help demonstrate molecular pathways and geometrical conformers. Classic physical chemistry experiments such as cyanine dyes, ring strain in cyclic carbonyls, potential energy curves and vibrational analysis are easily adapted to include calculations utilizing the platform. Entos Envision uses a semi-empirical method derived from density functional theory (the GFN1-xTB parameterization of the Geometry, Frequency, Noncovalent, eXtended Tight-Binding or GFN-xTB method). Although these calculations are performed at a low level of theory, the speed allows upper-level students to assess the accuracy of the method over a range of compounds, to build correction models for systems, and to design their own explorations. We have found that ease of use of the system allows faculty and students more time for visualization, analysis, and discussion.

Diversity of Discovery: Using Primary Literature to Learn About Discoveries Made by Scientists from Minoritized Backgrounds

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A major contributor to persistence of students from minoritized backgrounds in STEM fields is their sense of belonging and identity within the scientific community. One strategy aimed at increasing students' likelihood to identify as scientists and pursue careers in the STEM workforce is to see and experience other scientists with similar identities. To work towards this goal, I used primary literature published by scientists from minoritized backgrounds in STEM in a journal club-style seminar for senior undergraduate biochemistry majors. Students read and critically analyzed primary literature written by scientists from minoritized backgrounds. Each week, a student would present the paper that the group read, and we would discuss the authors, the major findings, and the broad contributions to the field. In presenting the work of the scientists, an emphasis was put on delving deeper into the life of the scientist. Primary literature included female and male researchers in both modern and historical contexts. Learning objectives for the seminar included learning how to communicate scientific findings, critically analyze primary literature, and value the contributions of scientists from minoritized backgrounds. Students reported feeling confident in recognizing the contributions made by scientists from minoritized backgrounds and one student mentioned that "The focus on the scientist themselves added relevancy and context to the discovery, which pushed me to learn more about the research." Overall, highlighting discoveries made by diverse scientists was an effective way to integrate primary literature into a senior biochemistry capstone lab course.

Ferroptosis and Transcatheter Chemoembolization for Treatment of Hepatocellular Carcinoma

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Liver cancer poses a significant threat worldwide as the sixth most common cancer and the third most common cause of cancer-related death. The recommended treatment for intermediate stage liver cancer is transcatheter arterial chemoembolization (TACE), which delivers high levels of compound to the tumor while reducing levels systemically. This technique can be effective but is often plagued by incomplete tumor cell death and resistance. Development of improved TACE chemotherapies relies heavily on drugs already approved for human use since the procedural logistics restrict the use of TACE in traditional murine preclinical model systems. Ferroptocide, a potent inducer of ferroptosis, is a promising compound for TACE due to its unique induction of cell death within the tumor and rapid clearance once it reaches systemic circulation. To explore ferroptocide's potential use in TACE, canine HCC patients can be leveraged as a clinically relevant model where size, vasculature, and tumor heterogeneity better reflect human patients. Together, exploring ferroptocide as a TACE chemotherapy and canines as model TACE patients promote a unique approach for the optimization and advancement of TACE-specific therapies.

Wrangling Reassessments with Python

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Reassessments or revisions without penalty are a core tenant for many alternative grading models. Students have an opportunity to learn from their mistakes and demonstrate growth in a subject without penalty. The downside of reassessments is the workload to write, distribute, and grade three or more versions of every assessment. Scaling alternative grading becomes even more challenging as the workload grows with large classes and variable enrollments. I present an open-source workflow using Python scripts to automate repetitive tasks and manage the reassessment avalanche. QR codes are used to label each assessment by learning target and identify the student it belongs to. Students receive an individualized set of assessments during retakes. Afterwards, papers are scanned to PDF and sorted by learning target and student in less than ten minutes for any class size. Assessments are graded on paper or as PDFs, and the final scores are read from each page into a sorted CSV file. Since the scripts are written in the free Python language, the system can be adapted for individual class designs and instructor preferences.