STEM Scholars 2019 ASC Projects

Row 2

Research Group	Winget
Project Title	**Probing the relationship between lipid composition in the body and brain diseases such as depression, with Infrared (IR) Spectroscopy**
Research Question, Hypothesis, or Conjecture	Research question: How does altering the ratio of phospholipids types in a sample of phospholipids alter the vibrational spectrum of that sample? Hypothesis: Interactions between short and long chain phospholipids in a mixture of a variety of phospholipids will cause a shift or change in the wavelengths of IR light typically absorbed when each phospholipid is studied separately
Project Description	The mental illness known as Major Depressive Disorder (MDD) is currently affecting large numbers of people, but the fundamental causes of the disease are not fully understood. However, there has been recent research linking MDD to issues with phospholipids, the lipids or fatty acids in cell membranes, in the human body. Researchers have also noted that the set of anti-depressant drugs known as tricyclic antidepressants, such as the drug Tofranil, appear to work by inhibiting the enzymes that break down phospholipids in the body, but the mechanism is still not fully understood. Depression occurs at a relatively high rate among people with coronary artery disease, and there is some thought that the ratio of different phospholipids in a person’s body could be linked to depression. As an aside, it is also known that lipid oxidation (lipid damage) is associated with general neurodegenerative disorders. It is possible to gain insight into the structures of phospholipids in the body using the vibrational spectroscopy technique of Infrared (IR) spectroscopy, where molecules (which are always vibrating) absorb some IR radiation and begin to vibrate with greater amplitude. This kind of research can be done because a molecule in a specific environment absorbs a very specific set of wavelengths of IR radiation, and these wavelengths can be plotted in a spectrum. The specific IR wavelengths absorbed by a wide variety of lipid types have previously been studied, and actually assigned to the various possible vibrations that occur inside lipid molecules. Vibrational spectroscopy techniques are now being used to study the molecules present in blood samples in the hopes of finding the fundamental causes of depression, with the logical next step being a hope that depression can be diagnosed by running a blood sample through an IR spectrometer. However, there are challenges in fully understanding the experimental results that are being obtained, as experimental spectra from biological samples are very complicated and it is difficult to tease out all of the overlapping information. I believe a combination of mathematically modeling these spectra computationally, alongside obtaining spectra from pure samples in the laboratory, could give significant insights into why the complex experimental spectra in the literature look the way that they do. This kind of research is said to follow the spiral feedback process. In spiral feedback, experimental work is obtained, computational work is done to predict the experimental work in order to understand the experimental work on a deeper level, then further experimental work is done to verify any conclusions drawn from the first round of computational work. The cycle continues until overall conclusions can be drawn, hence a spiral rather than a cycle or loop. Increasing the understanding of the spectra in the literature from biological samples, will hopefully shed more light on the structures of phospholipid molecules in patients with depression, and aid in the understanding of the full biochemical mechanism of this disease.
Introductory References	Reference 1: https://www.health.harvard.edu/blog/omega-3-fatty-acids-for-mood-disorders-2018080314414 Reference 2: http://deepimpact.umd.edu/science/spectroscopy.html
Project Timeline	Week 1: safety/training/background/literature review

(weekly)	Week 2: Repeating previous work – obtaining data (computational and experimental) from three individual phospholipids with different lengths of chains (we will call them A, B, C). Starting new work (both computational and experimental) - obtaining data, and analyzing data, from various mixtures of phospholipids (A with B, B with C, A with C, A with B and C). Week 3: Data acquisition with data analysis continues (both computational and experimental) Week 4: finish data acquisition with data analysis (both computational and experimental) and finish writing the report with discussion of conclusions and future work.
Expected Learning Outcomes	1. Compute spectra with the software Gaussian 16 along with the visualizer Gaussview 6. These are state-of-the-art computational programs seen in computational chemistry research laboratories in both industry and in academia today 2. Safely work in a research laboratory environment 3. Obtain spectra with a research-grade Infra-red (IR) spectrometer 4. Explain the IR spectrum of a molecule, including what causes each peak within the spectrum 5. Use the Scifinder database to search the latest literature 6. Use a laboratory notebook effectively 7. Write a scientific report, including discussion of conclusions and further work 8. Interact with professional chemists from outside of Agnes Scott College
Research Team	Dr. Winget and two undergraduate students
PI Last Name	Winget
PI FirstName	Sarah
PI Email	swinget@agnesscott.edu
Department	Chemistry
Mentor2 First Name	
Mentor2 Last Name	
Mentor2 Email	
4 or 8 Week Project	4 weeks
Project Dates	June 1 - 30, 2019
# of full-time student positions requested (1-3)	2
Novice Requirements	Students must have completed CHE150+L
Advanced Requirements	No Advanced Requirements
Recommended Preparation	N/A