Faculty Member Contact Information

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1 Funded, 2 Unfunded URCA Assistants

	This position is **ONLY** open to students who have declared a major in this discipline.	
	This project deals with social justice issues.	
X	This project deals with sustainability (green) issues.	
	This project deals with human health and wellness issues.	
	This project deals with community outreach.	
X	This mentor's project is interdisciplinary in nature.	

Are you willing to work with students from outside of your discipline? If yes, which other disciplines?

- Yes, Pharmacy, Materials Science and Civil and Manufacturing engineering

How many hours per week will your student(s) be required to work in this position? (Minimum is 6 hours per week; typical is 9)

- 9 hours

Will it be possible for your student(s) to earn course credit?

- Yes—CHEM 396 (2 credit hours)

Location of research/creative activities:

- Science West, Department of Chemistry, Research Lab 3270, and other rooms in the building for accessing instruments

Brief description of the nature of the research/creative activity?

Design of Cyclodextrin-Drug Inclusion Complexes to Scavenge Copper for Preventing CopperOverdose:

Copper overdose in the body can cause liver damage, nausea, diarrhea, cramps, and vomiting (Eske,2020). An abundance of Copper (in the form of Cu2+ ion) in the body often leads to Wilson's disease, a genetic disorder that causes the storage of unwanted copper in different tissues of the body, including the liver and brain. If untreated, Wilson's disease can cause liver failure, central nervous system dysfunction, and death (NORD, 2018). Most drug molecules that are meant to remove copper from an aqueous-based (physiological) environment suffer from poor water solubility of the molecules. Different modifications in the chemical structure of such drug molecules are performed through the synthesis and incorporation of functional groups that can aid water solubility. However, such modifications are challenging, limit the use to only water-soluble molecules, and are often toxic.

This project aims to develop a strategy to overcome the problem of water solubility of copper scavenging drug molecules by linking them to a biocompatible "carrier" in vitro. Through this mechanism, the "carrier" will not only solve the solubility issue but also transport the drug molecules to the affected organs. The "carrier" to be chosen for this research is Cyclodextrin (CD) which is a water-soluble macromolecule with multiple glucose subunits. The glucose subunits form a bucket-shaped structure with the hydrophobic cavity inside to encapsulate the poor water-soluble drug molecules forming an inclusion complex (Scheme 1). The copper-scavenging drug molecules(flavonoid and triazole derivatives) in the CD-drug inclusion complex will sense the presence of Cu2+ through a binding interaction that will lead to the measurement/quantification of copper in the affected area.

The copper binding mechanism of the drug in the CD-drug complex will be evaluated through different spectroscopic characterization methods such as absorption, fluorescence, and nuclear magnetic resonance (NMR) spectroscopy. In the beginning, the molecule's encapsulation mechanism in cyclodextrin will be understood through the spectroscopic modulation of the absorption and fluorescence spectra of the drug. A gradual wavelength shift of the drug molecule is expected in the CD environment, more specifically it will move to the lower wavelength region in the fluorescence spectrum. Such observation will substantiate the encapsulation process. After that, the dynamic light scattering (DLS)technique will be applied to assess the size change of the cyclodextrin cavity before and after drug encapsulation. Finally, copper binding of the molecule will be accomplished through NMR and fluorescence spectroscopy. The hypothesis is, that a colorimetric change (visible color change perceived through the naked eye) is expected in the drug molecule upon copper binding which will be reflected as a quenching of the intensity

in fluorescence spectroscopy (Landge, 2020). For 1H-NMR (proton NMR), the development of a new peak and shift in the aromatic protons is expected.

References:

Eske, J. (2020, December 1). Copper toxicity: Symptoms and treatment. Medical News Today.https://www.medicalnewstoday.com/articles/copper-toxicity

NORD - National Organization for Rare Disorders. (2018, March 7). Wilson Disease.https://rarediseases.org/rare-diseases/wilson-disease/

Landge, S.M.; Lazare, D.Y.; Freeman, C.; Bunn,J.; Cruz, J.I.; Winder*, D.; Padgett, C.; Aiken, K.S.; Ghosh*,D. 2020, Rationally designed Phenanthrene derivatized triazole as a dual chemosensor for fluoride and copper recognition, Spectrochimica Acta Part A: Molecular and Biomol. Spectroscopy, 228, 117758.

Brief description of student responsibilities?

Role of the Research Scholar:

1. During their time, the researcher will review the relevant literature to plan out the methodology.

2. They will be working towards generating pilot data on this research to:

(a) understand the fluorescence properties of the molecules under study in a cyclodextrin (CD)environment,

(b) assess the binding mechanism of the molecule with the metal ion (Cu2+) using UV-Vis and fluorescence spectroscopy in CD, and

(c) plan a systemic route to scavenge the metal ion that will conveniently be achievable.

URCA Assistant positions are designed to provide students with *research or creative activities* experience. As such, there should be measurable, appropriate outcome goals. What exactly should your student(s) have learned by the end of this experience?

The researcher working on this project will receive training in both qualitative and quantitative research methodology. They will be able to:

a) gather literature, explore and cite any previous work,

b) prepare appropriate concentration cyclodextrin solutions of different categories based on their diameter and functional groups,

c) encapsulate bioactive organic molecules in such colloidal environment and analyze the movement molecules using different spectroscopic techniques such as absorption, steady-state fluorescence, and fluorescence anisotropy,

d) disseminate research output through conference presentations and publish articles in highly impactful peer-reviewed journals.

e) The pilot data generated will help in developing a proposal for external funding agencies.

Requirements of Students

If the position(s) require students to be available at certain times each week (as opposed to them being able to set their own hours) please indicate all required days and times:

- I will work inclusively with students to set their timings. The recommendation is adjusted times on weekdays (M-F) between 8 am and 5 pm.

If the location of the research/creative activities involves off campus work, must students provide their own transportation?

- A part of the research project will include to use of testing outside of the facility in the building. The students must be able to provide their transportation in such circumstances.

Must students have taken any prerequisite classes? Please list classes and preferred grades:

- Preferred: Completed CHEM 121 A & 125A, 121B & 125B.
- Can consider: Completing CHEM 121 A & 125A, and taking CHEM 121B & 125B in their current semester.

Other requirements or notes to applicants:

- None