

Faculty Member: Brian Barngrover Faculty ID: 20224477
Department: Chemistry and Biochemistry Faculty Email: barngrbvbm@sfasu.edu
Have you previously received a SURE award? No If yes, when? _____

If yes, how did you disseminate results from previous awards (successfully published a paper or obtained a grant, submitted paper or grant based on results, presented results at external conference, etc.): _____

Student's Name: Samuel Keith Conlin Student ID: 20185559
Major: Chemistry Student Email: conlinsk@jacks.sfasu.edu
Have you previously received a SURE award? yes If yes, when? Summer 2018

Proposed SURE Project

Title of proposed SURE project: Modeling the Electrochemical Properties of Adrafinil

Description of proposed project (describe the scope of the project, including specific objectives):

The project will be to explore the electrochemical activity of adrafinil by a combination of physical experimentation using cyclic voltammetry and computational models. Previous indications of adrafinil being electrochemically active will be verified using a known pure reference sample, with a scan rate study and concentration study performed to determine the electrochemical response in laboratory conditions. Simulations of adrafinil in experimental conditions will be run to determine the functional groups that are oxidized during the suspected one electron, irreversible transfer

Is this a new project or a continuation of a current project? If a continuation, what new work will be done a part of SURE?

This project is a continuation of previous research. As part of SURE, new research will be performed to verify that adrafinil is the electrochemically active species, and the redox conditions will be simulated to determine the affected functional group.

Potential impact or significance of research:

This research will lead to a better understanding of adrafinil, a legal prodrug to modafinil, a drug used in treatment of narcolepsy and depression that is known to have mind altering side effects if abused. IN doing this research, the redox mechanism of adrafinil in lab conditions will be explored with the goal of determining its pKa.

Research Design (approach/methodology):

A pure sample of adrafinil will be obtained and tested using Cyclic Voltammetry under the same conditions as a previous set of adrafinil samples. The recorded peak currents and potentials will be compared to the previous data to determine if the electroactive species is indeed adrafinil. While the data is being analyzed, the molecule will be modeled in solution and manually oxidized, with the most energetically favorable reaction explored further.

Literature review for project (must provide at least five peer-reviewed sources):

T. Ziegler and A. Rauk, *On the calculation of Bonding Energies by the Hartree Fock Slater method. I. The Transition State Method*, Theoretica Chimica Acta 46, 1 (1977)

Remko, Milan et al. "A Comparative Study of Molecular Structure, pKa, Lipophilicity, Solubility, Absorption and Polar Surface Area of Some Antiplatelet Drugs" *International journal of molecular sciences* vol. 17,3 388. 19 Mar. 2016

Milgram, N. W.; Callahan, H.; Siwak, C. Adrafinil: A Novel Vigilance Promoting Agent. *CNS Drug Rev.* **2006**, 5 (3) 193–212.

P. NOROUZI, 1 M.R. GANJALI, 1 M. ZARE, 1 A. MOHAMMADI. Nano-Level Detection of Naltrexone Hydrochloride in Its Pharmaceutical Preparation at Au Microelectrode in Flowing Solutions by Fast Fourier Transforms Continuous Cyclic Voltammetry as a Novel Detector. *J. Pharm. Sci.* **2007**, 96 (8), 2010–2017.

Reynolds, J. E.; Josowicz, M.; Tyler, P.; Vegh, R. B.; Solntsev, K. M. Spectral and Redox Properties of the GFP Synthetic Chromophores as a Function of PH in Buffered Media. *Chem. Commun.* **2013**, 49 (71), 7788–7790.

Project timeline (activity/task and time to complete):

Week 1: Concentration Study of pure adrafinil using cyclic voltammetry.

Week 2: Scan Rate Study of pure adrafinil using cyclic voltammetry.

Week 3: Data Analysis and building computational models using SCM: ADF software.

Week 4: Running ADF simulations and determination of favorable energetics.

Week 5: Energetics study and pKa determination

Description of research and professional skills that the student will develop from the project:

The student will develop skills in computational chemistry and gain an understanding in the underlying DFT. This will allow the student to further apply these concepts in graduate school and provide them a useful tool that is becoming more required in chemical scientific publishing.

Description of the involvement and activities that the student and mentoring faculty will have in this project:

The mentoring faculty will be involved by teaching the student how to use the ADF software and explaining the underlying physical chemistry governing its use. The student and faculty will also interact in collaborating to develop a publication based upon their work.

Description of how you will disseminate results from the project:

The results from the project will be disseminated by poster at the end of the SURE program. The data collected and analysis performed will also be used in a future publication based upon the developments made during the program.

Budget (\$0-\$500 with justification):

None needed.

Amount requested for supplies from SURE: \$ 0

Amount requested for supplies from department: \$ 0

Amount department will fund faculty stipend: \$ _____

Amount department will fund student stipend: \$ _____

Chair approval: _____

Chair Signature

I have reviewed and agree to fulfill the expectations of the SURE award.

Student Signature


Faculty Signature

For internal purposes only:

Proposal Awarded _____ Proposal not awarded _____ Amount awarded: _____

Accounts to be used for award: _____