NDnano
Notre Dame Nanoscience and Technology

NDnano Summer Undergraduate Research 2021 Project Summary

1. Student name & home university: Jackson B. Vyletel, University of Notre Dame

2. ND faculty name & department: Dr. Matthew J. Webber, Chemical and Biomolecular Engineering

3. Summer project title: Binding of per- and polyfluoroalkyl substances (PFAS) to cucurbit[7]uril

4. Briefly describe new skills you acquired during your summer research:

I developed various techniques useful for chemical synthesis and analysis. A large portion of my work involves creating and iterating new materials. This requires me to construct organic synthesis routes, develop a deeper understanding of reaction kinetics, and gain new intuitions about chemical synthesis. In addition to chemical synthesis, I also gained skills in chemical analysis. I became familiar with Mass Spectrometry, Hydrogen Nuclear Magnetic Spectroscopy, separations columns, and dialysis. All these skills have helped me to become a better chemist and a more experienced researcher.

5. Briefly share a practical application/end use of your research:

This work could provide a novel method of PFAS toxin collection. As PFAS are dangerous to both the environment and human health, developing new methods for collection is of extreme importance.

6. 50- to 75-word abstract of your project:

Per- and polyfluoroalkyl substances (PFAS) have become increasingly problematic for health and the environment. This work demonstrates novel capture and detection of various PFAS molecules. We test multiple PFAS under varying pH conditions and model their respective association constants (Ka), showing technologies that capture PFAS with sufficient binding affinity. This shows promise for the applications of non-covalent binding of PFAS, with future sights set on industrial capture technologies for remediation of waste water and streams.

7. References for papers, posters, or presentations of your research:

[1] Centers for Disease Control and Prevention. (2020, June 24). Potential health effects of PFAS chemicals. Centers for Disease Control and Prevention. https://www.atsdr.cdc.gov/pfas/health-effects/index.html.
[2] KEMI, 7, Occurrence and use of highly fluorinated substances and alternatives (2020). Stockholm; KEMI.

[3] Muller, R., & Yingling, V. (2020, April). History and Use of Per- and Polyfluoroalkyl Substances (PFAS). Interstate Technology Regulatory Council. https://pfas-1.itrcweb.org/fact_sheets_page/ PFAS_Fact_Sheet_History_and_Use_April2020.pdf.
[4] Team, D. (2020, December 11). Understanding PFAS Regulations and Project Impacts. Dudek. https://dudek.com/ understanding-pfas-regulations/.

Introduction:

The broad consumer, industrial, and military uses of per- and polyfluoroalkyl substances (PFAS) have become increasingly problematic for health and the environment since the original classification of the toxins in the 1930s [1]. PFAS and other related molecules have been used for coatings for various surfaces and have a range of applications in the aerospace, photographic imaging, semiconductor, automotive, construction, electronics, and aviation industries [2]. While PFAS have proven useful for a number of applications, their limited natural degradation leads to bioaccumulation and ultimately harmful effects in animals and humans such as liver damage, damage to the immune system, and increased risk of kidney or testicular cancer [3]. In this work, we demonstrate a new route to capture and detect various PFAS molecules. We test multiple PFAS and model their respective association constants (K_a) in order to show technologies that capture PFAS with sufficient binding affinity. Furthermore, the pH dependence of these binding groups can be leveraged to modulate the affinity of capture. These studies ultimately show promise for the applications of non-covalent binding of PFAS, with future sights set on large-scale industrial capture technologies for remediation of contaminated waters and waste streams.

Results:

The figure below illustrates binding affinity obtained for PFAS capture:

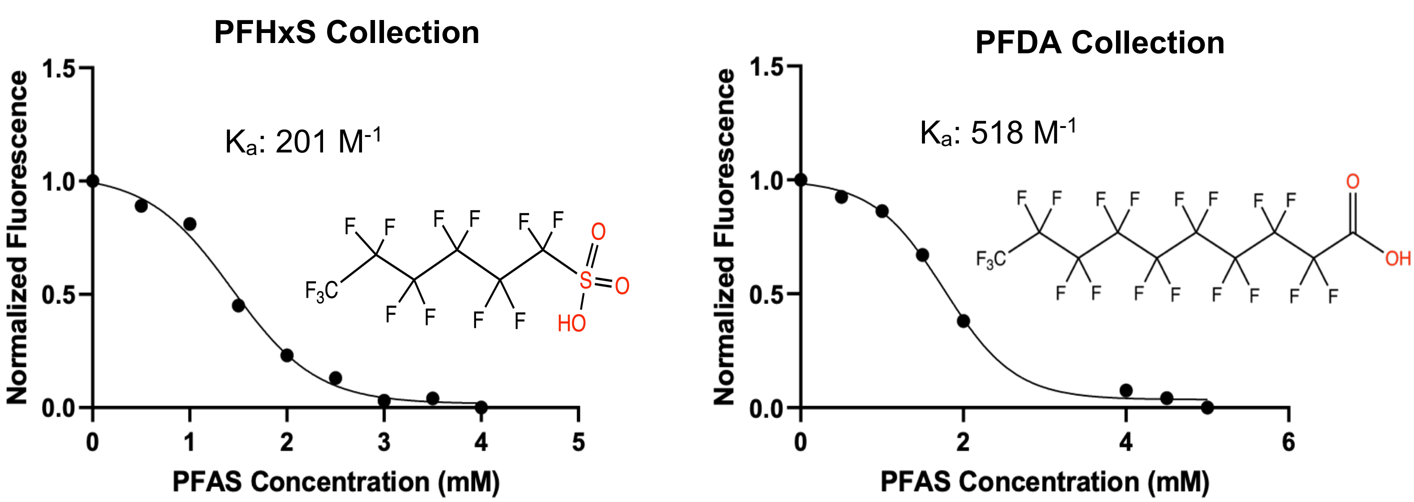

Figure 1: PFAS Collection and K_a

Although equilibrium binding has been modeled for multiple PFAS, there is still a need to improve upon this technique. Experiments will be conducted that give rise to an improved methodology and modeling practice.