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Fate and Transformation of Emerging Chemical Contaminants in Advanced Water/ Waste Treatment

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Faculty

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Project Summary

The world faces challenges surrounding water in terms of both quality and quantity due to rapid industrialization, environmental deterioration, population growth, and climate change. Contamination of aquatic environment with thousands of organic chemicals is one of the key water quality problems [1]. Two major sources of such contaminants are wastewater treatment plants (WWTPs) effluent and agricultural runoff. Pharmaceuticals and personal care products (PPCPs) represent an important contaminant category of concerns as conventional wastewater treatment processes are not efficient in their removal. WWTPs effluent along with agricultural runoff can flow or seep into rivers, lakes, and groundwater and contaminate freshwater systems. Furthermore, water shortage has increased the need for wastewater reclamation including direct/indirect potable reuse. As drinking water is supplemented with water sources of lower quality, it becomes more imperative to effectively degrade and remove these critical contaminants. However, one major technical challenge is to detect and quantify the contaminants of concern at trace level (ng/L to low µg/L) in the complex environmental matrices. In addition, the parent compounds may be degraded to unknown transformation products during treatment processes. Reduction of such contaminants cannot simply be characterized in the conventional percent removal through a treatment train because the transformation products can exceed the parent form in both concentration and toxicity [2]. Therefore, the transformation products also need to be identified. Here, we will fully utilize the state-of-art HPLC/Hybrid Ion Trap-Orbitrap Mass Spectrometer recently purchased through 2014/2015 UAH-RIF award. Carbamazepine is tentatively selected as the one of the target compounds based on the occurrence, concentration, and toxicity reported in the literature. Furthermore analytical procedures for the aforementioned compounds have been published [3]. Adaptation of these methods to our specific instrumental setup will be targeted first. Synthetic solution of the target compounds will first be treated using advanced oxidation processes to facilitate the investigation of transformation products. We may expect similar transformations as observed by Brezina et al. [4]. Finally, the target compounds will be spiked into real water/wastewater samples to further evaluate the treatment efficiency and

contaminants transformation. Due to complexity of the water matrices and typical low concentration of samples, an extraction protocol and subsequent mass spectrometric analysis first need to be developed with synthetic equivalents.

Student Duties

Under the PI's supervision, the student is expected to understand the characteristics of the target contaminants, be familiar with the detection method and procedure reported in the literature, and test/optimize the procedure for our applications. The student duties include: literature review, testing method development, sample preparation and analysis, and method optimization for our instrument. The student will learn how to review scientific papers, understand the water quality challenge we are facing, gain hands-on experience of standard water chemistry analysis as well as sample measurement and analysis using advanced instrument, and learn data analysis.

Mentor Supervision and Interaction

The undergraduate student will work closely with the faculty advisor and other students in the research group. Group meetings will be held weekly in TH S243, reviewing the progress, discussing any problems encountered, and developing future work plan. One-to-one meeting with the PI can also be set up as needed. In addition to the weekly progress report (oral or written), the student is expected to submit an 8 ~ 10 pages report at the end of summer, summarizing the research activities undertaken, progress and results. Upon mutual satisfaction, the student may continue working in the PI's research group as a student specialist after summer 2016.

References

1. Schwarzenbach, R. P. *et al.* The challenge of micropollutants in aquatic systems. *Science* **313,** 1072–7 (2006).
2. Stadler, L. B., Ernsto, A. S., Aga, D. S. & Love, N. G. Micropollutant Fate in Wastewater Treatment : Redefining ' Removal '. 10485–10486 (2012).
3. Miao X.-S., Metcalfe,C.D. Determination of Carbamazepine and Its Metabolites in Aqueous Samples Using Liquid Chromatography-Electrospray Tandem Mass Spectrometry, *Anal. Chem*., **75**, 3731-3738 (2003).
4. Brezina E, Prasse C., Wagner M., Ternes T.A.Why Small Differences Matter: Elucidation of the Mechanisms Underlying the Transformation of 2OH- and 3OH-Carbamazepine in Contact with Sand Filter Material. *Environ. Sci. Technol.* **49**, 10449−10456 (2015).