

Opportunity Title: EPA Transformation Pathways of Organic Chemicals

Fellowship

Opportunity Reference Code: EPD-ORD-CEMM-EPD-2020-03

Organization U.S. Environmental Protection Agency (EPA)

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Store or Google Play Store to help you stay engaged, connected, and informed during your ORISE experience and beyond!

A complete application consists of:

- An application
- Transcript(s) For this opportunity, an unofficial transcript or copy of the student academic
 records printed by the applicant or by academic advisors from internal institution systems may
 be submitted. All transcripts must be in English or include an official English translation. Click
 here for detailed information about acceptable transcripts.
- A current resume/CV, including academic history, employment history, relevant experiences, and publication list
- Two educational or professional recommendations. Click <u>here</u> for detailed information about recommendations.

All documents must be in English or include an official English translation.

If you have questions, send an email to EPArpp@orau.org. Please include the reference code for this opportunity in your email.

Application Deadline 10/30/2020 3:00:00 PM Eastern Time Zone

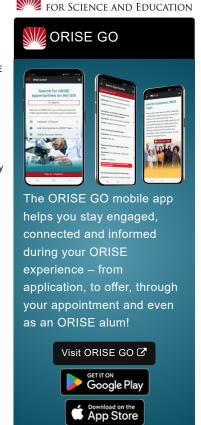
Description *Applications may be reviewed on a rolling-basis and this posting could close before the deadline. Click here for information about the selection process.

EPA Office/Lab and Location: A research opportunity is available at the Environmental Protection Agency (EPA), Office of Research and Development (ORD), Center for Environmental Measurement and Modeling (CEMM), Ecosystem Processes Division (EPD), in Athens, Georgia.

Research Project: This research project will focus on characterizing the likely transformation products of organic chemicals due to chemical and biological processes in aquatic, terrestrial and atmospheric systems. These transformations will be represented by reaction schemes associated with specific functional groups that may be present in an organic molecule. The primary objective of the research project is to assemble libraries of transformation pathways affecting the environmental fate of chemical classes that are a priority to the Agency. To accomplish this, data from published/completed experimental studies will be compiled and analyzed to characterize rates of transformation of various chemicals in the natural environment. This data will include the identity of transformation products, the fractional formation of the products, and the observed rates of transformation. The research project will further seek to elucidate the role of ambient conditions (e.g., pH, temperature and turbidity) and the presence of other reactive species in controlling the transformation pathway and reaction kinetics. This data will also form the basis for the development of Quantitative Structure Activity Relationships (QSARs) based on molecular properties for predicting transformation rates.

With guidance from the mentor, the research participant may be involved in the following training activities:

 Mining published literature and regulatory documents to extract information on organic chemical transformation pathways that are observed in aquatic ecosystems



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- · Synthesizing transformation pathway information from diverse sources to make inferences about the processes controlling chemical transformations
- · Incorporating process science understanding into existing cheminformatics-based software tools for the prediction of organic chemical transformation pathways
- · Developing algorithms to predict rates of transformation from molecular properties, structural attributes, and descriptors of ambient conditions
- · Evaluating the performance of software tools for predicting the identity of the dominant transformation products in natural environments

Learning Objectives: The research participant will benefit from interactions with an interdisciplinary research team with expertise in chemistry, microbiology, environmental modeling and software engineering. This team is presently working on the development and application of a suite of software tools that will provide the user with predicted reaction pathways, physicochemical properties, and transformation rates for Agency priority organic chemicals.

Mentor(s): The mentor for this opportunity is Caroline Stevens (<u>stevens.caroline@epa.gov</u>). If you have questions about the nature of the research please contact the mentor(s).

Anticipated Appointment Start Date: November/December 2020. All start dates are flexible and vary depending on numerous factors. Click here for detailed information about start dates.

Appointment Length: The appointment will initially be for one year and may be renewed up to three or four additional years upon EPA recommendation and subject to availability of funding.

Level of Participation: The appointment is full-time.

Participant Stipend: The participant will receive a monthly stipend commensurate with educational level and experience. Click here for detailed information about full-time stipends.

EPA Security Clearance: Completion of a successful background investigation by the Office of Personnel Management (OPM) is required for an applicant to be on-boarded at EPA.

ORISE Information: This program, administered by ORAU through its contract with the U.S. Department of Energy (DOE) to manage the Oak Ridge Institute for Science and Education (ORISE), was established through an interagency agreement between DOE and EPA. Participants do not become employees of EPA, DOE or the program administrator, and there are no employment-related benefits. Proof of health insurance is required for participation in this program. Health insurance can be obtained through ORISE.

Questions: Please see the FAQ section of our website. After reading, if you have additional questions about the application process please email EPArpp@orau.org and include the reference code for this opportunity.

Qualifications The qualified candidate should have received a master's or doctoral degree in one of the relevant fields, or be currently pursuing the degree and will reach completion by the start date of the

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appointment. Degree must have been received within five years of the appointment start date.

Knowledge of organic chemical reaction mechanisms and/or familiarity with cheminformatics software applications is desirable.

Eligibility Requirements

- Citizenship: U.S. Citizen Only
- **Degree:** Master's Degree or Doctoral Degree received within the last 60 months or anticipated to be received by 12/1/2020 12:00:00 AM.
- Academic Level(s): Graduate Students, Postdoctoral, or Post-Master's.
- Discipline(s):
 - Chemistry and Materials Sciences (4_●)
 - Computer, Information, and Data Sciences (1_●)
 - Earth and Geosciences (3_●)
 - Engineering (3_●)
 - Environmental and Marine Sciences (4_♥)
 - Life Health and Medical Sciences (1_●)
- **Veteran Status:** Veterans Preference, degree received within the last 120 month(s).

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