

Opportunity Title: EPA Postdoctoral Fellowship for Toxicokinetic Data Analysis

Opportunity Reference Code: EPA-ORD-CCTE-CCED-2022-06

Organization U.S. Environmental Protection Agency (EPA)

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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 [here](#) for detailed information about recommendations.

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

Application Deadline 1/6/2023 3:00:00 PM Eastern Time Zone

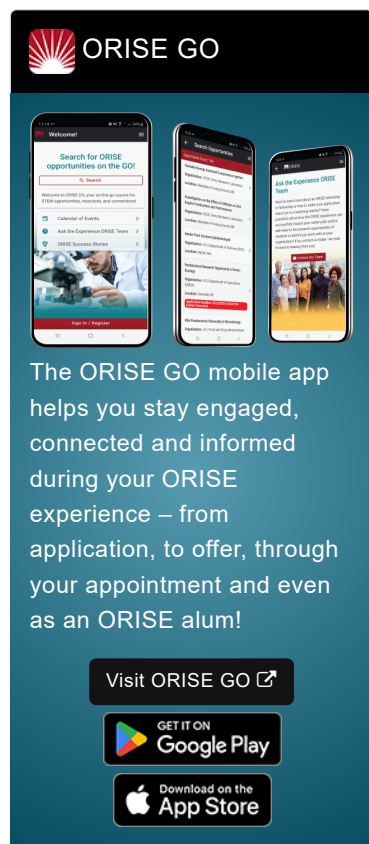
Description ***Applications may be reviewed on a rolling-basis and this posting could close before the deadline.** Click [here](#) for information about the selection process.

EPA Office/Lab and Location: A research opportunity is available at the Environmental Protection Agency (EPA), Office of Research and Development (ORD), Center for Computational Toxicology and Exposure (CCTE), Chemical Characterization & Exposure Division (CCED) located in Research Triangle Park, North Carolina.

Research Project: The EPA Center for Computational Toxicology and Exposure (CCTE) is responsible for developing new computational tools and providing quantitative analysis for improving public health and environmental risk assessments and regulatory decisions pertaining to chemical safety. This research project focuses on implementing and evaluating mathematical models for understanding the free chemical concentration within in vitro bioactivity assays. In vitro bioactive concentrations contribute to next generation risk assessment (NGRA), which aims to use human-relevant high throughput assays to replace animal toxicity testing. NGRA has the potential to understand the risks posed to the public health by chemicals in the environment and commerce.

The research participant will be a part of a multidisciplinary research team including scientists at EPA and multiple external partners.

This research project will reduce a key uncertainty in the use of new approach methodologies (NAMs) to provide key toxicity information. In vitro-in vivo extrapolation (IVIVE) is the science of relating chemical concentrations in the lab to real world exposures that might occur. A critical research need for IVIVE is to distinguish between the nominal



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concentration of the chemical added to the test system and the actual concentration at the site of action within the experimental system. Incomplete knowledge of in vitro disposition has the potential to be a significant source of error: For some chemicals the difference between nominal and effective chemical concentration has been shown to be greater than 100-fold. To the extent that nominal concentration fails to reflect actual media and/or target cell concentrations, IVIVE based on the nominal concentration will over- or under-predict doses that might cause adversity. In vitro disposition of chemicals in screening assays is a large uncertainty that impacts both accuracy and regulatory acceptance of bioactivity-based points of departure.

Mathematical models already exist to predict in vitro disposition based on physico-chemical properties; however, actual experimental data allowing evaluation have historically been extremely scarce. Most models either have not been evaluated or have been compared to data for fewer than ten chemicals. This research project will develop new modeling methods and analyze novel experimental data to address in vitro disposition of chemicals. The mathematical models studied will allow more accurate prediction in vivo toxicity through understanding the free chemical concentration within in vitro bioactivity assays.

Learning Objectives: Through this project the participant will gain education and training in mathematical modeling, computer programming, informatics, in vitro-in vivo extrapolation, and statistical analysis. The research participant will develop skills in Informatics and “Big Data” analytics using machine learning approaches, chemical non-targeted and suspect screening chemical (NTA/SSA), and statistical analysis. The research participant will receive training that includes co-authorship on peer-reviewed publications. The research participant will be supported in presenting project research at national meetings of professional societies and EPA work-in-progress seminars. The research participant will be involved in highly visible chemical safety efforts as part of the computational toxicology and exposure research projects and will be engaged with researchers world-wide.

Mentor(s): The mentor(s) for this opportunity is John Wambough (wambough.john@epa.gov). Collaborating researchers include Katie Paul-Friedman, Michael Devito, and Richard Judson. If you have questions about the nature of the research please contact the mentor(s).

Anticipated Appointment Start Date: **December 1, 2022.** 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 to 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

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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.

ORISE offers all ORISE EPA graduate students and Postdocs a free 5 year membership to the National Postdoctoral Association (NPA).

The successful applicant(s) will be required to comply with Environmental, Safety and Health (ES&H) requirements of the hosting facility, including but not limited to, COVID-19 requirements (e.g. facial covering, physical distancing, testing, vaccination).

Questions: Please see the [FAQ section](#) of our website. After reading, if you have additional questions about the application process please email ORISE.EPA.ORD@orau.org and include the reference code for this opportunity.

Qualifications The qualified candidate should have received a doctoral degree in one of the relevant fields (e.g. Biomedical Engineering, Informatics, Computer Science, Signal Processing, Machine Learning, Chemistry, Physics, Applied Mathematics, Statistics), or be currently pursuing the degree with completion before March 30, 2023. Degree must have been received within five years of the appointment start date.

Preferred Skills:

- Fluency in a modern programming language (for example, R, Python, Julia, C). This is a training position.
- Skills will be developed and previous experience is desired in applied mathematical modeling, for example:
 - Pharmacokinetics
 - Chemical engineering, biomedical engineering, applied mathematics, physics, and/or environmental engineering
 - Environmental fate and transport modeling
- Skills will be developed and previous experience is desired in statistical data analysis, for example:
 - Scientific software development in languages including R, Java, Perl, Python, Julia, C, and/or MATLAB.
 - Machine learning,
 - Quantitative structure-activity relationships,

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- Parallel computing
- Bayesian analysis via Markov Chain Monte Carlo,
- Applicants will conduct review of the scientific literature and ideally would be familiar with methods for extracting data from scientific publications.

- Eligibility**
- Requirements**
- **Citizenship:** U.S. Citizen Only
 - **Degree:** Doctoral Degree received within the last 60 months or anticipated to be received by 3/30/2023 11:59:00 PM.
 - **Discipline(s):**
 - **Chemistry and Materials Sciences** ([12](#) 👁)
 - **Computer, Information, and Data Sciences** ([17](#) 👁)
 - **Earth and Geosciences** ([21](#) 👁)
 - **Engineering** ([27](#) 👁)
 - **Environmental and Marine Sciences** ([14](#) 👁)
 - **Life Health and Medical Sciences** ([48](#) 👁)
 - **Mathematics and Statistics** ([11](#) 👁)
 - **Physics** ([16](#) 👁)
 - **Social and Behavioral Sciences** ([29](#) 👁)