

Opportunity Title: Postdoctoral Computational Toxicology Researcher **Opportunity Reference Code:** EPA-NSSC-0010-28

Organization U.S. Environmental Protection Agency (EPA)

Reference Code EPA-NSSC-0010-28

How to Apply Click <u>HERE</u> to apply.

Description The EPA National Student Services Contract has an immediate opening for a full time Postdoctoral Computational Toxicology Researcher position with the Office of Research and Development at the EPA facility in Duluth, MN.

The Office of Research and Development at the EPA supports high-quality research to improve the scientific basis for decisions on national environmental issues and help EPA achieve its environmental goals. Research is conducted in a broad range of environmental areas by scientists in EPA laboratories and at universities across the country.

What the EPA project is about

The Center for Computational Toxicology & Exposure (CCTE) is a scientific organization working to support Agency decisions by providing solutionsdriven research to rapidly evaluate the potential human health and environmental risks due to exposures to environmental chemicals and ensure the integrity of the freshwater environment and its capacity to support human well-being.

As part of their mission, the Great Lakes Toxicology and Ecology Division (GLTED) supports EPA's mission to protect human health and the environment by developing and applying innovations in computational toxicology. Specifically, through advancing methods in cross species extrapolation through developing methods and tools for the evaluation of species similarities and differences at the molecular level that can be used for predicting chemical susceptibility. Understanding chemical toxicity across the diversity of species from data generated with model organisms is essential to EPA's mission. Predictive computational tools for addressing such challenges in extrapolating data from one species to many (i.e., cross-species extrapolation) are needed to support research objectives in the Office of Research and Development and regulatory needs across Program Offices.

What experience and skills will you gain?

This position, in collaboration with Unilever scientists through a Cooperative Research and Development Agreement (CRADA), will jointly explore the utility of a battery of new approach methods (NAMs), which are non-animal based, for evaluating the safety and hazard of chemicals – establishing Next Generation Risk Assessments (NGRA). One of the primary missions of the US Environmental Protection Agency, Office of Research and Development, Center for Computational Toxicology and Exposure is to develop such methods. This includes high-throughput transcriptomics methods (HTTr) and bioinformatics approaches to predict chemical susceptibility across species (e.g., SeqAPASS; https://seqapass.epa.gov/seqapass/). Understanding the conservation and

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> relevance of targets and toxicity pathways, identified through HTTr screening using human and fish cell lines, across environmentally relevant species to inform chemical susceptibility and ultimately inform Environmental Risk Assessment (ERA) are major objectives of this training opportunity. This will be achieved using a suite of bioinformatics tools encompassing genomics and phylogenetics. The participant will be involved in the development of interoperable approaches to inform predictions of cross-species chemical susceptibility with demonstration of their application toward current challenges in ERA. Additionally, literature review will be conducted to capture cross-species biological pathway information linking mechanisms of chemical perturbation to adverse effects .

> As a team member, you will be trained in predictive toxicology aimed at characterizing the similarities and differences across species that drive chemical sensitivity. The position will primarily be computationally-based research taking place in an office setting with the potential to apply molecular techniques in the laboratory to validate computational results. You will provide database management, file management, data curation and extraction, quality control, as well as performing qualitative and quantitative data analysis. The team member will be a member of a multidisciplinary research team and support the development, maintenance, and expansion of analysis for the SeqAPASS data, tools, and web application.

Data Development and Analysis responsibilities will include:

- Estimating points of departure (e.g., lowest observed effect concentrations, benchmark doses) from high throughput toxicity testing data including ToxCast data and omics data sets;
- Comparing points of departure from alternative methods with those derived from traditional animal testing;
- Designing workflows and data analysis pipelines for automated and standardized analysis of large data sets;
- Developing and implementing a data archiving and storage system;
- Automate data collection and collation processes;
- Propose solutions and strategies to improve existing web-based U.S. EPA tools, particularly considering interoperability with other internal and external tools;
- Extend existing software programs, web-based interactive tools, or database queries as analysis needs evolve;
- Explore and operate molecular modeling, molecular docking, virtual screening, and molecular dynamic simulation programs to support research;
- Development of methods for streamlining molecular docking and virtual screening for cross species comparisons of chemical-protein interactions;
- · Quality control of computational derived data;
- Development of manuscripts and fact sheets supporting the data products; and
- Literature review, including the use of systematic methods.

Communications-related responsibilities will include:



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- Participating as a member of a multi-disciplinary research team;
- Interacting with other members of the development team as well as EPA scientists;
- Documenting code, methods, and tool/pipeline development efforts; and
- Presenting work performed at a scientific conference as required.

Required Knowledge, Skills, Work Experience, and Education

- Demonstrated education and/or experience in informatics and/or bioinformatics, ideally with protein molecular modeling, molecular docking, molecular dynamic simulations, and/or virtual screening;
- Experience with computational toxicology in answering biological questions;
- Previous research experience in molecular biology, beyond lab-oriented course work alone; and
- Strong written, oral, and electronic communication skills.

Desired Knowledge, Skills, Work Experience, and Education

- Previous experience working with omics data and/or high throughput data sets such as those from EPA's ToxCast program;
- Experience programming in R, Phython, or other scripting languages; and
- Experience using Molecular Operating Environment (MOE), AutoDock Vina, and/or similar software.

Location: This job will be located EPA's facility in Duluth, MN.

Salary: Selected applicant will become a temporary employee of ORAU and will receive an hourly wage of \$44.60 for hours worked.

Hours: Full-time.

Travel: Occasional overnight travel may be required.

Expected start date: The position is full time and expected to begin July 2024. The selected applicant will become a temporary employee of ORAU working as a contractor to EPA.

For more information, contact EPANSSC@orau.org. Do not contact EPA directly.

Qualifications • Be at least 18 years of age and

- Have earned at least a doctoral degree in the fields of bioinformatics, computational toxicology, genetics, pharmacology, health sciences, or a related field **and**
- Be a citizen of the United States of America or a Legal Permanent Resident.

EPA ORD employees, their spouses, and children are not eligible to participate in this program.



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Eligibility	 Citizenship: LPR or U.S. Citizen
Requirements	Degree: Any degree .
	 Discipline(s):
	 Life Health and Medical Sciences (<u>6</u>

Affirmation I certify that I am at least 18 years of age; a recent graduate with at least a doctoral degree in the fields of bioinformatics, computational toxicology, genetics, pharmacology, health sciences, or a related field of study from an accredited university or college within the last 24 months; a citizen or a Legal Permanent Resident of the United States of America; and not a current employee of EPA ORD or the spouse or child of an EPA ORD employee.

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