Opportunity Title: Postdoctoral Researcher - Computational Toxicology
Opportunity Reference Code: EPA-NSSC-0010-21

Organization U.S. Environmental Protection Agency (EPA)

Reference Code EPA-NSSC-0010-21

How to Apply Click HERE to apply.

Description The EPA National Student Services Contract has an immediate opening for a full time Postdoctoral Researcher - Computational Toxicology 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 solutions-driven 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?

As a team member, you will provide data management, data curation and data analysis support for a project aiming to translate the analysis and findings of 3D molecular modeling efforts (e.g., molecular docking studies and protein-ligand interaction fingerprints) to generate and inform virtual high-throughput screening (vHTS) techniques such as pharmacophore-based ligand screening and ligand-based conformational modeling to be used in the elucidation of chemical effects to support cross species extrapolation. Additionally, the team member will utilize existing systematic literature review methods to create a corpus of literature specific for site-directed mutagenesis studies to identify amino acid changes that lead to

altered binding, activity, or function. This corpus of literature will be used to collate these changes in amino acids and incorporate design of features in the Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS; https://seqapass.epa.gov/seqapass/) tool to predict susceptibility from these data. The team member will provide database management, file management, data curation and extraction, quality control, as well as performing qualitative and quantitative data analysis. The candidate will be a member of a multi-disciplinary research team and will support the development, maintenance, and expansion of analysis for the SeqAPASS data, tools, and web application.

How you will apply your skills

Data Development and Analysis responsibilities will include:

- 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:

- 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 protein molecular modeling, molecular docking, molecular dynamic simulations, and/or virtual screening;
- Experience with computer science in the context of using the approaches to answer biological questions (e.g., bioinformatics approaches evaluating gene or protein data); and
- Strong written, oral and electronic communication skills.

Desired Knowledge, Skills, Work Experience, and Education

- Experience programming in R or other scripting languages; and
- Experience using Molecular Operating Environment (MOE), AutoDock Vina, and/or similar software.

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

Salary: Selected applicant will become a temporary employee of ORAU and will receive an hourly wage of $43.73 for hours worked.

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Hours: Full-time.

Travel: Occasional overnight travel may be required.

Expected start date: The position is full time and expected to begin May 2023. The selected applicant will become a temporary employee of ORAU working as a contractor to EPA. The contract renews each May through 2025.

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, or a related field from an accredited university or college within the last 24 months **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.

Eligibility Requirements

- **Citizenship:** LPR or U.S. Citizen
- **Degree:** Doctoral Degree received within the last 24 months or currently pursuing.
- **Overall GPA:** 2.00
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (12 👁)
  - **Communications and Graphics Design** (2 👁)
  - **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 👁)
  - **Science & Engineering-related** (2 👁)
  - **Social and Behavioral Sciences** (28 👁)

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, or a related field 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.

Click HERE to apply!

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