

Opportunity Title: Computational Modeling Support

Opportunity Reference Code: EPA-NSSC-0009-62

Organization U.S. Environmental Protection Agency (EPA)

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How to Apply Click [HERE](#) to apply!

Description The EPA National Student Services Contract has an immediate opening for a full time Computational Modeling Support position with the Office of Research and Development at the EPA facility in Research Triangle Park, NC.

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 and Exposure (CCTE) supports ORD by providing solutions-driven research to rapidly evaluate the potential human health and environmental risks due to exposures to environmental stressors and ensure the integrity of the freshwater environment and its capacity to support human well-being. CCTE researchers are developing and applying cutting edge innovations in methods to rapidly evaluate chemical toxicity, transport, and exposure to people and environments. Within CCTE, the Chemical Characterization and Exposure Division (CCED) performs research to develop and advance analytical chemistry, computational chemistry, and cheminformatic approaches that are critical to the rapid characterization of the presence, structural characteristics, and properties of chemicals that underlie chemical exposure, environmental fate, toxicokinetics, and toxicity.

What experience and skills will you gain?

As a team member, you will support research under the Chemical Safety for Sustainability (CSS) research program in the Informatics, Synthesis, and Integration (ISI) Research Area. The Informatics, Synthesis, and Integration (ISI) Research Area will develop approaches to present, manage, and utilize the voluminous empirical and predicted data derived from CSS research efforts and relevant external data sources. ISI efforts include designing systems and approaches to integrate these diverse data streams into knowledge transfer modules, platforms, and/or workflows with the expressed objective of informing decision-making for multiple problem formulations associated with evaluation of environmental chemicals.

Paramount to this research area is the need to effectively share quantitative structure-activity relationship (QSAR) models with relevant stakeholders, including those internal and external to EPA. Historically, QSAR models have been developed by research scientists using a plethora of computational software and programming languages. This necessitates a standardized system, a model management system, to share the various



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models associated with scientific publications in the same form as detailed in those papers. The incumbent will help advance this model management system by developing software to facilitate the storage and deployment of models using technologies such as the Predictive Model Markup Language (PMML) and open source Java libraries as well as working with the research scientists producing QSAR models to ensure their storage and retrieval needs are adequately addressed throughout the development process.

The duties of the team member will include, but are not limited to:

- Developing, modifying, and integrating public-facing software to perform specific aspects of QSAR modeling.
- This may include the development of novel machine learning models and developing and using existing (or new) application programming interfaces (APIs) between databases and applications.
- Developing, modifying, and integrating existing (or new) web services to facilitate model storage, deployment, and use by the public.
- Architect and maintain databases (e.g., MySQL, PostgreSQL, SQLite) for storage of modeling data.
- Respond to data requests from colleagues as needed (e.g., retrieve data according to specified criteria) through development of SQL queries and API scripts; and
- Participate in curation of chemical information and physchem datasets.

Communication-related responsibilities will include:

- Participate as a member of a multi-disciplinary research team;
- Engage with and participate in the scientific process, including presenting results at internal meetings and learning the necessary background to communicate the greater impact of their work;
- Interact with other members of the development team as well as EPA scientists;
- Thoroughly document all work as directed by EPA mentor to comply with EPA quality assurance procedures for transparency and reproducibility of work; and
- Summarize work in internal reports/memos to be used by EPA scientists.

Required Knowledge, Skills, Work Experience, and Education

- Experience with SQL, database structure, and data storage practices;
- Knowledge of basic chemistry in terms of molecular structure and chemical properties;
- Experience programming in Java, object-oriented Scala, or any objected-oriented programming language (i.e., Python, etc.);
- Experience in designing and modifying web applications, APIs, and software tools as well as familiarity in using frameworks such as Hibernate, Flask, and/or Spring Boot; and
- Strong reading comprehension skills and experience logically interpreting pieces of data.

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Desired Knowledge, Skills, Work Experience, and Education

- Understanding of software development practices (Agile, etc.)

Location: This job will be located EPA's facility in Research Triangle Park, NC.

Salary: Selected applicant will become a temporary employee of ORAU and will receive an hourly wage of \$31.38 for hours worked.

Hours: Full-time.

Travel: Occasional overnight travel is not required

Expected start date: The position is full time and expected to begin October 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 master's degree in physics, chemistry, biology, engineering, applied sciences, environmental health, exposure science, computer sciences, information technology, data science, or a related discipline (i.e., cheminformatics) 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:** Master's Degree received within the last 24 month(s).
- **Discipline(s):**
 - **Business** ([11](#) 👁)
 - **Chemistry and Materials Sciences** ([12](#) 👁)
 - **Communications and Graphics Design** ([6](#) 👁)
 - **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](#) 👁)
 - **Other Non-Science & Engineering** ([13](#) 👁)
 - **Physics** ([16](#) 👁)
 - **Science & Engineering-related** ([2](#) 👁)
 - **Social and Behavioral Sciences** ([29](#) 👁)

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Affirmation I certify that I am at least 18 years of age; a recent graduate with at least a Master's degree in physics, chemistry, biology, engineering, applied sciences, environmental health, exposure science, computer sciences, information technology, data science, or a related discipline (i.e., cheminformatics) 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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