Opportunity Title: QSAR modeling for PFAS
Opportunity Reference Code: EPA-NSSC-0009-30

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 Ph.D. level QSAR modeling for PFAS 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 on PFAS (Per- and Polyfluoroalkyl Substances). PFAS are a group of man-made chemicals that are very persistent in the environment and in the human body – meaning they don't break down and they can accumulate over time. There is evidence that exposure to PFAS can lead to adverse human health effects. Physicochemical (or physchem) properties are needed to be able to assess human exposure to these chemicals.

Since there is a paucity of experimental physchem data for PFAS, the goal of this project to develop QSAR (quantitative structure activity relationship) models to estimate properties from molecular structure. It is desired to develop models for a variety of properties/endpoints such as water solubility, Henry's law constant octanol water partition coefficient, and the log10BCF (bioconcentration factor) in fish.

How you will apply your skills

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

- Development of modeling data sets from raw experimental data;
  - This will require careful analysis of metadata to determine valid modeling records.
- Developing models to predict physical properties from molecular structure;
  - Modeling approaches may include random forest (RF), support vector machines (SVM), and k nearest neighbor (kNN) methods.
  - Models will be written using machine learning libraries in Python, online model development tools, or custom in-house computer code written in Java.
- Developing web services to perform specific aspects of QSAR modeling; and

- Respond to data requests from colleagues as needed (e.g. retrieve data according to specified criteria) through development of programming scripts or SQLqueries.

Communications-related responsibilities will include:

- Participate as a member of a multi-disciplinary research team;

- 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 computational or mathematical modeling (i.e. cheminformatics or QSAR modeling) and data science techniques;

- Knowledge of basic chemistry in terms of molecular structure and physicochemical properties;

- Experience programming in the Java or Pythonlanguages;

- Experience with quantitative techniques, basic statistics, and use of spreadsheets; and

- Strong reading comprehension skills and experience logically interpreting pieces of data.

Desired Knowledge, Skills, Work Experience, and Education

- Experience with databases (e.g. MySQL).

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

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Salary: Selected applicant will become a temporary employee of ORAU and will receive an hourly wage of $43.31 for hours worked.

Hours: Full-time.

Travel: Overnight travel is not required.

Expected start date: The position is full time and expected to begin August 2021. The selected applicant will become a temporary employee of ORAU working as a contractor to EPA. The initial project is through May 14, 2022, with up to 3 additional option periods.

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

Qualifications
- Be at least 18 years of age **and**
- Have earned a Doctorate in physics, chemistry, biology, engineering, applied sciences, environmental health, exposure science, computer sciences, information technology, data science, or a related discipline 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 month(s).
- **Overall GPA:** 2.00
- **Discipline(s):**
  - **Computer, Information, and Data Sciences** (17 👁)
  - **Engineering** (27 👁)
  - **Life Health and Medical Sciences** (46 👁)
  - **Mathematics and Statistics** (10 👁)
  - **Physics** (16 👁)

Affirmation I certify that I am at least 18 years of age; a recent graduate with a Doctorate in physics, chemistry, biology, engineering, applied sciences, environmental health, exposure science, computer sciences, information technology, data science, or a related discipline 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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