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Opportunity Title: Chemical Compound Curation Research
Opportunity Reference Code: EPA-NSSC-0009-61

Organization U.S. Environmental Protection Agency (EPA)

Reference Code EPA-NSSC-0009-61

How to Apply Click HERE to apply!

Description The EPA National Student Services Contract has an immediate opening for a full time Chemical Compound Curation Research 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 QACs (quaternary ammonium compounds). QACs are a large class of chemicals that have seen increased use as disinfectants during the COVID-19 pandemic. In order to assess any risk associated with this class of chemical, it is necessary to capture the entirety of the chemical space defined by molecules having the quarternary ammonium substructure.

The initial goal is to aid in the refinement of QAC nomenclature as well as defining the QAC structure space, including the enumeration of complex substances to establish training data for the automated translation of structure to compound name.

Once the QACs dataset is complete, data will be gathered for additional classes of chemicals, such as PFAS, including physicochemical properties, toxicology, and exposure data.

This support consists of data entry, online searches, curation, and

computer programming to aid in the enhancement of existing chemical data sets. The data will be obtained from a variety of literature sources including online databases, websites, and journal articles.

The team member will assist with data organization and extraction needs, including acquisition and development of datasets containing QACs, development of semi-automated protocols for data identification and collection, basic summaries and analyses of data, and extraction and curation of data from original sources.

The work of the team member may include gathering additional datasets from online sources, formatting datasets into standard templates and uploading into databases, applying out-of- the-box thinking to improve automated data collection, and completing QA workflows to ensure data quality and provenance.

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

- Collecting, curating (e.g., drawing chemical structures), and organizing data in databases on QACs including relevant metadata (e.g., CAS number, chemical name, physicochemical properties);
- Respond to data requests from colleagues as needed (e.g., retrieve data according to specified criteria) through development of programming scripts or SQL queries; and
- Development of novel data models and text analytics methods for identifying data sources containing QACs and nomenclature similarities between QAC subclasses.

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

- Knowledge of basic chemistry in terms of molecular structure, chemical naming conventions, and physicochemical properties
- Experience programming in the Java, R, and/or Python languages
- Experience with quantitative techniques, basic statistics, and use of spreadsheets
- Strong reading comprehension skills and experience logically interpreting pieces of data

Desired Knowledge, Skills, Work Experience, and Education

- Master’s coursework in statistics, data science, user experience and

design, and/or data analysis;
- Experience with computational or mathematical modeling (i.e. cheminformatics) and data science techniques; and
- Experience with databases.

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 August 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 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 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).
- **Overall GPA:** 2.00
- **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 👁)

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- **Social and Behavioral Sciences** (29 👁)

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 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.