Opportunity Title: EPA Computational Chemistry and QSAR Models Fellowship
Opportunity Reference Code: EPA-ORD-CCTE-BCTD-2020-03

Organization U.S. Environmental Protection Agency (EPA)

Reference Code EPA-ORD-CCTE-BCTD-2020-03

How to Apply ***Connect with ORISE...on the GO!*** Download the new ORISE GO mobile app in the Apple App Store or Google Play Store to help you stay engaged, connected, and informed during your ORISE experience and beyond!

A complete application consists of:

- An application
- Transcript(s) – For this opportunity, an unofficial transcript or copy of the student academic records printed by the applicant or by academic advisors from internal institution systems may be submitted. All transcripts must be in English or include an official English translation. Click here for detailed information about acceptable transcripts.
- A current resume/CV, including academic history, employment history, relevant experiences, and publication list
- Two educational or professional recommendations. Click here for detailed information about recommendations.

All documents must be in English or include an official English translation.

Application Deadline 10/20/2020 3:00:00 PM Eastern Time Zone

Description ***Applications may be reviewed on a rolling-basis and this posting could close before the deadline.** Click **here** for information about the selection process.

EPA Office/Lab and Location: A research opportunity is available at the Environmental Protection Agency (EPA), Office of Research and Development (ORD), Center for Computational Toxicology and Exposure (CCTE), Biomolecular & Computational Toxicology Division (BCTD) located in Research Triangle Park, North Carolina.

The EPA CCTE is responsible for developing new computational tools and providing quantitative analysis for improving environmental risk assessments and regulatory decisions pertaining to chemical safety and sustainability.

Research Project: This research project aims to develop computational models to predict the safety of chemicals without running tests on whole animals. The tools to be used include databases of chemicals of environmental interest, previously run animal studies, data from in vitro experiments, and outputs of various predictive models of chemical action. The project integrates data science, software engineering, applied statistics, and predictive mathematical modeling.

Under the guidance of a mentor, the research participant will learn to develop novel computational chemistry applications to predict properties of interest for risk assessment. These will include chemical properties and toxicological endpoints. Research activities may include: (1) the development of a generic QSAR infrastructure that could be used to automate computation of a large number of chemical endpoints on hundreds of thousands of chemicals and store them in relational databases;

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(2) development of methods to curate data used to build models; (3) evaluation of existing models and integration of these into in-house modeling pipelines; (4) develop of consensus models (i.e. models that rely on multiple other models as input).

Learning Objectives: The research participant will gain education and training in the general areas of computational chemistry, bioinformatics data science, mathematical modeling, data management, and computational toxicology in preparation for future career opportunities.

The research participant may author or co-author on peer-reviewed publications and may present at local and national meetings. The participant will be a member of a multi-disciplinary research team.

Mentor(s): The mentor for this opportunity is Richard Judson (Judson.richard@epa.gov). If you have questions about the nature of the research please contact the mentor(s).

Anticipated Appointment Start Date: Summer/Fall 2020. All start dates are flexible and vary depending on numerous factors. Click **here** for detailed information about start dates.

Appointment Length: The appointment will initially be for one year and may be renewed up to four additional years upon EPA recommendation and subject to availability of funding.

Level of Participation: The appointment is full-time.

Participant Stipend: The participant will receive a monthly stipend commensurate with educational level and experience. Click **here** for detailed information about full-time stipends.

EPA Security Clearance: Completion of a successful background investigation by the Office of Personnel Management (OPM) is required for an applicant to be on-boarded at EPA.

ORISE Information: This program, administered by ORAU through its contract with the U.S. Department of Energy (DOE) to manage the Oak Ridge Institute for Science and Education (ORISE), was established through an interagency agreement between DOE and EPA. Participants do not become employees of EPA, DOE or the program administrator, and there are no employment-related benefits. Proof of health insurance is required for participation in this program. Health insurance can be obtained through ORISE.

Questions: Please see the FAQ section of our website. After reading, if you have additional questions about the application process please email EPArpp@orau.org and include the reference code for this opportunity.

Qualifications The qualified candidate should have received a doctoral degree in one of the relevant fields, or be currently pursuing the degree and will reach completion by September 2020. Degree must have been received within five years of the appointment start date.

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Proficiency in the development of computational chemistry applications, including machine learning models in R or Python, and in the use of relational databases is preferred.

Eligibility Requirements

- **Citizenship:** U.S. Citizen Only
- **Degree:** Doctoral Degree received within the last 60 months or anticipated to be received by 9/30/2020 11:59:00 PM.
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (5 👁)
  - **Computer, Information, and Data Sciences** (3 👁)
  - **Engineering** (1 👁)
  - **Environmental and Marine Sciences** (3 👁)
  - **Life Health and Medical Sciences** (45 👁)
  - **Mathematics and Statistics** (1 👁)
  - **Other Non-Science & Engineering** (1 👁)
  - **Physics** (1 👁)
- **Veteran Status:** Veterans Preference, degree received within the last 120 month(s).