

Opportunity Title: Development of QSAR Models and Delivery

Opportunity Reference Code: EPA-ORD-NCCT-2017-03

Organization U.S. Environmental Protection Agency (EPA)

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How to Apply A complete application consists of:

- An application
- Transcripts – [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 references

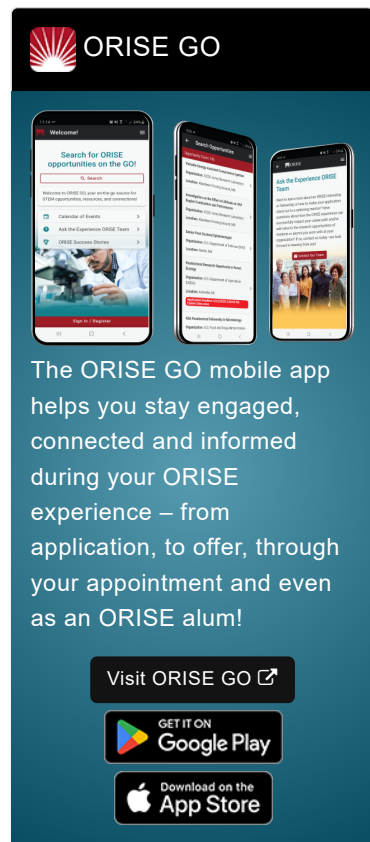
All documents must be in English or include an official English translation.

If you have questions, send an email to EPArpp@orau.org. Please include the reference code for this opportunity in your email.

Description A postdoctoral research opportunity is currently available at the U.S. Environmental Protection Agency's (EPA) Office of Research and Development (ORD). The appointment will be served with the National Center for Computational Technology (NCCT) in Research Triangle Park, NC.

NCCT 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. This project aims to enhance existing data curation and standardization workflows to prepare data for modeling. Models will be developed to support predictions of various endpoints including toxicity and physchem (specifically to support analytical chemistry analysis).

The participant will collaborate with a multidisciplinary research team including scientists at EPA and other partners. The research activities will include. (1) exploring approaches for automated data extraction, standardization and curation; (2) integrating chemical structure, physicochemical, toxicity and bioactivity data and information to generate SAR/QSAR/QSPR models; (3) exploring the application of QSAR models to the analysis and validation of analytical data supporting mass-spectrometry non-targeted analysis studies. Activities will include: a) adapting existing open source software code to enhance workflows for data conversion, standardization and curation. b) enhancing existing datasets and developing new datasets to underpin predictive models. c) integrating the data and models into existing databases and web-based tools; c) engaging with NCCT researchers and collaborators in the application of the models and workflows to diverse research projects. The participant will be trained in developing new workflows, predictive models and prototype tools for data-analysis and dissemination of all research outputs. Predictive models and associated data will be made available via NCCT online tools (e.g. CompTox Chemistry Dashboard at <http://comptox.epa.gov>) and delivered within the agency to other offices to support their research programs. The training the participant will receive, coupled with a productive publishing



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record, should make it possible for them to move into any of these areas or continue down a transdisciplinary path at their discretion. The research participant will be involved in highly visible predictive toxicology efforts as part of the computational toxicology research projects and will be engaged with researchers world-wide.

In the course this research project, research findings will be disseminated and communicated through web-based dashboards, research-in-progress seminars, peer-reviewed publications, and national meetings of professional societies. The research participant will be involved in highly visible predictive toxicology efforts as part of the computational toxicology research projects and may be engaged with researchers world-wide. S/he will be published in peer-reviewed journals and present research results at local and national meetings. S/he will perform under a research project plan and instructions provided by the mentor. S/he will have latitude in exercising independent initiative and judgment in the research commensurate with the level of training. Through this project, the participant will gain education and training in the general areas of data management, modeling and computational toxicology. Prior experience in these areas would clearly be of value.

This program, administered by ORAU through its contract with the U.S. Department of Energy to manage the Oak Ridge Institute for Science and Education, was established through an interagency agreement between DOE and EPA. The appointment is full time for one year and may be renewed upon recommendation of EPA and contingent on the availability of funds. The participant will receive a monthly stipend. Funding may be made available to reimburse the participant's travel expenses to present the results of his/her research at scientific conferences and stakeholder venues. No funding will be made available to cover travel costs for pre-appointment visits, relocation costs, tuition and fees, or participant's health insurance. The participant must show proof of health and medical insurance. **The participant does not become an EPA employee.**

The mentor for this project is Anthony Williams (williams.antony@epa.gov). The desired start date for this appointment is July 17, 2017.

Qualifications Postdoctoral degree in chemistry, biochemistry, toxicology, physics, applied math, statistics, or computer science within five years of the desired start date, or completion of all requirements for the degree should be expected prior to the starting date.

- Eligibility Requirements**
- **Degree:** Doctoral Degree received within the last 60 month(s).
 - **Discipline(s):**
 - **Chemistry and Materials Sciences** ([12](#) )
 - **Computer, Information, and Data Sciences** ([6](#) )
 - **Environmental and Marine Sciences** ([3](#) )
 - **Life Health and Medical Sciences** ([45](#) )
 - **Mathematics and Statistics** ([10](#) )