Opportunity Title: Drug Target Prediction Fellowship - FDA CDER
Opportunity Reference Code: FDA-CDER-2018-0303

Organization U.S. Food and Drug Administration (FDA)

Reference Code FDA-CDER-2018-0303

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 FDArpp@orau.org . Please include the reference code for this opportunity in your email.

Description An opportunity is available at the U. S. Food and Drug Administration (FDA), Center for Drug Evaluation and Research (CDER) in Silver Spring, Maryland.

The Office of the Center Director and Controlled Substances Staff (CSS), working with the Drug Enforcement Agency (DEA) has requested that Office of Translational Sciences (OTS) Office of Clinical Pharmacology (OCP) Division of Applied Regulatory Science (DARS) develops computational models to help determine whether chemical substances are a risk to public safety and should be temporarily placed into Schedule I of the Controlled Substances Act (CSA) (21 U.S.C. 811 (h)). This project will develop and validate three dimensional (3D) quantitative structure-activity relationship (QSAR) models to predict the binding affinity of opioids, cannabinoids and stimulants. These new models can be rapidly deployed and used to provide science-based evidence in the absence of in vitro data to support scheduling needs.

Under the guidance of a mentor, the participant will be trained in: collecting experimental assay data from databases, literature, or proprietary sources and evaluating the accuracy and assisting in the enhancement of one or more target prediction models of receptors of interest from the Protein Data Bank (PDB) and importing into the Molecular Operating Environment (MOE) software; generating chemical structures for substances; converting to a computer-readable format; importing into MOE and docked using molecular interactions identified by the software; scoring for each pose; calculating and comparing to the empirical binding data; and conducting an additional validation.

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 FDA. The initial appointment is for one year, but may be renewed upon recommendation of FDA contingent on the availability of funds. The participant will receive a monthly stipend commensurate with educational level and experience. Proof of health insurance is required for participation in this program. The appointment is full-time at FDA in the Silver Spring, area. Participants do not become employees of FDA, DOE or the program administrator, and there are no employment-related benefits.

The Homeland Security Presidential Directive-12 (HSPD-12) mandates a background check be completed for both U.S. Citizens and foreign nationals. Foreign nationals must have resided in the U.S. for at least three (3) of the past five (5) years in order for FDA to be able to complete a

background check.

Qualifications

Doctoral or master's degree in chemistry, the health sciences, or a related field received within the last five years required

Knowledge of drug toxicology and chemical/biological data mining desired.

Eligibility Requirements

- **Degree:** Master's Degree or Doctoral Degree received within the last 60 month(s).
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (11)
  - **Environmental and Marine Sciences** (1)
  - **Life Health and Medical Sciences** (45)