Opportunity Title: FDA Fellowship in Cheminformatics and Computational Chemistry
Opportunity Reference Code: FDA-NCTR-2023-07

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

Reference Code FDA-NCTR-2023-07

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
- Transcripts – Click here for detailed information about acceptable transcripts
- A current resume/CV, including academic history, employment history, relevant experiences, and publication list
- One educational or professional recommendation. Your application will be considered incomplete, and will not be reviewed until one recommendation is submitted.

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

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

Application Deadline 10/31/2023 3:00:00 PM Eastern Time Zone

Description ***Applications will be reviewed on a rolling basis.**

A postdoctoral fellowship opportunity is currently available in the Bioinformatics Branch in Division of Bioinformatics and Biostatistics at the National Center for Toxicological Research (NCTR) of the U.S. Food and Drug Administration (FDA) Jefferson Laboratories Campus located in Jefferson, Arkansas.

The candidate will collaborate with the Principal Investigator (PI) and Co-PIs across different centers in FDA on research projects aimed at the Identification and validation of immutable vaccine targets in severe acute respiratory syndrome–coronavirus 2 (SARS-CoV-2) spike glycoprotein. The candidate will learn various techniques in 1) collecting comprehensive sets of SARS-CoV-2 S gene sequences from GISAID, GenBank, FDA-ARGOS and other sources and curate the dataset to select high-quality sequences for computational analysis, obtain next-generation sequence data from NCBI Short Read Archive and assemble S gene sequences from high-quality data; (2) identifying amino acid residues that have been subject to strong, pervasive negative (purifying) selective pressure; (3) refining SARS-CoV-2 S glycoprotein 3D structure model and map identified sites to the 3D structure. (4) mapping existing published knowledge, including information on glycans, to better evaluate the predicted functionally significant critical amino acid sites; and (5) mutating the critical amino acid residues within the 3D structure to predict the impact on structure and function.

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 Jefferson, Arkansas area. Participants do not become employees of FDA, DOE or the program

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administrator, and there are no employment-related benefits.

Completion of a successful background investigation by the Office of Personnel Management is required for an applicant to be on-boarded at FDA. OPM can complete a background investigation only for individuals, including non-US Citizens, who have resided in the US for a total of three of the past five years.

FDA Ethics Requirements

If an ORISE Fellow, to include their spouse and minor children, reports what is identified as a Significantly Regulated Organization (SRO) or prohibited investment fund financial interest in any amount, or a relationship with an SRO, except for spousal employment with an SRO, and the individual will not voluntarily divest the financial interest or terminate the relationship, then the individual is not placed at FDA. For additional requirements, see FDA Ethics for Nonemployee Scientists.

FDA requires ORISE participants to read and sign their FDA Education and Training Agreement within 30 days of his/her start date, setting forth the conditions and expectations for his/her educational appointment at the agency. This agreement covers such topics as the following:

- Non-employee nature of the ORISE appointment;
- Prohibition on ORISE Fellows performing inherently governmental functions;
- Obligation of ORISE Fellows to convey all necessary rights to the FDA regarding intellectual property conceived or first reduced to practice during their fellowship;
- The fact that research materials and laboratory notebooks are the property of the FDA;
- ORISE fellow's obligation to protect and not to further disclose or use non-public information.

Qualifications

The qualified candidate should have received or be currently pursuing a doctoral degree in one of the relevant fields (e.g. chemistry, physics or engineering with a strong emphasis in nanotechnology). Degree must have been received within five years of the appointment start date.

Preferred Skills:

- Protein structure modeling
- Molecular dynamics simulations
- Database development
- Proficiency with at least one programming language (Python, Perl, Java, C, etc.)
- Experience with computational chemistry software packages such as Schrodinger, AMBER, AutoDock, and PyMOL.
- Candidates should also possess excellent oral and written communication skills, good judgment, clear sense of purpose, and accountability.

Eligibility Requirements

- **Degree:** Doctoral Degree received within the last 60 months or currently pursuing.
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (2 👁)
  - **Computer, Information, and Data Sciences** (5 👁)
  - **Life Health and Medical Sciences** (3 👁)
  - **Mathematics and Statistics** (1 👁)

Affirmation

I have lived in the United States for at least 36 out of the past 60 months. (36 months do not have to be consecutive.)

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and

I have read the FDA Ethics Requirements.