

Translational Science Interagency Postdoctoral Fellowship (Cheminformatics/AI-ML/NAMs)

Organization

National Institutes of Health (NIH), National Center for Advancing Translational Sciences, Rockville, Maryland, United States

U.S. Food and Drug Administration (FDA), White Oak Campus, Silver Spring, Maryland

Scientific focus areas

- Cheminformatics, AI/ML, Computational Chemistry
- Bioengineering and Biomedical Engineering, Biology, Biochemistry, Chemistry, Physics, Pharmacology, and Basic Biomedical Sciences

The NIH National Center for Advancing Translational Sciences, Division of Preclinical Innovation, in collaboration with the FDA Division of Applied Regulatory Science, Office of Clinical Pharmacology, Office of Translational Sciences, (CDER) is now seeking a qualified postdoctoral fellow for the Early Translation Branch.

About the fellowship

The National Center for Advancing Translational Sciences (NCATS), a major research component of the National Institutes of Health (NIH), invites applications for a postdoctoral fellow through the Translational Science Interagency Fellowship (TSIF) program, a three-year long collaborative training program between NCATS and the U.S. Food and Drug Administration (FDA).

This fellowship offers a unique opportunity to train at the interface of computational modeling, drug discovery, and regulatory science, with direct exposure to how computational models and human-relevant experimental platforms can influence real-world drug development and safety evaluation. The fellow will be co-mentored by investigators at NCATS and FDA and will contribute to developing AI/ML-driven approaches for mechanism-based drug safety assessment and drug repurposing, as well as experimental validation using cutting-edge New Approach Methodologies (NAMs) and complex in vitro models (CIVMs). Fellows are expected to spend three years in combined training at the FDA and NCATS. The exact timing of the transition between the two agencies will be project and mentor dependent.

Responsibilities of this fellowship include:

- Curate, harmonize, and analyze a large-scale target class profiling datasets and construct compound-level activity signature vectors
- Design, develop, and optimize multi-task machine learning models to predict target-specific and cross-target inhibition patterns
- Integrate target class activity signatures *within silico* ADME and organ toxicity predictions into a unified compound prioritization framework
- Actively participate in laboratory-based research activities utilizing human-relevant *in vitro* models.

- Apply CIVMs and other NAMs to experimentally evaluate and confirm computational model predictions related to organ-specific adverse events, including hepatotoxicity, cardiotoxicity, and CNS toxicity
- Collaborate closely with experimental scientists, regulatory science colleagues at FDA, and interdisciplinary teams across NCATS
- Present research findings in internal meetings and at external scientific conferences and contribute to peer-reviewed publications.

Training & Development Opportunities:

- Receive comprehensive training in human induced pluripotent stem cell-derived techniques, gaining hands-on experience with cutting-edge cellular models used in regulatory science
- Gain an in-depth understanding of how human-relevant in vitro models advance the principles of regulatory science and public health protection
- Develop expertise in emerging NAMs and AI/ML methodologies with direct regulatory application
- Gain meaningful exposure to government regulatory science and the drug evaluation process at one of the world's leading public health agencies
- Build a professional network spanning NIH, FDA, and the broader translational and regulatory science communities

Qualifications

Prospective applicants should possess a Ph.D. in computational chemistry, cheminformatics, computer science, data science, , bioengineering, pharmacology or a related discipline, with demonstrated experience in data-driven research, including machine learning or statistical modeling. Strong programming skills in languages such as Python or R are required, along with excellent written and oral communication skills and the ability to complete projects both independently and collaboratively in a multidisciplinary research environment. Experience with large-scale biological or chemical datasets, QSAR modeling, or familiarity with AI/ML methods and/or in vitro experimental platforms is preferred.

This fellowship is not eligible for full-time remote participation, and NIH does not permit trainees to telework from overseas locations.

Disclaimer/Fine Print

Applicants must meet the following qualifications:

- Have a Ph.D., M.D. or other doctoral degree in a related discipline or have documentation that all degree requirements will be completed before the start of the fellowship in September 2026. Assurance to this effect must be supplied in writing by the chair of the dissertation committee (for Ph.D. candidates) or the dean of the medical school (for M.D. candidates).
- Be a citizen or permanent resident of the United States at the time of application. Applicants must have resided in the United States for three of the last five years.
- Be within two years of their terminal degree and have no more than two years of prior postdoctoral training before joining this fellowship program.
- Be able to pass a federal background check using Standard Form-85 (or SF 85). Section 14 of the form asks, “In the last year, have you used, possessed, supplied or manufactured illegal drugs?”

The question pertains to the illegal use of drugs or controlled substances in accordance with federal laws, even though permissible under state laws. Applicants will be required to complete a conflict-of-interest assessment.

- An NCATS/FDA Translational Science Interagency 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. If the individual will not voluntarily divest the financial interest or terminate the relationship, then the individual is not placed at the FDA. For additional requirements, see [FDA Ethics for Nonemployee Scientists](https://www.fda.gov/about-fda/office-chief-scientist/fda-ethics-non-employee-scientists) (<https://www.fda.gov/about-fda/office-chief-scientist/fda-ethics-non-employee-scientists>).

How to Apply

Please submit a cover letter that includes a research summary and describes your interest in the fellowship, a current curriculum vitae with a complete bibliography, and contact information for at least three references to Min Shen, Ph.D., at shenmin@mail.nih.gov.

Application reviews will begin promptly and continue until the fellowship is filled. Fellows must be able to start no later than September 21, 2026.