Computational Science (Cheminformatics) Postdoctoral Fellow
Division of Preclinical Innovation, NCATS/NIH
Drug Metabolism and Pharmacokinetics

National Institutes of Health (NIH)
National Center for Advancing Translational Sciences (NCATS)
Division of Preclinical Innovation (DPI)
Drug Metabolism and Pharmacokinetics
Rockville, Maryland, USA

Description

NCATS, a major research component of NIH, seeks applications from exceptional scientists to serve as a computational science (cheminformatics) postdoctoral fellow — for preclinical development projects involving drug metabolism and pharmacokinetics (DMPK) — within the Center's **Division of Preclinical Innovation**.

The DMPK Core partners with collaborators (academic institutions, foundations, and private industry) to conduct preclinical discovery and development studies leading to Investigational New Drug (IND) applications for new therapeutics. These projects play a leading role in NCATS' mission to develop new ways to reduce, remove or bypass bottlenecks across the entire continuum of translational science and to address rare and neglected diseases.

Core Responsibilities

The selected candidate will work collaboratively with team members to evaluate, develop and implement *in silico* absorption, distribution, metabolism and excretion (ADME) models for assigned projects. Specific duties include analyzing DMPK data using state-of-the-art methods and exploring new computational methodologies and approaches from the literature in a constant effort to improve existing models and reveal useful medicinal chemistry insights. The selected candidate also will be responsible for developing new structure-based computational models for predicting DMPK properties. They will collaborate with chemists and researchers across different teams within NCATS to address project-specific needs (e.g., development of local models for a particular project team). Additional duties include disseminating research via peer-reviewed publications and participating in scientific conferences and meetings.

The selected candidate should possess strong oral and written communication skills. They also should possess excellent interpersonal skills, including the ability to communicate clearly and succinctly in a timely manner. The selected candidate will be expected to demonstrate a proven ability to work collaboratively with colleagues to achieve project, team and organizational goals.

Qualifications

Applicants to this postdoctoral fellow position should possess a Ph.D. in bioinformatics, cheminformatics, computational biology, pharmaceutical science, chemistry, structural biology or a related field. A proven track record of coding in Python and applying machine/deep learning techniques to drug discovery data using popular Python libraries (e.g., Scikit-learn, TensorFlow, Keras and PyTorch) is highly desired. Candidates with advanced knowledge and skills in graph neural networks or equivariant neural networks will receive preferential consideration. Experience working on cloud platforms — such as Amazon Web Services or Microsoft Azure (or a similar high-performance computing environment) — will be considered favorably. Applicants also should

possess strong oral and written English communication skills and be able to work in a highly collaborative team setting.

Stipends/Benefits

The salary will be commensurate with experience, based on the **NIH Postdoctoral Intramural Research Training Award and Visiting Fellow scale**; medical insurance coverage will be provided. The position is renewable for up to five years.

How to Apply

Please email a cover letter describing your interest in the position, including a career synopsis (one to two pages); a current curriculum vitae with a complete bibliography; and the names of and contact information for at least three references to Pranav A. Shah, Ph.D., (**pranav.shah@nih.gov**(link sends e-mail)) and Xin Xu, Ph.D. (**xin.xu3@nih.gov**(link sends e-mail)). Review of applications will begin on Feb. 7, 2022, and will continue until the position is filled.