

Job Opportunity: Assistant Professor in Department of Computational Drug Discovery and Design

Medical Research Laboratory (MRL) of Institute of Science Tokyo (Science Tokyo) invites applications for a faculty position (Assistant Professor) in the field of Computational Drug Discovery and Design.

1. Position

Assistant Professor

2. Areas of Research

The Division of Computational Drug Discovery and Design aims to elucidate the molecular mechanisms underlying biomolecular function and to develop methods for molecular design and functional modulation for drug discovery by integrating computational physical chemistry and information science. Our research focuses particularly on enzymes and membrane proteins, using molecular dynamics (MD) simulations, quantum chemical calculations, and machine learning to investigate their structures, functions, and reaction mechanisms, as well as to advance protein design (<https://cddlab.io/research.html>).

We seek a researcher with expertise in biochemical and cell biological approaches to the functional characterization of enzymes and membrane proteins, and a strong motivation to elucidate the mechanisms of transporters and membrane enzymes. In particular, candidates should have experience in functional studies using cultured cells and in vitro experiments, including the reconstitution of purified proteins into liposomes, and be capable of establishing and developing experimental and analytical workflows for structural studies using cryo-electron microscopy and related techniques. Hands-on experience in computational research, particularly molecular dynamics simulations of proteins and protein design using deep generative models, is desirable. We welcome candidates who are eager to build on this experience to investigate reaction mechanisms through QM/MM calculations and experimentally validate the functions of computationally designed proteins. We encourage applications from individuals who are enthusiastic about collaborating with researchers from diverse backgrounds, both within and outside the laboratory, to advance mechanistic understanding and drug discovery by integrating experimental and computational approaches.

3. Terms and Conditions of Employment

The contract of Full-time position will start from April 1, 2027 and will not exceed five years period, renewable based on an evaluation according to the rules and regulations of Science Tokyo once.

Salary will be determined by the annual salary system outlined by Science Tokyo regulations.

Female applicants are strongly encouraged to apply for this position, as Science Tokyo

promotes gender-equality work environment. We provide career support programs for all staff that enable them to balance work and life, such as childbirth and child rearing.

Status of measures to prevent second-hand smoke : No smoking on the premises

4. Application Forms

- (1) Resume (Curriculum Vitae, etc.) (free form).
- (2) List of publications (free form).
- (3) Reprints of representative publications (up to 3 papers, photocopies acceptable).
- (4) Summary of the representative publications (100 words each).
- (5) List of research grants and patents (free form).
- (6) Summary of previous research contributions and future research and education plans (in 500 words).
- (7) A list of other achievements (Awards etc).

5. Work Location

Medical Research Laboratory, Institute of Science Tokyo
1-5-45 Yushima, Bunkyo-ku, Tokyo 113 - 8510, JAPAN

6. Deadline

October 20, 2026, Japan Standard Time.

7. Inquiry

Yushima Research Institute Administration Division, Institute of Science Tokyo

E-Mail: pr.mri.adm@tmd.ac.jp

Tel: +81-3-5803-4504

8. How to Apply

All the application documents must be sent to Administration Division. To apply, please enter the following [E-mail contents] at pr.mri.adm@tmd.ac.jp

Please contact us by E-mail by October 19, 2026.

We will send the URL and manual for submission to the university to the "destination email address".

[E-mail contents]

- Subject: "Application for the Assistant Professor position in the Computational Drug Discovery and Design"
- Full name
- Destination email address

All information will be treated with the strictest confidentiality in accordance with pertinent laws and rules.