Indian Institute of Technology (ISM) Dhanbad
Office of the Dean (Research & Development)

Sanction No and Date:DAR/27/2026-27	**IIT (ISM) Project No.** SRDP1415 F	Date: 16/11/2026

Project Staff (JRF/SRF/RA/Project Assistant/Project Associate) position under Gates Foundation

Applications are invited under the sponsored project. The details of the project are as under:

Position	Research Associates-I
Number of Position (s)	01
Title of The Project	Predictive Tools for Antibiotic Discovery in Klebsiella pneumoniae
Principal Investigator	Dr. Niladri Patra, Associate Professor, Department of Chemistry and Chemical Biology, IIT(ISM) Dhanbad
Tenure of Project	Two years, or until the completion of the project, whichever comes earlier.
Job Description (in maximum 100 words)	The initial tenure will be for 01 (one) year. Upon completion of the first year, the tenure may be extended based on annual performance evaluation and project requirement. Can structural biology-based computational models reliably distinguish antibiotics with known efflux challenges from those that evade efflux, and can this be turned into a validated predictive tool for early-stage efflux liability assessment? The selected PDF is expected to conduct all-atom Molecular Dynamics (MD) simulations, alchemical free energy calculations (SAFEP), non-equilibrium egress profiling, and network analysis, paired with conditional AI/ML surrogate modelling of efflux pumps.
Essential Qualification	• PhD in Computational and theoretical Chemistry/Biology or a closely related field. Experience in MD simulations and free-energy calculations of biomolecules with AI/ML modelling is mandatory, with proven publications in high-impact-factor journals.
Desirable Qualification	Experience in Molecular Dynamics and enhanced sampling simulation, machine learning, data analytics
Age and Relaxation (if any)	As per the norms of the Govt. of India
Fellowship	Rs. 58,000.00 PM + HRA as per rules of IIT(ISM) Dhanbad
Last Date & Time	• Interested candidates should mail a single PDF containing (i) CV (ii) Related Publicationsets (iii) proof of work experience (if any) to PI npatra2@iitism.ac.in 30th November 2026. • Candidate should write **"Application for the position of PDF under Gates Foundation project"** in the subject of the email.

Shortlisted candidates will be informed on the date of interview. Mere possession of the minimum qualification does not guarantee an invitation to the interview. Candidates will be shortlisted based on their merit and as per the requirements of the project. All candidates should make their own arrangements for their stay at Dhanbad, if required. No TA/DA will be paid to attend the interview.