Jamia Millia Islamia (A Central University)
New Delhi-110025, India

ADVERTISEMENT FOR THE POST OF

PROJECT RESEARCH SCIENTIST-I (NON-MEDICAL)

FOR AN ICMR-FUNDED PROJECT

Project Details:

Project Title: Developing DdpMPyPEPhU as a multitargeted drug for breast cancer using AI-guided enumeration-based optimisation, synthesis and preclinical evaluation in PDX model.

Position: Project Research Scientist- I (Non-Medical), **Duration:** 2 Years

Salary: 56,000/- + 30% HRA= 72,800/- pm or as per ICMR guidelines.

Deadline: April 20, 2026

Application: Fill out the Google Form: https://forms.gle/VScsvLVDdCGEkTCZ8

Minimum Essential Qualifications:

1. First Class Post Graduate Degree, including the integrated PG degrees
   OR
2. Second Class Post Graduate Degree, including the integerated PG degrees with PhD
   OR
3. For Engineering/IT/CS- First Class Graduate Degree of Four Years

Desirable: Experienced in applying artificial intelligence in drug design, computing and handling drug descriptor data, and good coding skills in Python/R. Also, the candidate should have hands-on experience in molecular modelling, drug library screening, DFT, WaterMap, MD simulations, or binding free energy computations and analysis.

Upper age limit: 35 years

Brief Description of the Project

Cancer is a complex and heterogeneous group of diseases characterised by uncontrolled cell proliferation, often leading to metastasis. Our preliminary research has identified **DdpMPyPEPhU** as a promising anticancer inhibitor for breast cancer (doi: 10.1371/journal.pone.0344028). To accelerate drug discovery and development, we aim to employ advanced in-silico methodologies for comparative reassessment and validation of existing breast cancer drugs alongside our developed candidate, DdpMPyPEPhU. This includes molecular docking, DFT, WaterMap, MD simulations, MMGBSA, and binding affinity predictions. Furthermore, we plan to develop **AI-driven drug enumeration techniques** to enhance the design and formulation of novel compounds while ensuring optimal physicochemical properties, binding affinity, and stability. These computational approaches aim to streamline drug discovery and optimise lead compounds for clinical translation. Collaborating with our **synthetic chemistry team**, we will synthesise and characterise DdpMPyPEPhU and its optimised analogues using **NMR spectroscopy, mass spectrometry, TLC, and FT-IR**. The **biochemistry team at AIIMS** will subsequently conduct ***in-vitro* validation** using multiple breast cancer cell lines, benchmarking the results against standard control drugs. Promising candidates demonstrating significant anticancer activity will undergo ***in-vivo* validation** to assess their therapeutic potential.

Contact Details (Principal Investigator):

Dr. Khalid Raza

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