**Job Title: Scientist - Insilico**

**Location:** Bengaluru, Karnataka, India
**Company:** Quantumzyme

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**About Quantumzyme**

Quantumzyme is a leading biocatalysis company leveraging advanced computational chemistry, AI, and enzyme engineering to deliver sustainable and efficient solutions for chemical and pharmaceutical manufacturing. Our mission is to revolutionize chemical production through greener, cost-effective, and precision-driven enzyme design.

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**Position Overview**

We are seeking a highly motivated **Scientist (Computational Chemistry / Computational Biology / Bioinformatics)** with **0.6 to 4 years of post-PhD experience** to join our Bengaluru team.

This role requires a **strong hands-on computational researcher** who can independently execute projects while mentoring junior team members. The candidate will be responsible for **on-time project delivery**, working on industrial and academic collaborations, with a strong emphasis on **MD simulations for enzyme engineering and catalytic mechanism**.

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**Key Responsibilities**

- Perform hands-on computational research in molecular simulations and enzyme modelling.

- Lead specific project modules while mentoring junior researchers.

- Ensure timely completion and delivery of project milestones.

- Perform **Molecular Dynamics (MD) simulations** of biological macromolecular systems (proteins, enzymes, protein–ligand complexes).

- Design and execute **QM/MM simulations** to:

    o   Study enzyme catalytic mechanisms

    o   Model reaction pathways

    o   Perform transition state and electronic structure calculations

    o   Evaluate reaction energetics and free energy profiles

- Apply enhanced sampling techniques such as:

    o   Umbrella Sampling

    o   Meta dynamics

    o   FEP

o MMPBSA / MMGBSA

- Automate simulation setup, workflow pipelines, and post-MD analysis using scripting.

- Work efficiently in Linux-based HPC environments.

- Contribute to reports, technical documentation, and publications.

- Analyse reaction mechanisms and interpret computational results to guide experimental design.

- Collaborate with interdisciplinary teams and communicate scientific insights effectively.

**Qualifications**

- PhD in Computational Chemistry / Computational Biology / Bioinformatics or related field

- **0.6 – 4 years of post-PhD hands-on research experience**

- Strong background in enzyme systems and biomolecular simulations

**Mandatory Skills**

**Core Computational Biology/Chemistry**

- **GROMACS (Minimum 3 years hands-on experience)**

- **CP2K**

- Molecular Dynamics (MD) simulations

- QM/MM simulations

- Reaction mechanism analysis

- Umbrella Sampling, Metadynamics, Free Energy methods

- Protein–ligand and enzyme system modelling

- Experience working with biological macromolecules (proteins, enzymes, AI-assisted workflows)

**Visualization & Analysis**

- VMD

- PyMOL

- Chimera

- Discovery Studio

- ChemDraw / Biovia Draw

**QM/MM & Electronic Structure Tools**

Experience with one or more of:

- CP2K

- Gaussian

- ORCA

- ChemShell

- Turbomole

**Programming & Automation:**

- **Python**

- **BASH**

- Shell scripting for automation

- C / C++

- Workflow automation for MD simulations

- Post-processing and trajectory analysis scripting

- Experience working in Linux / HPC clusters


**Additional Skills (Preferred)**

**Enzyme Engineering & Bioinformatics**

- Enzyme structure–function analysis

- Active-site modelling

- Mutational scanning and hotspot prediction

- Sequence alignment & homology modelling (BLAST, Clustal Omega, MEGA)

- Understanding of enzyme kinetics and catalytic selectivity

**Advanced Sampling & AI**

- Replica MD, aMD, REMD

- TI, LIE, MMPBSA

- Exposure to AI/ML tools (scikit-learn, PyTorch, TensorFlow)

- RF Diffusion