

Open Position for PhD Students in Computer-Aided Drug Design

The University

Johannes Gutenberg University Mainz (JGU) is one of the largest universities in Germany. Almost all of its institutes are located on a single campus close to the Mainz city center – creating a lively academic culture for researchers, and students from every continent.

The Role

The research team of *Molecular Simulations and AI-driven Molecular Design* (<https://palomino.uni-mainz.de/>) at the Institute of Physical Chemistry, Mainz has an open position for a PhD student in collaboration with the University Medical Center (UMC) Mainz, in the framework of the Focus Program Translational Neurosciences (FTN).

This position involves the development of novel small molecules to modulate inflammatory processes through simulation of biomolecular receptors to understand their conformational behavior, discovery of novel hits based on virtual screening, and generation of novel chemical matter through AI-driven generative modelling. The most promising molecules will be experimentally tested in UMC Mainz.

This position will be jointly supervised by Dr. Oscar Palomino (JGU Mainz) and Dr. Christina Vogelaar (UMC Mainz). **The position is scheduled to begin in the third quarter of 2025; thus, candidates who are available to start within this timeframe will be given priority.**

The candidate profile

The candidate must hold an M. Sc. degree in chemistry, interdisciplinary natural sciences, physics, or related. The M. Sc. should preferably include some computational work.

English language skills are required (Common European Framework of Reference B2), German is beneficial but not mandatory.

Additionally, basic knowledge in any of the following areas is beneficial for the position:

- Drug discovery and structure-based design.
- Simulations of biomolecules through molecular dynamics or Monte Carlo techniques.
- Machine learning techniques in chemistry

JGU values diversity and welcomes applications from qualified candidates of all backgrounds. **Please note that applications with unrelated academic or professional backgrounds, as well as incomplete submissions, will not be considered.**

The offer

- Monthly PhD Stipendium (2,030 €)
- Job ticket for the entire Rhine-Main area.
- Extensive HR development offer.
- Flexible working time arrangements.

The doctoral position is limited to a period of three years with a possibility of extension.

How to apply?

For the application, prepare three files:

- Tabular Curriculum Vitae with references.
- Grade certificates including coursework
- Motivation letter (one page), that highlights (i) why are you interested in this position, and (ii) why your previous experience makes you a good candidate.

Send these files (with the application ID “PhDSep2025” in the e-mail subject) to: palomino.applications@uni-mainz.de. **The application deadline is May 9, 2025; however, applications will be reviewed immediately, so early submission is strongly encouraged.**

For questions and further information please contact Oscar Palomino by e-mail: opalomin@uni-mainz.de.