

The Department of Natural Sciences and Sustainable Resources, Institute of Molecular Modeling and Simulation is currently seeking a

Postgraduate Research Associate

project employment

(Reference code 86)

Extent of employment: 30 hours per week

Duration of employment: 1st of June 2026, limited to 31st of May 2029

Workplace: 1190 Vienna, Muthgasse 18

Allocation in compliance with the Collective Agreement for University Staff to job group:
B1

Gross monthly salary: (depending on previous eligible experience) at least: € 2.832,10
(payable 14 times per year)

Responsibilities

The project is part of the Christian Doppler Laboratory "Molecular Informatics in the Biosciences". In Module 2 of this CD-laboratory, we focus on protein structure and dynamics to understand and modulate the interactions between biomolecules of interest. In this project, we focus on the recently developed accelerated enveloping distribution sampling (AEDS) method in three different use cases:

- Efficient screening of a series of compounds or mutations, after optimization of the AEDS parameters in a reference simulation
- Free-energy calculations of the affinity or stability of such a series of compounds or mutations after further refinement of the AEDS parameters
- Combining endstate simulations with AEDS simulations to reach efficient multistate free-energy calculations from a handful of simulations

We aim to benchmark and improve the applicability of the method at the hand of real-life examples from our industrial partners. The work is expected to lead to high-quality scientific publications and a doctoral thesis.

Required skills and qualifications

- Diploma degree in Chemistry / Biotechnology / Molecular Sciences or other equivalent university degree
- Language skills: fluent in English

- Experience in molecular dynamics simulations

Desirable skills and qualifications

- Knowledge of statistical thermodynamics
- Experience with programming
- Enthusiasm for working in research team

Applications can be submitted until: 11th of May 2026

University of Natural Resources and Life Sciences Vienna seeks to increase the number of its female faculty and staff members. Therefore qualified women are strongly encouraged to apply. In case of equal qualification, female candidates will be given preference unless reasons specific to an individual male candidate tilt the balance in his favour.

People with disabilities and appropriate qualifications are specifically encouraged to apply.

Please send your job application incl.

- motivation letter
- CV

to HR Management, BOKU University, Peter-Jordan-Straße 70, 1190 Vienna;

E-Mail: recruiting@boku.ac.at. (**Reference code: 86**)

We regret that we cannot reimburse applicants travel and lodging expenses incurred as part of the selection and hiring process.

www.boku.ac.at