PhD position in Computational Chemistry

Computer-aided drug design based on protein-ligand interactions analysis

We are looking for a motivated and talented **PhD Student** to join our laboratories of **Computational Biology and Biomolecular NMR Spectroscopy** (https://www.maxperutzlabs.ac.at/research/research-groups/konrat, University of Vienna) and **Computer-Aided Molecular Design** (CAMDgraz.com, Medical University of Graz).

The PhD Student will work in the implementation of a computational framework for the prediction of protein-ligand interactions with views of the design of new drugs with our industrial partner. Computer techniques such as molecular dynamics (MD) and quantum mechanics/molecular mechanics (QM/MM) simulations, free energy calculations, and machine learning methods will be used for the quantification of fragment-protein interactions. Theoretical results will be cross-validated with experimental techniques such as NMR in combination with selective side-chain labeling carried out at the Department of Structural and Computational Biology (Vienna).

The contract (3 years) will be established according to the FWF personal cost scheme (Doctoral candidate). The selected candidate is expected to start **October 1st 2021**.

Requirements

- MSc degree on Theoretical Chemistry, Physics, Biophysics, Biochemistry or Mathematics.
- Experience with Linux operating systems and hands on molecular dynamics simulations
- Knowledge in MD simulation, QM and QM/MM methods
- Knowledge in programming languages like Python, R and/or Shell scripting
- Knowledge in machine learning is desirable
- Excellent command of English

How to apply

If you are interested in the position, please send the following documents to **pedro.murcia@medunigraz.at** before **July 10th 2021**:

- Curriculum Vitae
- Letter of Motivation
- 2 Letters of recommendation

The selected candidates will be invited to a virtual hearing at the end of July 2021.