

# Postdoctoral position for a junior scientist in the Laboratory of Molecular Modeling, Faculty of Chemistry, University of Gdańsk, Poland

**Project title:** “Data-assisted modeling of the ensemble structure of intrinsically disordered proteins and their assemblies”

**Project leader:** prof. dr hab. Józef Adam Liwo

**Position name:** Postdoctoral Associate (adiunkt naukowy)

## Requirements:

1. Ph.D. degree in Chemistry, Physics, Biology or related disciplines.
2. Command of English sufficient to read scientific papers and for communication.
3. Knowledge of molecular dynamics and experience in running MD simulations and analyzing and interpreting the results of simulations. The knowledge of MD extensions (replica exchange and Hamiltonian replica exchange) is desirable.
4. Knowledge of experimental methods for protein-structure determination, in particular those based on nuclear magnetic resonance, at least regarding the quantities available from experiments and using them in data-assisted structure modeling.
5. Experience in modeling MD-based data-assisted modeling of protein structures.
6. Ability to work with UNIX-operated workstations at least at the medium-advanced level, including the ability to write UNIX scripts.
7. Literacy in Fortran/C/C++ at least at the basic level.
8. Reliability and ability to solve scientific problems independently.

## Project information and task description:

The goal of the project is to develop the Ensemble Oriented Data Assisted Molecular Dynamics (EODAMD) approach to determine the dynamic structure of the Intrinsically Disordered Proteins (IDPs) and other flexible multistate proteins (such as, e.g., molecular chaperones). The method will be based on MD simulations with Hamiltonian replica exchange with the coarse-grained UNRES force field, designed in the laboratory of the project leader. The experimental restraints will be imposed on the whole conformational ensemble by their averaging over replicas and simulation windows. This is a collaborative project run together with the group of Prof. Chun Tang, Peking University. The postdoc employed in the project will carry out the following tasks:

1. Development of a method for the computation of backbone proton,  $^{13}\text{C}$  and  $^{15}\text{N}$  chemical shifts, and the RDCs for a given coarse-grained geometry.
2. Development of the extended replica-exchange molecular dynamics algorithm, with time- and replica averaged restraints to take into account conformationally-averaged experimental restraints, and testing the methodology with multistate proteins for which the experimental data are already available.

3. Application of the methodology to study the structures of IDPs, IDRs, and to study peptide association in solution.

### **Conditions of employment:**

1. Full-time 1-year job contract.
2. Gross-gross salary: 10000 PLN. The gross-gross salary includes health insurance and pension plan.
3. Approximate start date: April 1, 2024.

### **Application package must include the following:**

1. Cover letter.
2. CV including the list of publications.
3. A copy of Ph.D. diploma or documented proof that the applicant will obtain the Ph.D. degree (scan/electronic version acceptable).
4. At least one recommendation letter from a previous supervisor; applicants who apply for the first postdoc position must supply the recommendation letter from the Ph.D. work supervisor.

**The applicant is obliged to submit, together with the documents listed above, the information clause (agreement to process personal data for the purpose of application), which can be downloaded from the page of the University of Gdańsk or obtained from the project leader.**

The application package can be submitted in person to the Office of the Dean of the Faculty of Chemistry, University of Gdańsk, ul. Wita Stwosza 63, 80-308 Gdańsk, Poland, mailed to Prof. J.A. Liwo to the above address or, preferably, emailed to Prof. J.A. Liwo to **adam.liwo@ug.edu.pl**; the cover letter can be included in the email body, scans of the other documents attached to the email.

Selected candidates will be invited for an interview, which will be conducted in person at the Faculty of Chemistry, University of Gdańsk or online. The candidates will be notified of the time and form of the interview by email.

Any questions should be sent by email to Prof. Liwo at **adam.liwo@ug.edu.pl** or **adam.liwo@gmail.com**.

**Application deadline: March 6, 2024**