Graduate (Ph.D.) position 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: Graduate Student (stypendysta/doktorant)

Requirements:

1. M.Sc. degree in Chemistry, Physics, Biology or related disciplines.
2. Command of English at least sufficient to read scientific papers and for communication.
3. Knowledge of molecular quantum mechanics, statistical mechanics, and methods of computational chemistry.
4. Experience in using molecular-modeling software (Gaussian, Mopac, Gamess, Amber, Charmm) desired.
5. Knowledge of the basic principles of protein structure organization.
6. Ability to work with UNIX-operated workstations at least at the medium-advanced level, including the ability to write UNIX scripts. Basic literacy in Fortran/C/C++ desirable.

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 graduate student will participate in carrying out the following tasks:

1. Evaluation of the extended replica-exchange molecular dynamics algorithm, with time- and replica-averaged restraints to take into account conformationally-averaged experimental restraints.
2. Investigation of the phase separation tendency, i.e., coacervating or aggregating into liquid droplets or fibrils of the selected IDPs, in relation to the monomeric structure of the IDP.

Conditions of employment:

1. 1-year stipend contract based on project funds, extension depending on funds availability, for 3 years maximum.
2. Monthly gross stipend from project funds: 5000 PLN for 3 years. This sum includes obligatory social security taxes.
3. The successful candidate will be enrolled in the Graduate School of Exact and Natural Sciences at the University of Gdańsk.
4. Start date: February 19, 2023.

Application package must include the following:

1. Cover letter.
2. CV including the list of publications.
3. A copy of M.Sc. diploma or a certificate that the applicant has the M.Sc. degree (scan/electronic version acceptable).
4. Recommendation letter from the supervisor of the M.Sc./B.Sc. work or other mentor.

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 downloades 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 adres **adam.liwo@gmail.com**; 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: November 30, 2023