The Institute of Biochemistry and Biophysics PAS

is looking for a <u>PhD student for 36 months</u> for the execution of OPUS scientific project entitled: "Assessing protein-ligand complexes with ML/DL models trained on molecular dynamics-based descriptors", financed by the National Science Centre.

Project description:

Discriminating binders from non-binders in a computationally efficient and accurate manner is an important step in the search for new therapeutic agents and/or tool compounds. This project builds on the hypothesis that characterizing the dynamic nature of protein–ligand complexes is beneficial for differentiating binders from non-binders and selecting proper ligand poses from conformational ensembles provided by current molecular docking procedures. We propose to merge dynamic information obtained from MD simulations to develop and explore protocols for discriminating, especially for targets that are currently difficult for rigid or semi-flexible docking and scoring procedures.

The project is highly multidisciplinary in nature, at the interface of computational chemistry, biology and machine learning/deep learning. It has an ambitious goal of changing the perspective of ligand-receptor binding assessment from a single snapshot-like complex into a dynamical system with many more properties and features which are currently not considered.

Scope of work:

The PhD student will be using data wrangling techniques for acquisition and filtering. She/he will make extensive use of computational techniques such as molecular docking, molecular mechanics and dynamics simulations. She/he will develop machine learning models, training and testing.

Required professional qualifications:

1. Programming skills (Python and/or R)
2. Knowledge of basic chemistry and/or computational chemistry will be preferred.
3. Cheminformatics skills (rdkit, openbabel, knime, etc) will be a bonus.
4. Basic knowledge of ML/DL frameworks (Tensorflow and/or PyTorch).

The anticipated average fellowship: 4 800 PLN/month (brutto/brutto) for 36 months with possible extension.

Deadline for submitting offers: September 20, 2021, 23:59

Applications should be sent by e-mail to the project manager: dr hab. Paweł Siedlecki, pawel@ibb.waw.pl.

NCN call for proposals type: OPUS – ST

Required documents:

- CV
- Motivation letter with justification of the matching to the project
- Copy of masters' degree diploma
- Letter of support from the master thesis supervisor
- a declaration of consent to the processing of personal data