UNIWERSYTET WARSZAWSKI

Wydział Chemii

Warsaw, 23.03.2023

WCH.1210-19/2022

An announcement for **adjunct (postdoc)** position

Position for **adjunct (post doc)** who will connect theoretical chemistry with thermodynamics by molecular dynamics simulations, to rationally design a novel bioisosteric replacement for the forefront of drug discovery in project entitled " **True Bioisosteres - Structural and Thermodynamic Classification of Molecular Fragments for Ligand Design**" financed by **National Science Centre (NCN)** is open for application.

Project leader: **dr Maura Malińska**

Grant Decision: Nr DEC-2021/42/E/ST4/00229

Available positions: 1 (a group of researchers operating in the field of natural sciences, in discipline of Chemistry).

Overview

One cannot predict enthalpy and entropy of binding, in other words, the unforeseen recognition event changes both the structure and dynamics of each counterpart. Yet, many strategies in medicinal chemistry and crop protection rely on the identification and quantification of similar molecules (bioisosteres) with a related thermodynamic profile. We propose that a group of molecules/molecular fragments may be called bioisosteric if they are all complementary to the same host site in three key elements i.e. steric fit, electrostatic fit, and hydrophobic effect. Only understanding the role of a molecular shape, weak non-covalent interactions, and the role of water in the formation of a complex can provide a more powerful method of prediction of true, diverse bioisosteres.

Malinska's scientific group at Faculty of Chemistry, University of Warsaw is pioneering experimental and computational approaches for quantification of molecular similarities and bioisosteric replacements. This gives deeper insight into molecular recognition and the role of solvent molecules that often dominates the thermodynamic effect of binding.

We seek to recruit a self-driven and creative theoretical chemist to join our team to work on SONATA BIS project entitled "True Bioisosteres - Structural and Thermodynamic Classification of Molecular Fragments for Ligand Design". You will help to connect theoretical chemistry with thermodynamics by molecular dynamics simulations, to rationally design a novel bioisosteric replacement for the forefront of drug discovery.

Responsibilities include

- conducting theoretical calculations for guest-host systems, in particular, the enthalpy and entropy of binding;
- validation of theoretical results against ITC experimental results;
- keeping scientific documentation;
- creating publications from research results;
- training of Ph.D. students and undergraduates in theoretical research.

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Qualifications

- Ph.D. in Computational Chemistry or related field, held on the first day of the contract.

Required:

- Team player skills
- Good knowledge of English (at least B2)
- Good knowledge of molecular dynamics simulations and DFT calculations;
- Skilled in docking algorithms and results evaluation;
- Good knowledge of scientific article preparation
- Self-driven, proactive attitude.

Considered a plus:

- Molecular dynamics simulation of crystal system;
- Experience in several areas from ligand- and structure-based virtual screening, multi-parameter optimization, conformational analysis, pharmacophore development, QSAR, data mining, and target assessment strategies;
- Programming.

Personal attributes:

- Highly organized, conscientious, and reliable team player, with strong attention to detail;
- Excellent communication and presentation skills to share complex ideas and results with non-experts;

The candidate must meet the requirements of art. 113 of the Act - Law on Higher Education and Science dated July 20, 2018 (Journal of Laws of 2022, item 574).

Your benefits:

- The total salary before taxing (brutto/brutto) is 12 000PLN/month;
- Ample support to grow your skills;
- Contract with the University of Warsaw (full-time position/employment contract) for 30 months with the possibility of extension.

Please send your

- CV;
- information on the processing of personal data (the template available at: http://www.chem.uw.edu.pl/oferty-pracy/);
- declaration of reading and acceptance of the rules for conducting competitions at the University of Warsaw (a template available at: http://www.chem.uw.edu.pl/oferty-pracy/;
- motivation letter;
- two references,
- publication record;
- a brief description of the most important scientific achievement.

no later than 12.05.2023 to mmalinska@chem.uw.edu.pl, adding "Post Doc position" to the subject of your email. The results of the competition will be given by e-mail till 1.06.2023.

Selected candidates will be informed about the date of the interview by e-mail. In justified cases, the interview may also take place via the Internet. Only those who submit complete documentation will be considered in the recruitment procedure.

The competition is the first stage of the employment procedure as an academic teacher, and its positive outcome is the basis for further proceedings.