Post Doc Position

True Bioisosteres - Structural and Thermodynamic Classification of Molecular Fragments for Ligand Design

Faculty of Chemistry, University of Warsaw

Warsaw, Poland

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 PhD students and undergraduates in theoretical research.

Qualifications

- PhD in Computational Chemistry or related field

Required:

- Good knowledge of molecular dynamics simulations and DFT calculations;
- Skilled in docking algorithms and results evaluation;

- Self-driven, proactive, and forward-thinking 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;
- Fluency in English.

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 2018, item 1668 as amended).

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) from 1.07.2022 to 31.12.2024 with possible extension.

Please send your

- CV,
- motivation letter,
- publication record,
- 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/,
- references

no later than **May 10th** 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 June 1st, 2022.