

Ph. D Student 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 student to join our team to work on SONATA BIS project entitled "True Bioisosteres - Structural and Thermodynamic Classification of Molecular Fragments for Ligand Design".

Responsibilities include

- conducting research within the project (crystal structure diffraction experiments, crystallization, ITC measurements for host-guest system, molecular dynamics simulations and DFT computations);
- active participation in conducting research and entire publication process (from idea to writing the final draft);
- cooperation and effective communication with the team and external research groups
- participation in determining research strategies and new research directions

Qualifications

- MSc degree in chemistry, physics, or similar (or thesis close to being defended)

Required:

- Self-driven, proactive, and forward-thinking attitude;

Considered a plus:

- Programming.

Personal attributes

- Highly organized, conscientious, and reliable team player, with strong attention to detail;
- Good knowledge of the English language

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

- Full-time Ph.D. scholarship for 48 months in the amount of 5000 PLN net/month scholarship from the Doctoral School in the standard recruitment time in June. Non-standard recruitment time results in significantly lower scholarship (5000 PLN gross);
- Co-authorship of publications in recognized scientific journals;
- Ample support to grow your skills;
- Participation in international conferences

Please send your

- CV, if you are a co-author of publications, please describe your contribution in their creation
- motivation letter;
- information on the processing of personal data (the template available at: <http://www.chem.uw.edu.pl/oferty-pracy/>);
- references

no later than **May 1st** to mmalinska@chem.uw.edu.pl, adding “PhD position” to the subject of your email. The results of the competition will be announced on the website crystal.chem.uw.edu.pl no later than 14 days after the competition is adjudicated.