PhD open Position October 2025 CRM2 BioMIMIC group.

New Electrostatic Descriptor for Molecular Recognition & Drug Design

KEYWORDS
Electrostatic Energy, Ultra High-Resolution Crystallography - Molecular modelling – Crystal Engineering – Drug design – Protein/ligand interactions

We are seeking a highly motivated and skilled candidate with a master's degree in physics, molecular modelling, bioinformatics, cheminformatics, or biophysics to join our team as a PhD researcher.
The BioMIMIC team at CRM2 laboratory has integrated a patented descriptor into the MoProSuite software to analyze electrostatic complementarity on the Hirshfeld surface of molecular assemblies. Based on molecular electron density, this tool maps interatomic interactions—whether strong or weak—and determines their favorable or unfavorable nature. Initially developed for analyzing crystal packings, it is also applicable to protein-ligand complexes, providing a score to assess the quality of docking poses.
In this PhD project, a novel and more advanced descriptor, directly linked to the electrostatic energy of intermolecular interactions, will be developed. The PhD researcher will work on its creation and integration into our MoProViewer software, evaluating its effectiveness on both crystal structures and protein-ligand complexes using experimental data.
This research is part of international collaborations, including virtual screening and ligand optimization projects for drug targets, with opportunities for research stays abroad. The approach may also be complemented by machine learning techniques in collaboration with a Parisian laboratory. Ultimately, this functionality will be applied to molecular docking results, including correct and decoy poses, to quantify and compare its performance with other scoring methods used in popular docking software.
The candidate will contribute to the development of new functionalities related to the scoring function in MoProSuite, using the C++ programming language.

CANDIDATE PROFILE
We are seeking a highly qualified PhD candidate with a strong academic background, evidenced by exceptional grades at the Master's level, in line with the high standards of our PhD program. Applicants must hold a Master's degree in physics, biophysics, physical chemistry, bioinformatics, or chemo-informatics. Proficiency in computer programming, such as Fortran, Python, or C++ would be highly valued. A solid level of English, both written and spoken, is essential.