

## **PhD position :**

### **Development of a scoring function for evaluating drug docking poses**

**Location : Nancy, France. CRM2 University of Lorraine.**

Laboratoire Cristallographie Résonance Magnétique & Modélisations

A PhD position is open in the BioMIMiC team. Our team focuses on developing and applying new methods to understand interactions within biomolecular entities and crystal structures ( 10.1107/S2059798321008433 ; 10.1021/acs.jpca.9b05051).

We are seeking a highly motivated and skilled individual with a PhD in molecular modelling, bioinformatics, chemo-informatics, biophysics, to join our team as a doctoral researcher. The successful candidate will work on the development of a physics-based interaction potential to re-score docking poses and analyse ligand/protein interactions. This scoring function is based on explicit representation of both receptor and ligand electron densities for electrostatic and induction components. The researcher will work on the development of specific terms in the scoring function, including the dispersion, non-polar solvation and entropic terms.

In a subsequent stage, the research project consists in the training of the developed scoring function using a benchmark dataset of protein/ligand complexes associated to experimental binding constants. Machine learning approaches will be applied in collaboration with a Parisian laboratory. The trained function will eventually be applied to molecular docking results including correct and decoy poses in order to quantify and compare its performance with other approaches proposed in popular docking computer programs. In addition, the candidate will be involved in the software development of functionalities related to the scoring function in the MoProSuite software developed by the team, using the C++ programming language.

#### **Profile requirements**

To be successful in this role, the ideal candidate will have preferably a master degree in bioinformatics, computational chemistry, biophysics or physics.

Proficiency in at least one programming language, preferably C++, is required.

Additionally, proficiency in English language is necessary.

#### **Responsibilities**

- Conduct scholarly research, develop new methods and analysis codes with all required annotations and documentation.
- Contribute to publication writing and scientific progress reports, and present research findings at seminars/conferences.
- Supervise junior lab members during their internship.

We offer a dynamic and collaborative research environment, competitive compensation, and opportunities for further professional development. If you are interested in this 3 years PhD opportunity, please submit your CV with cover letter.

Contacts: [christian.jelsch@univ-lorraine.fr](mailto:christian.jelsch@univ-lorraine.fr) [benoit.guillot@univ-lorraine.fr](mailto:benoit.guillot@univ-lorraine.fr)