

## Master project 2020-2021

### Personal Information

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### Project

## Web development & bioinformatic tools

### Project Title:

A web server to generate conformational ensembles of highly-flexible proteins

### Keywords:

Web server, Intrinsically Disordered Proteins (IDPs), Sampling, Conformational ensemble models

### Summary:

Contrarily to what was thought in past decades, not all proteins fold into a relatively stable functional structure. Many proteins remain highly flexible in solution, possibly forming local transient structural elements. These proteins are usually called Intrinsically Disordered Proteins (IDPs). They play crucial roles in multiple biological processes and are directly involved in several pathologies, including cancer and neurodegeneration. The high flexibility of IDPs has notably hampered their study. Experimental biophysics technics such as Nuclear Magnetic Resonance (NMR) and Small-Angle X-ray Scattering (SAXS) provide information on conformational trends [1]. However, the quantitative interpretation of these experimental data requires the use of computational approaches that account for their ensemble averaging properties. These computational approaches are based on the construction of large conformational ensembles. We have recently developed a new method to model conformational ensembles of IDPs [2], which provides a more accurate representation than existing approaches. This method will be of great interest for the scientific community working on the understanding of IDPs. The goal of this project is to provide easy access to this method through a web server, as we did a few years ago for another molecular modeling application (<http://moma.laas.fr>) [3]. By the end of the project, aiming to disseminate our work, we plan to submit an article describing the new web server for publication in a high-impact scientific journal. The student will work in a team involving other students (PhD and master level), researchers and software engineers working on related topics. He/she will take part in the design phase and the full-stack web development (both front-end and back-end). We aim to use the most recent languages and technologies at both levels (in particular, the Django web framework). Particular importance will be given to the ergonomics of the proposed solution.

### References:

[1] T.N. Cordeiro, F. Herranz-Trillo, A. Urbanek, A. Estaña, J. Cortés, N. Sibille, P. Bernadó (2017) Small-angle scattering studies of intrinsically disordered proteins and their complexes. *Current Opinion in Structural Biology*, 42:15-23. [2] A. Estaña, N. Sibille, E. Delaforge, M. Vaisset, J. Cortés, P. Bernadó (2019) Realistic ensemble models of intrinsically disordered proteins using a structure-encoding coil database. *Structure*, 27(2):381-391 [3] D. Devaurs, L. Bouard, M. Vaisset, C. Zanon, I. Al-Bluwí, R. Iehl, T. Siméon, J. Cortés (2013) MoMA-LigPath: a web server to simulate protein-ligand unbinding. *Nucleic Acids Research*, 41(W1):W297-W302.

**Expected skills::**

Good programming skills are mandatory, mainly C++ and Python. Teamwork skills are also very important for the achievement of the project.

**Possibility of funding::**

Yes

**Possible continuity with PhD: :**

To be discussed

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