



Master project 2021-2022

Personal Information

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Project

Structural bioinformatics

Project Title:

Frag-AA

Keywords:

Computational Chemistry, Molecular Modeling, python, Fragment Growing, Peptides

Summary:

We are currently developing packages to automate and standardize protocols oriented to use PELE, one of our proprietary softwares, for specific purposes in drug discovery. In this context, we have recently developed FragPELE, a new tool for in silico hit-to-lead drug design, capable of growing a fragment from a small molecule bound core while exploring the protein-ligand conformational space. This project will be focused on the development of FRAG-AA, a specific adaptation of FragPELE code to growing peptide-like molecules with the aim of developing protein-protein peptide-like inhibitors.

Expected skills::

Computer Sciences, Chemistry-Physics, Programming skills

Possibility of funding::

Yes

Possible continuity with PhD: :

To be discussed

Comments:

Initial duration: 6 months

