



Master project 2021-2022

Personal Information

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Project

Structural bioinformatics

Project Title:

In silico rational discovery of novel molecular glue degraders

Keywords:

Computational Chemistry, Molecular Modeling, Molecular Glues, Drug Design

Summary:

Molecular glue (MG) degraders induce protein-protein interactions that lead to ubiquitin-mediated protein degradation, catalysing the rapid depletion of previously inaccessible targets. This project consists in developing a computational protocol for the design of novel MG compounds, based on a Monte Carlo-based ligand landscape sampling within the possible protein-protein complex through the automatic combination of consecutive calls of pyDock and PELE, two of our proprietary softwares.

Expected skills::

Biochemistry with programming skills or knowledge

Possibility of funding::

Yes

Possible continuity with PhD: :

Yes

Comments:

Initial project duration: 6-8 months

