Master project 2020-2021

Personal Information

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Project

Structural bioinformatics

Project Title:

ML victual Screening

Keywords:

Docking, coronavirus, PELE, deep learning

Summary:

We aim at developing a Deep Docking (DD) approach to screen billions of compounds in a fast manner. It will be integrated in a hierarchical pipeline combining commercial docking techniques and our Monte Carlo scheme (PELE). The application field will include real targets a current project to screen for pancoronavirus (polypharmacology) inhibitors.

References:

https://doi.org/10.1002/minf.202000028,

Expected skills::

Previous knowledge on docking and machine learning will be a plius.

Possibility of funding::

Yes

Possible continuity with PhD: :

Yes