Universitat Pompeu Fabra Barcelona

Master in Bioinformatics for Health Sciences

Master project 2021-2022

Personal Information

Supervisor	Victor Guallar
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Group	EAPM

Project

Structural bioinformatics

Project Title:

CovPELE

Keywords:

Drug design, covalent ligands, pharmacology, PELE, ligand binding, ligand diffusion

Summary:

We are seeking for a master student to develop and implement a new protocol for mapping covalent ligands diffusion and binding in pharmacological targets. The student will be part of a larger team and be responsible of: i) benchmark development, ii) protocol development, iii) protocol implementation (validation)

References:

A general view of PELE: Monte carlo techniques for drug design: the success case of PELE. JF Gilabert, D Lecina, J Estrada, V Guallar - Biomolecular Simulations in Structure-Based Drug Design, 2018 Adaptive simulations, towards interactive protein-ligand modeling. D Lecina, JF Gilabert, V Guallar. Scientific reports 7 (1), 1-11 (2017) An example of a recent implementation in PELE: FragPELE: Dynamic Ligand Growing within a Binding Site. A Novel Tool for Hit-To-Lead Drug Design. C Perez, D Soler, R Soliva, V Guallar. Journal of chemical information and modeling 60 (3), 1728-1736 (2020)

Expected skills::

Molecular modeling, python programming

Possibility of funding::

Yes

Possible continuity with PhD: :

Yes