Universitat Pompeu Fabra Barcelona

Master in Bioinformatics for Health Sciences

Master project 2024-2025

Personal Information

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Group	Computational Drug Design

Project

Structural bioinformatics

Project Title:

New Structure-based Methods for Fragment Screening

Keywords:

Fragment Screening, Structure-based Drug Design, Protein Docking, Molecular Dynamics, Generative Chemistry

Summary:

Fragment-based drug discovery has become a key approach to identify chemical structures that serve as starting points from which medicinal chemists can generate novel bioactive small molecules. Chemotargets has developed an AIDD platform that includes a fragment screening phase. This project aims at developing and validating new methods to virtual fragment screening that achieve good levels of performance compared with their X-ray counterparts.

References:

Z. Chilingaryan et al. Fragment-based Screening by Protein Crystallography: Successes and Pitfalls. Int. J. Mol. Sci. 2012, 13, 12857-12879.

Expected skills:

Good programming skills; good level of English

Possibility of funding:

Yes

Possible continuity with PhD:

Yes