Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

Master project 2020-2021

Personal Information

Supervisor	Jordi Villà-freixa
Email	jvilla@uic.cat
Institution	Universitat Internacional de Catalunya
Website	http://mon.uvic.cat/cbbl
Group	Computational Biochemistry and Biophysics Lab

Project

Structural bioinformatics

Project Title:

Finding epitope-MHC interactions through deep learning and molecular simulations

Keywords:

Molecular simulations, MHC, Deep Learning

Summary:

Several Machine Learning methods have been established to classify antigen-MHC interactions with somehow good success. However, precise classification of the binding characteristics within those complexes is still elusive if only classification methods are used. Here we will work in a combination of state of the art deep learning tools with structure based molecular simulations.

References:

"Structure Based molecular simulations" Submitted. Martin Floor, Li Keng Jie, Luís Agulló, Jenn K. Hwang, Jordi Villà-Freixa

Expected skills::

Python, Molecular simulations, Machine Learning

Possibility of funding::

To be discussed

Possible continuity with PhD: :

Yes