Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

Master project 2020-2021

Personal Information

Supervisor	Magdalena Scharf
Email	magdalena.scharf@pharmazie.uni-marburg.de
Institution	Philipps-University Marburg
Website	www.kolblab.org
Group	Peter Kolb

Project

Structural bioinformatics

Project Title:

In silico prediction of novel ligands for a chemokine receptor

Keywords:

Chemoinformatics, homology modelling, docking calculations, GPCRs, computer-aided drug design

Summary:

Your project will evolve around one member of the chemokine receptors. The ultimate goal is to find novel ligands that modulate the activity of this target. Since there are no crystal structures available for the target receptor, the first step is to prepare a three dimensional structure of it by homology modelling. This model will then be used in docking calculations to screen a large library of molecules against it.

Expected skills::

basic chemical knowledge to evaluate protein-ligand interactions

Possibility of funding::

To be discussed

Possible continuity with PhD: :

To be discussed