Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

Master project 2020-2021

Personal Information

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Project

Pharmacoinformatics & systems pharmacology

Project Title:

Drug discovery and drug design for COVID-19 treatment

Keywords:

COVID-19, SARS-CoV-2, drug discovery, drug design

Summary:

The project aims to find new drugs that can be used for the treatment of COVID-19 and related patologies. In order to do that, the student will use structural information of therapheutic targets for COVID-19 treatment to define energy-based pharmacophores that allow him to mine in commercial databases of small molecules for finding those that can bind with high affinity to the target of interest. Then, the most promosing hits of this virtual screening will be used in hit-to-lead computational experiments to find more potents derivatives. The project will involve different drug-discovery or drug design technologies such protein-ligand docking, shape & electrostatic comparisons, FEP+. To achieve this project, the student will be trained in the use of the most common drug discovery & design suites (Schrödinger, OpenEye and Cresset). The result of his/her research project will be the several drugs for COVID-19 treatment.

References:

Understanding the variability of the S1' pocket to improve matrix metalloproteinase inhibitor selectivity profiles. Gimeno A, Beltrán-Debón R, Mulero M, Pujadas G, Garcia-Vallvé S. Drug Discov Today. 2020 Jan;25(1):38-57 Mining large databases to find new leads with low similarity to known actives: application to find new DPP-IV inhibitors. Ojeda-Montes MJ, Casanova-Martí À, Gimeno A, Tomás-Hernández S, Cereto-Massagué A, Wolber G, Beltrán-Debón R, Valls C, Mulero M, Pinent M, Pujadas G, Garcia-Vallvé S. Future Med Chem. 2019 Jun;11(12):1387-1401. The Light and Dark Sides of Virtual Screening: What Is There to Know? Gimeno A, Ojeda-Montes MJ, Tomás-Hernández S, Cereto-Massagué A, Beltrán-Debón R, Mulero M, Pujadas G, Garcia-Vallvé S. Int J Mol Sci. 2019 Mar 19;20(6). Combined Ligand- and Receptor-Based Virtual Screening Methodology to Identify Structurally Diverse Protein Tyrosine Phosphatase 1B Inhibitors. Gimeno A, Ardid-Ruiz A, Ojeda-Montes MJ, Tomás-Hernández S, Cereto-Massagué A, Beltrán-Debón R, Mulero M, Valls C, Aragonès G, Suárez M, Pujadas G, Garcia-Vallvé S. ChemMedChem. 2018 Sep 19;13(18):1939-1948 Activity and selectivity cliffs for DPP-IV inhibitors: Lessons we can learn from SAR studies and their application to virtual screening. Ojeda-Montes MJ, Gimeno A, Tomas-Hernández S, Cereto-Massagué A, Beltrán-Debón R, Valls C, Mulero M, Pujadas G, Garcia-Vallvé S. Med Res Rev. 2018 Sep;38(6):1874-1915.

Expected skills::

Good skills with Python and shell scripting

Possibility of funding::

No

Possible continuity with PhD: :

To be discussed
