SJSU | DEPARTMENT OF CHEMISTRY

CHEMISTRY Departmental Seminar

Spring 2022
CHEM 285/191 Schedule
Tuesday at 4:30-5:45PM
Duncan Hall 250

March 1st, 2022

Dr. Sara Capponi
IBM

AI-driven Predictions of Binding Trends of SARS-CoV-2 Variants from Atomistic Simulations

Protein-protein interactions are fundamental for cellular processes underlying functions such as signal transduction, cell regulation, or immune response activation among others. However, in silico characterization at atomistic level of the binding process between two proteins can be computationally demanding due to the long timescale of typical binding/unbinding events. To address this challenge, several approaches have been developed to estimate the binding free energies between two molecules and weigh mutation effects. Here, we present a novel technique to predict binding affinity between two molecules from full-atom molecular dynamics simulations. The technique uses a neural network algorithm applied to a series of images generated by the simulation data and representing the distance between two molecules in time. The algorithm is capable of distinguishing with high accuracy low vs high binding affinity of non-hydrophobic mutations, indicating that our method excels on the inference of the binding affinity trends for charged and/or polar amino acid mutations. Moreover, it shows high accuracy in prediction using a small subset of the simulated data, therefore requiring a much shorter simulation time. We apply our algorithm to the binding between several variants of the SARS-CoV-2 spike protein and the human receptor ACE2.

For more information: Prof. Muller at gilles.muller@sjsu.edu
or Prof. Wang at ningkun.wang@sjsu.edu

Revised 01/24/2022