

MASTER « *In Silico* Drug Design »
2ème année

PROPOSITION DE STAGE
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Ecole doctorale de rattachement : Médicament, Toxicologie, Chimie, Imageries (MTCI ED 563)

Spécialité du stage : Recherche ☒ Professionnel ☐

Indiquez par quelques mots clés, l'orientation scientifique du sujet :

SARS-Cov2, molecular dynamics simulation, MM/PBSA analysis

Titre du stage : Study of the interaction between antibodies and Spike protein variants.

Ce sujet constitue-t-il un premier pas vers un travail de thèse : Oui

Description du sujet (quelques lignes):

Since its emergence in December 2019, SARS-Cov-2 (Severe Acute Respiratory Syndrome Coronavirus 2) has been responsible for the deaths of more than 4.7 million people worldwide. Several vaccines were developed in record time and have been available to the global population since December 2020. At the same time, however, several variants have emerged in different parts of the world, mainly in England, Brazil, South Africa, and, more recently, in India. These variants give SARS-Cov-2 the ability to increase its virulence or transmissibility and more easily evade the immune response by reducing the ability of antibodies to bind to the virus.

To understand which residues are most important in the interaction between the wild-type Spike protein and the human ACE2 receptor and to identify the regions to be targeted to prevent this interaction, we developed a molecular modeling protocol combining molecular dynamics simulations, MM/PBSA (Molecular Mechanics/Poisson-Boltzmann Surface Area) analyses and PockDrug analyses.

It is now important to consider the emergence of new variants of SARS-Cov-2. Several variants have become of real concern for human health, because mutations in the Spike protein induce an increase in its affinity for the ACE2 receptor or a decrease in its recognition by the body's antibodies. In this internship, we want to study the mutations effects in 2 variants (Indian and Brazilian) on the affinity of the antibodies for the Spike protein. Thus, we want to apply the previously described protocol to evaluate the affinity between several antibodies and the mutated Spike proteins using MM/PBSA analysis of molecular dynamics simulations.

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