IN SILICO STUDY ON SPIKE PROTEIN OF SARS-COV-2 VIRUS

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The COVID-19 pandemic is a global outbreak of the novel coronavirus (SARS-CoV-2). It was first identified in Wuhan, China in December 2019 and has since spread to become a global pandemic, affecting many countries and continents. The virus is highly contagious and spreads primarily through respiratory droplets from infected individuals. In this study, molecular docking experiments were performed to several promising natural products and anti-hypertensive molecules to test their potential against coronavirus, and more specifically, the inhibition of the spike protein bound ACE2 (Angiotensin Converting Enzyme 2). As regards Molecular Docking studies were performed in three different binding sites. The first binding site was defined in ACE2, the second binding site was defined in Spike protein. Finally, Durdagi *et al.* suggested the third binding site, located at the junction of spike protein and ACE2. The docking results demonstrated that salvianolic acid, quercetin and rosmarinic acid present the most favorable docking scores. The stability of the three aforementioned complexes were further investigated via molecular dynamics simulations. Additionally, in collaboration with the research laboratory of Professor S. Durdagi, *in vitro* experiments were accomplished where the inhibitory activity of the compounds was measured.

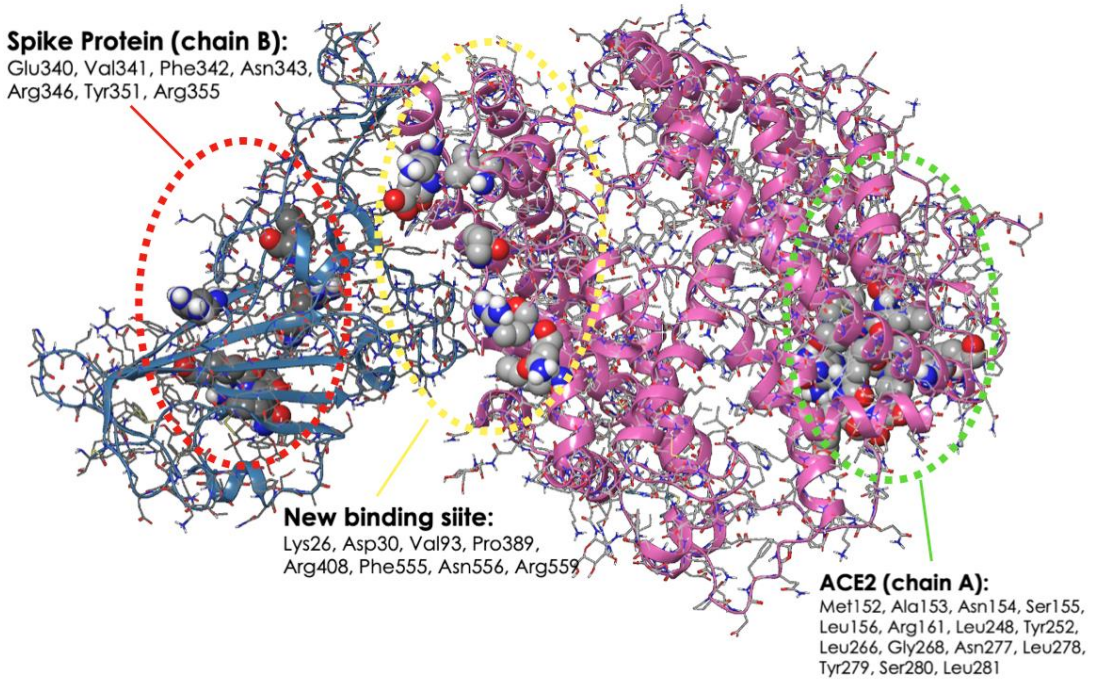

Figure 1. The three selected binding sites of Spike Protein bound with ACE2 (PDB id: 6M0J).

1. S. Durdagi, T. Avsar, M. D. Orhan, *et al*, *Molecular Therapy*, **30**, 1 (2021)