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### Computational Approach investigation Bioactive Molecules from *Saussurea Costus* Plant as SARS-CoV-2 Main Protease Inhibitors Using Reverse Docking, Molecular Dynamics Simulation, and Pharmacokinetic ADMET Parameters

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SARS-COV-2 virus causes (COVID-19) disease; it has become a global pandemic since 2019 and has negatively affected all aspects of human life. Scientists have made great efforts to find a reliable cure, vaccines, or treatment for this emerging disease. Efforts have been directed towards using medicinal plants as alternative medicines, as the active chemical compounds in them have been discovered as potential antiviral or anti-inflammatory agents. In this research, the potential of *Saussurea costus* (*S. Costus*) or QUST Al Hindi chemical consistent as potential antiviral agents was investigated by using computational methods such as Reverse Docking, ADMET, and Molecular Dynamics with different proteases COVID-19 such as PDB: 2GZ9; 6LU7; 7AOL, 6Y2E, 6Y84. The results of Reverse Docking the complex between 6LU7 proteases and Cynaropicrin compound being the best complex, as the same result, is achieved by molecular dynamics. Also, the toxicity testing result from ADMET method proved that the complex is the least toxic and the safest possible drug. In addition, the 6LU7-Cynaropicrin complex obeyed Lipinski rule; it formed  $\leq 5$  H-bond donors and  $\leq 10$  H bond acceptors, MW < 500 Daltons, and octanol/water partition coefficient < 5.

#### Biography

Yuqi Xin has expertise in adolescent mental health and health education promotion, specializing in psychometric and statistical methods. At the same time, she has a passion for improving the health and well-being of adolescents. She studies the changes in mental health of adolescents from different generations in their environment (society, family, etc.) to provide new ideas for promoting healthy adolescent development. She has voluntary part-time positions in the Society for Preventive Medicine, the Society for the Promotion of International Exchange, and the Society for Family Education, aiming to study adolescent health and environmental improvement.

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