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Contribution of Artificial Intelligence in the Studies of Natural Compounds Against SARS-COV-2

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Abstract : We have carried out extensive and in-depth research to search for bioactive compounds based on Algerian plants. A selection of 50 ligands from Algerian medicinal plants. Several compounds used in herbal medicine have been drawn using Marvin Sketch software. We determined the three-dimensional structures of the ligands with the MMFF94 force field in order to prepare these ligands for molecular docking. The 3D protein structure of the SARS-CoV-2 main protease was taken from the Protein Data Bank. We used AutoDockVina software to apply molecular docking. The hydrogen atoms were added during the molecular docking process, and all the twist bonds of the ligands were added using the (ligand) module in the AutoDock software. The COVID-19 main protease (Mpro) is a key enzyme that plays a vital role in viral transcription and mediating replication, so it is a very attractive drug target for SARS-CoV-2. In this work, an evaluation was carried out on the biologically active compounds present in these selected medicinal plants as effective inhibitors of the protease enzyme of COVID-19, with an in-depth computational calculation of the molecular docking using the Autodock Vina software. The top 7 ligands: Phloroglucinol, Afzelin, Myricetin-3-O- rutinosidTricin 7-neohesperidoside, Silybin, Silychristinthat and Kaempferol are selected among the 50 molecules studied which are Algerian medicinal plants, whose selection is based on the best binding energy which is relatively low compared to the reference molecule with binding affinities of -9.3, -9.3, -9, -8.9, -8 .5, 8.3 and -8.3 kcal mol-1 respectively. Then, we analyzed the ADME properties of the best7 ligands using the web server SwissADME. Two ligands (Silybin, Silychristin) were found to be potential candidates for the discovery and design of novel drug inhibitors of the protease enzyme of SARS-CoV-2. The stability of the two ligands in complexing with the Mpro protease was validated by molecular dynamics simulation; they revealed a stable trajectory in both techniques, RMSD and RMSF, by showing molecular properties with coherent interactions in molecular dynamics simulations. Finally, we conclude that the Silybin ligand forms a more stable complex with the Mpro protease compared to the Silychristin ligand.

Keywords : COVID-19, medicinal plants, molecular docking, ADME properties, molecular dynamics
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