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Abstract

Identification of New Anti-SARS CoV-2 Agents through theVirtual Screening of Phytoconstituents Extracted from Moroccan Plants †

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Abstract: The rapid spread of fatal diseases forces us to reconsider our position as researchers in the field of drug development assisted by computers. On the other hand, new drugs are constantly being developed from natural compounds using computer-aided methods. Virtual screening is carried out in accordance with the protocols established by accredited organizations and is based on the structure of the ligands or the structure of the target proteins. The formation of a database based on phytotherapy is the best option because Morocco is known for its wealth of plants and their traditional uses in medicine, which encourages us to better utilize our cultural heritage and the natural diversity of our country in the therapeutic field. The combination of these fields of CADD and phytotherapy can yield positive results in terms of the development of molecules with the goal of their use as drugs that are capable of inhibiting a pathological protein. In the present study, deep research was performed to collect a set of phytoconstituents extracted from Moroccan plants in order to evaluate their ability to limit the proliferation of SARS-CoV-2. Molecular docking was performed in the active sites of the 6lu7 and 6m0j proteins to assess their binding affinity. The structural stability of the target proteins was validated by redocking. The compounds with good binding affinity values were further subjected to Lipinski's rule of five, chemical absorption and toxicity analysis. The results revealed that only two of the compounds presented a good binding affinity towards the target proteins and are able to be used as orally available medication for SARS-CoV-2.

Keywords: SARS-CoV-2; Moroccan plants; virtual screening; molecular docking

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