University of Zabol
Graduate school
Department of Chemistry

The Thesis Submitted for The Degree of Master of sciences
(In the field of Analytical Chemistry)

Qsar modeling and molecular docking for identifying 3CLpro and RdRp inhibitors as potential therapeutics for COVID-19

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Abstract

With the coronavirus pandemic, the medical system of many countries started trying to develop effective treatments to save human lives and help society to return to everyday life due to the high rate of infection and death caused by this disease. Computer-aided drug design facilitates the discovery of promising drug candidates for diseases. In this research, QSAR models have been developed for a data set of 2377 compounds defined as either active or inactive against 3-CLpro and RdRp. Pharmacophore structure-based modeling, molecular docking, virtual screening, and in silico ADMET studies of against 3-CLpro and RdRp inhibitors with the aim of finding new and potent against 3-CLpro and RdRp inhibitors, was done. Virtual screening of ZINC, CHEMBEL, Molport and MCULE databases using a pharmacophore structure-based structure model constructed was carried out. The effective method of molecular docking was applied as the last step of virtual screening on the obtained hits from pharmacophore screening and Druglikeness rules. The proposed compounds from the process were checked on their pharmacokinetics properties.

Keywords: QSAR, Molecular docking, Virtual screening, pharmacophore, Coronavirus