ORIGINAL RESEARCH ARTICLES

IN SILICO MOLECULAR DOCKING STUDIES OF COUMARIN-CHALCONE HYBRIDS AGAINST SARS-COV-2 MAIN PROTEASE (6LU7)

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ABSTRACT

The present work aimed to explore efficient lead molecules to combat against COVID-19. Despite the extensive usage of repurposed medications for COVID-19 therapy due to their inadequacy to proper control of endangered pandemic, there is an urgent need to discover innovative compounds that are very effective against the COVID-19 pandemic. Newly synthesized coumarin-chalcone hybrids were assessed for their efficacy to inhibit main protease 6LU7(M^{pro}) and compared it with some repurposing COVID-19 drug activity through *in silico* technique. Among all synthesized hybrids, **d11**, **a11**, **c12**, **b11** and **c5**, showed highest binding affinities with the least docking score against protease (PDB ID: 6LU7) protein comparable to repurposed drugs currently used against COVID-19. The selected hybrics having coumarin, chalcone, and dihydropyridine pharmacophores are promising for their anti-COVID-19 activity. However, further extensive research is required through suitable *in vitro* and *in vivo* methods.

Keywords: Coumarin-chalcone, main protease, drugs repurposing, hybrids; SARS-CoV-2; molecular docking, 6LU7

were already more than 6 corona viruses that produced respiratory syndromes in human beings; SARS-CoV-2 is the 7th corona virus that shares structural similarity with SARS-