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ORIGINAL ARTICLE

In silico studies on phytochemicals to combat the emerging COVID-19 infection

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Abstract The current COVID-19 pandemic, caused by the severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) and its variants, remains a serious health hazard globally. The SARS-CoV-2 Mpro and spike proteins, as well as the human ACE2 receptor, have previously been reported as good targets for the development of new drug leads to combat COVID-19. Various ligands, including synthetic and plant-derived small molecules, can interact with the aforementioned proteins. In this study, we investigated the interaction of eight phytochemicals, from selected medicinal plants (*Aegle marmelos*, *Azadirachta indica*, and Ocimum sanctum) commonly used in Indian traditional medicine, with SARS-CoV-2 Mpro (PDBID: 6LU7), SARS-CoV-2S spike protein (PDB

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