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In-silico Screening of potent Phytoconstituents of Indian medicinal plantsPossess Antiviral Activity against COVID 19 spike protein usingComputational based Screening Methods and Pharmacophoric Mapping

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ABSTRACT:

The deadly effect of corona virus has severely affected World .Presently the scheme of treating Virus with antiviral or antimalarial drugs or in combination with anti-Ebola medicine,. In researches conducted in China researchers revealed that phytoconstituents like Betulinic acid ,Emodin Ursolic acid and Menthol showed better activity against COVID 19. In this work Indian Medicinal plants carry these phytoconstituents searched then their ligands were selected from online databases then their biopharmaceutical ,physiochemical, and druggable, properties were compared and Target prediction of these plant constituents were done. Pharmacophoric Mapping was also done for all the phytoconstituents so that the mechanism of ligand protein interaction can be identified Phytoconstituents exhibited better target prediction then subjected for Docking .The result of Docking between the COVID 19 Viral protein and phytoconstituents based ligands showed that out of four potential Emodin proved best ligand since they fit in the first pocket 224.704 area and 180.763 volume of COVID 19 spike Viral protein more suitably shows by distance and their binding affinity was also better since it carried 3 hydrogen bond donor for binding with the viral protein .

Keywords: Emodin, Ursolic acid, Betulinic acid, Menthol, phytoconstituents.

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