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(71)**Name of Applicant :**
1)Dr. Varsha Tiwari
Address of Applicant :Pharmacy Academy, IFTM University, Lodhipur-Rajput, Moradabad (U. P.)-244102 ---------- ----------
2)Dr. Abhishek Tiwari
3)Dr. Navneet Verma
Name of Applicant : NA
Address of Applicant : NA
(72)**Name of Inventor :**
1)Dr. Varsha Tiwari
Address of Applicant :Pharmacy Academy, IFTM University, Lodhipur-Rajput, Moradabad (U. P.)-244102 ---------- ----------
2)Dr. Abhishek Tiwari
Address of Applicant :Pharmacy Academy, IFTM University, Lodhipur-Rajput, Moradabad (U. P.)-244102 ---------- ----------
3)Dr. Navneet Verma
Address of Applicant :Pharmacy Academy, IFTM University, Lodhipur-Rajput, Moradabad (U. P.)-244102 ---------- ----------

(57) Abstract :
Researchers are seeking for phyto-candidates that can inhibit or stop SARS-CoV-2 because of the present pandemic. The main protease (Mpro) of SARS-CoV-2 and spike glycoprotein (S) are both suppressed by bioactive compounds found in plants that work by docking them together. The Mpro proteins 6LU7 (complex with an inhibitor N3) and 5C3N (space group C2221) were employed in docking research. PyRx and AutoDock Vina software was used as a docking engine. 22 phytoconstituents were identified and selected from IMPPAT, a manually curated database on the basis of their antiviral effects. Docking results showed that phytoconstituents ß-amyrin (-8.4 kcal/mol), Withaferin A (-8.3 kcal/mol), Oleanolic acid (-7.8 kcal/mol) and Patentiflorin A (-8.1 kcal/mol) have shown best results against 5C3N Mpro whereas Kuwanon L (-7.1 kcal/mol), ß-amyrin (-6.9 kcal/mol), Oleanolic acid (-6.8 kcal/mol), Cucurbitacin D (-6.5 kcal/mol) and Quercetin (-6.5 kcal/mol) against 6LU7 Mpro Protein. All the compounds were examined for their ADMET characteristics using SwissDock. Present research reports the phytoconstituents along with docking score will be helpful for future drug development against Covid-19 drugs.

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