

(54) Title of the invention : A system to explore the phytochemical intervention of Terminalia chebula as a therapeutic potential against Covid-19

<p>(51) International classification :A23L 331050, A61K 361850, A61P 190200, A61P 311400, C12N 050783</p> <p>(86) International Application No :PCT// Filing Date :01/01/1900</p> <p>(87) International Publication No : NA</p> <p>(61) Patent of Addition to Application Number :NA Filing Date :NA</p> <p>(62) Divisional to Application Number :NA Filing Date :NA</p>	<p>(71)Name of Applicant : 1)Brainware University, Kolkata Address of Applicant :398, Ramkrishnapur Rd, Near Jagadighata Market, Barasat, Kolkata, West Bengal 700125 ----- -----</p> <p>Name of Applicant : NA Address of Applicant : NA</p> <p>(72)Name of Inventor : 1)Mr. Rajorshi Sen Gupta Address of Applicant :Research Scholar, Department of Computational Science, Brainware University, 398, Ramkrishnapur Rd, near Jagadighata Market, Barasat, Kolkata, West Bengal 700125, SACT 2, Department of Computer Science and Applications, Malda College, Rathbari, Rabindra Avenue, Malda Town, West Bengal 732101. -----</p> <p>2)Dr. Sandip Roy Address of Applicant :Professor and HOD, Department of Computational Science, Brainware University, 398, Ramkrishnapur Rd, near Jagadighata Market, Barasat, Kolkata, West Bengal 700125. -----</p> <p>3)Dr. Rajesh Bose Address of Applicant :Professor and Director Research, Department of Computational Science, Brainware University, 398, Ramkrishnapur Rd, near Jagadighata Market, Barasat, Kolkata, West Bengal 700125. -----</p>
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(57) Abstract :

The present invention relates to in-silico study to find COVID-19 Mpro-inhibitors from phytochemicals of T. chebula. With the help of Dr. Duke's database, 56 secondary metabolites were selected as the phytochemicals of T. chebula and were taken for the druggability study. A screening was done based on Lipinski's rule of 5, and 14 unique phytochemicals were selected for toxicity studies with Protox II and based on their toxicity class 5 or very low toxicity and 6 or no toxicity. 7 phytochemicals were selected that participated in virtual screening with macromolecule 6LU7.

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