ORIGINAL RESEARCH ARTICLES

IN SILICO BASED SCREENING EMPLOYED TO ASSESS THE ACTIVITY OF PHYTOCHEMICAL, SYNTHETIC AND MARINE COMPOUNDS ON THE SARS-COV-2 MAIN PROTEASE

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ABSTRACT

Our study focuses on screening ligands against the target 6Y2E using the iGemDock docking program, encompassing phytochemical, synthetic and marine sources, suggesting suitability for oral use against SARS-CoV-2 Main protease. Docking process involves iGemDock program for assessment, Argus Labs, for binding energy determination, Swiss ADME for evaluating pharmacological properties, and Chimera for visualizing interactions. Docking score gauges how effectively a ligand inhibits SARS-CoV-2 M^{pro}, with compounds ranked based on their docking scores. Rosmarinic acid, a phytochemical compound, achieved a docking score of -117.629 and energy of -11.051. Remdesivir, a synthetic compound, attained a docking score of -118.091 and energy of -9.31522. Spongouridine, a marine compound, secured a docking score of -83.1317 and energy of -6.38, making them the top-ranked molecules in the docking process.