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Investigation on the binding affinity of five drug-like sulphonamides on SARS-CoV-2 targets: A computational study

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Covid-19 is a dreadful pandemic of the 21st century. Many people have lost their lives and those who recovered are ailing from serious health issues. Even though preventive vaccinations are being carried out all over the world, lack of effective drugs to cure the patients increases the casualties. Scientists are in search of effective pharmaceuticals to fight against coronavirus. Computational methods are used for the discovery of new drugs. In the present course of investigation, we have performed docking studies of fifteen molecules on various targets of SARS-CoV-2, and five drug like molecules having high binding scores have been selected and reported. The molecules under investigation have been selected from spirochem and ChemBL databases. They are the derivatives of benzene sulphonamide and consist of cubane or cyclopropane or cyclobutane ring systems. Web Servers like Swissdock and SwissADME have been used for docking studies and ADME prediction respectively. Softwares such as Chimera and Biovia Discovery Studio have been employed for the modeling of the protein ligand-complex. Structures of drug targets of coronavirus have been downloaded from Protein Data Bank. Ligands w045 and 2059020 have been effective against the main protease of SARS-CoV-2. The nucleoprotein of the virus is well inhibited by 205913 and 2059020. The envelope protein of the virus shows great attraction towards the molecule 2059020. The same ligand also shows better binding capacity on the surface of the spike protein of the covid-19 virus.

Keywords: SARS-CoV-2, Docking, Sulphonamide, SwissADME