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Abstract

In Silico Investigations of Dihydrophenanthrene Derivatives as Potential Inhibitors of SARS-CoV-2 †

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Abstract: Since its appearance in Wuhan in December 2019, finding ways to manage the COVID-19 pandemic has become the biggest challenge the world is facing. In this investigation, we used a quantitative structure-activity relationship (QSAR) study, an absorption, distribution, metabolism, excretion, and toxicity (ADMET) analysis, and computational molecular docking simulations to screen and assess the efficacy of 39 bioactive 9,10-dihydrophenanthrene analogues. The density functional theory (DFT) using the B3LYP/6-31G (d, p) level was used for the calculations of molecular descriptors, and principal component analysis (PCA) was used to eliminated redundant and non-significant descriptors. After that, statistically robust models were developed using the multiple linear regression (MLR) method. All the derived models were then subjected to thorough external and internal statistical validations, Y-randomization, and applicability domain analysis. These validations were carried out as per the Organisation for Economic Co-operation and Development (OECD) principles. The best built model was used to design new molecules that have good values of inhibitory activity against SARS-CoV-2. The pharmacokinetics properties were then determined using an ADMET analysis to weed out any that would be harmful to the human body or cause adverse effects. Through the use of computational molecular docking simulations, in silico research was conducted on the deigned compounds to forecast their SARS-CoV-2 activity and determine the stability of the evaluated ligands during their contacts with the proteins of the desired activity.

Keywords: SARS-CoV-2; QSAR; MLR; dihydrophenanthrene; molecular docking

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