In silico Research of the Potential Role of a Number of Compound Class N-acylethanolamines as Inhibitors of E-protein Coronavirus SARS-CoV-2

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Nowadays, global coronavirus SARS-CoV-2 pandemic exerts special emphasis on the search of non-toxic biological active compounds, that are able to have an anticoronavirus effects and can be used to develop a cure. N-acylethanolamines is a class of minor lipids, that demonstrate high biological activity and properties. These molecules are included in the endocannabinoid retrograde neurotransmitters systems of humans and mammals. Early works of Department of lipid biochemistry of the O.V. Palladin Institute of biochemistry shown that saturated N-stearoylethanolamine possesses powerful antiviral activity to H1N1 influenza virus, herpes simplex and hepatitis C viruses. Also it was identified that E-protein plays important role in coronavirus genome implementation,and therefore can be used as a target of different antiviral substances. In this project, method of molecular docking was used for In silico modeling of the potential ability of N-acylethanolamines to bind with active sites of coronavirus SARS-CoV-2 E-protein. Molecular docking and preparation of spatial structures (N-acylethanolamines), were carried out in the program AutoDock 1.5.6. After conducting molecular docking modeling, we obtained affinity data to active site of each N-acylethanolamines, then calculated inhibition constant and determinated the binding sites with suitable receptors. The results indicate, that all n-acylethanolamines can bind with active site of E-protein of coronavirus SARS-CoV-2, but N-stearoylethanolamine possesses highest affinity to active site and inhibition constant. My results support the hypothesis of using n-stearoylethanolamine as potential anti coronavirus SARS-CoV-2 active molecule in the human organism.

Awards Won:

Drug, Chemical &amp

Associated Technologies Association (DCAT): $1,000 scholarship will will be awarded &#x0D

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