QSAR-Quantum Mining on Chern-Simons Topological Geometrics for the generation of a Ligand Targeting COVID-19-SARS-COV-2 SPIKE D614G Binding Sites.

Ioannis Grigoriadis[1]

[1]Biogenea Pharmaceuticals Ltd

March 30, 2022

Abstract

SARS coronavirus 2 (SARS-CoV-2) in the viral spike (S) encoding a SARS-COV-2 SPIKE D614G mutation protein predominate over time in locales revealing the dynamic aspects of its key viral processes where it is found, implying that this change enhances viral transmission. It has also been observed that retroviruses infected ACE2-expressing cells pseudotyped with SG614 that is presently affecting a growing number of countries markedly more efficiently than those with SD614. The availability of newer powerful computational resources, molecular modeling techniques, and cheminformatics quality data have made it feasible to generate reliable algebraic calculations to design new chemical entities, merging chemicals, fragmentizing natural products, and a lot of other substances fuelling further development and growth of this AI-quantum based drug design field to balance the trade-off between the structural complexity and the quality of such biophysics predictions that cannot be obtained by any other method. In this paper, we strongly combine topology geometric methods targeting at the atomistic level the protein apparatus of the SARS-COV-2 virus that are simple in machine learning anti-viral characteristics, to propose computer-aided rational drug design strategies efficient in computing docking usage, and powerful enough to achieve very high accuracy levels for this in-silico effort for the generation of the AI-Quantum designed molecule the RoccustyrnaTM small molecule, a multi-targeting druggable scaffold 2-({[fluoro({[(2E)-5-oxabicyclo [2.1.0]pentan-2-ylidene]cyano-lambda6-sulfanyl}) methyl]phosphorylidene} amino)-4,6-dihydro-1H-purin-6-onetargeting the COVID-19-SARS-COV-2 SPIKE D614G mutation using Chern-Simons Topology Euclidean Geometric in a Lindenbaum-Tarski generated QSAR automating modeling and Artificial Intelligence-Driven Predictive Neural Networks.

Hosted file

`RoccustyrnaiJcamOmgt7HK__ Grigoriadis_Ioannis_.doc` available at https://authorea.com/users/389434/articles/562756-qsar-quantum-mining-on-chern-simons-topological-geometrics-for-the-generation-of-a-ligand-targeting-covid-19-sars-cov-2-spike-d614g-binding-sites