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Marine Alga *Ulva fasciata*-Derived Molecules for the Potential Treatment of SARS-CoV-2: An *In Silico* Approach

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Abstract: SARS-CoV-2 is the causative agent of the COVID-19 pandemic. This in silico study aimed to elucidate therapeutic efficacies against SARS-CoV-2 of phyco-compounds from the seaweed, *Ulva fasciata*. Twelve phyco-compounds were isolated and toxicity was analyzed by VEGA QSAR. Five compounds were found to be nonmutagenic, noncarcinogenic and nontoxic. Moreover, antiviral activity was evaluated by PASS. Binding affinities of five of these therapeutic compounds were predicted to possess probable biological activity. Fifteen SARS-CoV-2 target proteins were analyzed by the AutoDock Vina program for molecular docking binding energy analysis and the 6Y84 protein was determined to possess optimal binding affinities. The Desmond program from Schrödinger's suite was used to study high performance molecular dynamic simulation properties for 3,7,11,15-Tetramethyl-2-hexadecen-1-ol—6Y84 for better drug evaluation. The ligand with 6Y84 had stronger binding affinities (−5.9 kcal/mol) over two standard drugs, Chloroquine (−5.6 kcal/mol) and Interferon α-2b (−3.8 kcal/mol). *Swiss ADME* calculated physicochemical/lipophilicity/water solubility/pharmacokinetic properties for 3,7,11,15-Tetramethyl-2-hexadecen-1-ol, showing that this therapeutic agent may be effective against SARS-CoV-2.

Keywords: SARS-CoV-2; *Ulva fasciata*; iGEMDOCK; PASS; *Swiss ADME*; VEGA QSAR; Schrödinger; Desmond software

1. Introduction

Marine macroalgae (also known as seaweed) are macroscopic, multicellular, eukaryotic photosynthetic organisms that belong to the Plantae kingdom [1]. These salt-dwelling marine plants are found on rock surfaces, corals, shells, pebbles, other plants, as well as the seabed or solid underlying layers of rock. Marine algae commonly grow in tidal and subtidal regions of the ocean in optimal availability of light. They can survive in harsh conditions (i.e., withstand heat, cold, UV radiation, salinity and desiccation) due to their easy adaptation to physiological changes by producing stress tolerant substances [2,3]. With this survival, they produce a variety of primary and secondary metabolites. Marine