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POTENTIAL OF INHIBITING THE RECEPTOR BINDING MECHANISM OF SARS-COV-2 USING PHYTOCHEMICAL EXTRACTS OF MEDICINAL HERB; MOLECULER DOCKING STUDY

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ABSTRACT

The Corona Viral Infective Disease (COVID-19), which leads to Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) is caused a pandemic situation globally. World Health Organization (WHO) declared that COVID-19 as a Public Health Emergency of International Concern (PHEIC) on January 30, 2020. Intend of this study is divulge the chemistry behind the phenomenon of viral (SARS-CoV-2) attachment on human epithelial cells as well as evaluate the receptor blocking abilities of selected herbal compounds. Significant anti-viral compounds were identified via review process of medicinal plants and Ferula asafetida, Glycyrrhiza glabra, Curcuma longa, Zingiber officinale etc. are widely used plant species for drugs against viral infectious diseases in Ayurveda medicine. Molecular docking prognosis have been carried out to demonstrate any possible secondary metabolites present in several anti-microbial herbs that could act as blocking agents of ACE2 and GRP78 receptors of epithelial cells to baffle the binding of receptor-binding domain (RBD) sections of SARS-CoV-2. Computational findings reveal that Phyto-chemicals such as Conferone, Samarcadin, Bdrakemin Farnesiferol A, Fernesiferol C and Galbanic acid isolated from Ferula asafetida have intensive binding energies for ACE2 receptor binding process. Apart from that Hederagenin and Ursolic also shows highest inhibitory potential towards human ACE2. When considering GRP78, almost all isolated compounds in oligo-gum resins of Ferula asafetida trot out perfect binding ability towards the active site of GRP78 receptor. Hence, it is worth to pay more attention on natural phytochemicals for mitigating of human viral infections.

INTRODUCTION

COVID ‘19 was first reported in Wuhan, Hubei province, China in December 2019 [1] and is now an intricate endemic in the world and as of today, 16th of April 2020, the number of coronavirus cases has exceeded 1,914,916 and more than 123,010 deaths were confirmed [2]. These numbers are increasing on a daily basis. The Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) first occurred 17 years ago [3] and the novel coronavirus, SARS-CoV-2 is the seventh coronavirus known to infect humans. Among the other strains, SARS and MERS were the most widely known strains of coronaviruses, and each caused nearly 800 deaths [4]. WHO declared a public Health Emergency of international concern on 30th January 2020 for COVID ’19 [2]and it has become a burden to public health as well as to the world economy.

According to the Phylogenetic analysis, the SARS-CoV-2 virus belongs to lineage B of the beta-coronavirus [5]. The researchers analyzed genomic data available from SARS-CoV-2 and other coronaviruses, showing that the receptor-binding domain (RBD) sections of SARS-CoV-2 spike proteins are optimized for receptor binding [6]. The angiotensin-converting enzyme (ACE) - related carboxypeptidase, ACE2 is a type 1 (Hydrolase) integral membrane protein of 805 amino acids that contains one HEXXH + E zinc-binding consensus sequence [7]. Crystal structures of the native (PDB ID: 1R42) and inhibitor bound (PDB ID: 1R42) forms of ACE2 extracellular domains were solved to 2.2- and 3.3-Å resolution and deposited in RSCB protein data bank. When it considers tissue distribution of ACE2 protein, a remarkable expression found on lung alveolar epithelial cells and enterocytes of the small intestine. And also ACE2 present in arterial and venous endothelial cells, arterial smooth muscle cells [8] and, renal tissues [9]. It has proved a higher expression of ACE2 in the human failing heart [10].