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Molecular Docking Studies of some Antiviral and Antimalarial Drugs *Via* Bindings to 3CL-Protease and Polymerase Enzymes of the Novel Coronavirus (SARS-CoV-2)

Najim A. Al-Masoudi [1,*], Rita S. Elias [2], Bahjat Saeed [3]

[1] Department of Chemistry, College of Science, University of Basrah, Basrah, Iraq. Present address: Constance, Germany
[2] Department of Pharmaceutical Chemistry, College of Pharmacy, University of Basrah, Basrah, Iraq
[3] Department of Chemistry, College of Education of Pure Science, University of Basrah, Basrah, Iraq
* Correspondence: najim.al-masoudi@gmx.de;

Scopus Author ID 7003637680
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Abstract: The rapid spread of the novel coronavirus (SARS-CoV-2) as a serious threat to the world public health is in dire need of finding potential therapeutic agents. Chinese have tested several antiviral and antimalarial drugs as potent inhibitors for the novel virus, such as remdesivir, chloroquine, hydroxychloroquine, umifenovir and favipiravir. In this study, we used the molecular docking models to study the binding interactions between these pharmaceuticals, as well as our proposed remdesivir analogue (AZCV-20) with the 3CLpro and RNA-dependent RNA polymerase (RdRp) of the SARS-CoV-2, using MEO and Autodock4 methods. Our study provides insight into the possible role of structural flexibility and efficacy during interactions between 3CLpro, RdRp and the drugs.

Keywords: Antiviral and antimalarial drugs; Molecular Docking; SARS-CoV-2; 3CLpro; RNA-dependent RNA polymerase (RdRp).

1. Introduction

A novel severe acute respiratory syndrome coronavirus (SARS-CoV-2) was identified from respiratory illness patients in Wuhan, China in December 2019 [1, 2], which is closely related to severe acute respiratory syndrome CoV (SARS-CoV). Today, no specific drugs are available to treat this disease. Thus, there remains an urgent need for the development of specific antiviral therapeutics toward SARS-CoV-2. A number of pharmaceuticals already being tested [3-5], but a better understanding of the underlying pathobiology is required. Due to the similarities of SARS-CoV-2 with the original SARS-CoV, several laboratories are focusing on the viral genome structural proteins like spike glycoprotein (S), a small envelope protein (E), matrix glycoprotein (M), nucleocapsid protein (N) [6, 7], the 3CLpro, the main protease required for the maturation of coronaviruses, the protease polymerase (RdRp) is vital for the viral life cycle, making it an attractive target of anti-coronavirus drug development.

Drugs like ribavirin, interferon-alpha, lopinavir-ritonavir (kaletra), required for the maturation of coronaviruses (3CLpro) [8, 9] and the RNA-dependent RNA umifenovir, favipiravir, emtricitabine/tenofovir alafenamide, corticosteroids, and cyclophilin have been tested in patients with SARS or MERS, although the efficacy of some drugs remains controversial [10], whereas other antiviral drugs such as oseltamivir, and ganciclovir have been