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Anti-Dengue potential, Molecular Docking Study of Some Chemical Constituents in the leaves of *Isatis tinctoria*

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ABSTRACT

Dengue infection is a major public health challenge in several parts of the world, especially the subtropical and tropical regions. The development of agents that are able to inhibit the dengue virus (DNV) replication is therefore of utmost significance. *I. tinctoria* is one of the most investigated Chinese herbs, which has been recognised to be effective in the treatment of dengue fever. However, the mechanisms through which it exhibits such biological activity of great importance are still unclear. A total number of about 27 compounds isolated from *I. tinctoria* leaves which have been identified and reported in the literature to be effective against dengue fever were investigated for their inhibitory potencies against dengue virus as novel drugs for treating early attacks of dengue fever. The compounds were optimized by employing a method of Density functional theory (DFT) and a basis set of B_3LYP (6-31G**). The results of Molecular docking investigation between the compounds and the dengue viral protein (PDB: 6MO1) revealed that three of the compounds (GB-20, GB-19, and GB-6) possessing best binding energy in of -27.051, -26.193 and -24.664 kcal/mol respective were observed to inhibit the target through hydrogen bonds and hydrophobic interactions with amino acids residue of the protease binding site. The results of these studies would offer relevant insight into structural requirements for the development of effective and specific treatment against dengue virus infection.

1. Introduction

Dengue infection is a mosquito-borne infection caused by a virus called Dengue virus (DNV) which belongs to *Flavivirus* members commonly found in tropical regions of the world [1]. The virus is transmitted to persons by infested females especially *Aedes aegypti*, the Aedes genus [2-3]. The number of people infected with the dengue virus is over 390 yearly, with about 20–25% cases with clinically apparent symptoms [4].

These infections, in some cases, may also develop into a dengue hemorrhagic fever or dengue shock syndrome; a more acute phase of the fatal infection [5-7], these constitute a serious fatal threat in major dengue cases, about 2.5 % from 500,000 clinical cases [5]. The West Nile virus and the Zika virus are serotypes of DNV [8].

The NS3-NS2B proteases, NS3 helicase, as well as the RNA polymerase of NS5, which are the essential proteins of the dengue virus, have been the drug able targets studied for the development of antiviral inhibitors in the past 4 years [9-12].

Currently, there is no reliable vaccine or antiviral treatment for dengue virus infection [13]. This necessitates the need to discover novel and highly potent drugs to battle the menace of this disease. In pursuant of this effort, several molecular drug targets have been identified to develop new drug candidates.

In 2016, Suganya and Mahendran carried out molecular docking studies of chemical compounds

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