Asian Journal of Pharmaceutical Research and Development
(An International Peer-Reviewed Journal of Pharmaceutical Research and Development)
www.ajprd.com
ISSN 2320-4850

Research Article

VIRTUAL DOCKING STUDIES OF FLAVONOID COMPOUNDS AGAINST CELL WALL PROTEINS OF *MYCOBACTERIUM TUBERCULOSIS*

D. Gnanslin Sheeba[1], V. Subha*[2], Dr. K. Suseela Gomathi[3] and Dr T.Citarasu[4]

[1]. Biotechnology, Udaya College of Arts and Science, Vellamodi, KK District, **Tamil Nadu, India,**
[2]. Bioinformatics, Dept. of Biotechnology, College of Agriculture, Trivandrum, **Kerala, India,**
[3]. Santhigiri IGNOU Community College, Trivandrum, **Kerala, India**,
[4]. Centre for Marine Science and Technology, Rajackamangalam, KK District, **Tamil Nadu, India**.

Received: 20 June 2013, ***Revised and Accepted: 16 July 2013***

ABSTRACT

Tuberculosis continues to be a major cause of morbidity and mortality throughout the world. Considering the world–wide TB problems, there is an urgent need to develop relatively inexpensive new drugs to treat this deadly disease. The two main avenues of drug discovery are: identifying new microbial proteins for which to direct drug discovery efforts, and designing innovative drugs that target existing proteins. Natural products isolated from plants have played an important role in discovery of drugs against infectious diseases. In this present study, 50 ligand molecules (basically secondary metabolites, flavonoids) which were commonly present in the plants were docked with the selected Mycobacterium tuberculosis receptors (PDB ID- 1DQY, 1KPI and 1TQ8) using iGEMDOCK. Among them, five compounds had a significant inhibitory activity with the receptors at a very low energy value. This was also found to obey the Lipinski's Rule of five and showed the drug likeliness and bioavailability. Since it is from a natural source the compound is non toxic and has reduced side effects.

Keywords: *Cell wall proteins, docking, flavonoids, iGEMDOCK, Mycobacterium tuberculosis.*