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IN-SILICO DOCKING ANALYSIS OF SELECTED FLAVONOIDS AND PROTECTIVE ANTIGEN

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Abstract

Anthrax toxin released by virulent strains of the bacterium, Bacillus anthracis, plays key factor in anthrax disease.

The main purpose of this study was to investigate the interaction between four flavonoid ligands including Rhamnetin, Apigenin, Tectochrysin, Pinocembrin and protective antigens.

Bioinformatics checking was done by means of Molegro virtual docker and Chimera 1.7. Also, in order for more accuracy, servers like Swiss Dock and BSP-SLIM, and all outputs obtained from this software were compared with each other. The results demonstrated that Apigenin interacted with the Glu117 which is crucial part of binding to its ligand with -12.3453 kca/mol. Also, the highest Fullfitness among these four ligands attributed to Rhamnetin with -994.80 kcal/mol and the ΔG =-7.06 kcal/mol.

Results demonstrated that every four ligands possessed interaction with protective antigen and so have inhibitory effect on its interaction with cell membranes but the inhibitory activity of Apigenin and Rhamnetin in interaction is stronger than others flavonoids. Results shown above bring up laboratory studies based on these flavonoids in order to produce an efficacious drug against anthrax.

Keywords: *Rhamnetin, Apigenin, Tectochrysin, Pinocembrin, protective antigens, Willebrand factor*

Introduction

Anthrax, charbon (France), Milzbrand (Germany) is derived from Greek anthrakos, meaning coal, emanating from the black color of the eschar in the human skin. Bacillus anthracis (so named by Cohn in 1875) is agent for anthrax which is peracute, acute or subacute disease involving a broad range of animal including humans, mammals and even birds [*Turnbull P, 2002*] it can occur generally in three forms cutaneous anthrax, gastrointestinal anthrax and inhalational anthrax [*Nickell Z, Moran M, 2017*] leading not only to high mortality rate also indirectly can affect Gross national product [*Siamudaala V et al., 2006*]. Lack of accurate controlling system and difficulty of counting number of infected people throughout the world contributes to lack of precise evaluation. The distribution of anthrax is now in agricultural regions of South and Central America, sub-Saharan Africa, central and southwestern Asia, and southern and eastern Europe [*Sitali D et al., 2017*]. Etiological

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