Short Communication

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Journal of Genomics & Gene Study

2020
Vol. 3 ISS. 3

Insights from molecular modeling and docking analysis of invasive protein SipB of Salmonella Typhi -A novel drug target for Salmonellosis

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the emergence of MDR Salmonella typhimuruium is a worldwide problem.Salmoella enterica serotype typhimurium multilocus sequence type (ST) 313 has been reported as an emerging cause of invasive salmonellosis and its infection is associated with high rates of drug resistance, blood stream infections, and death. Salmonellosis is one of the most common and widely distributed foodborne diseases caused by Salmonella enterica serovar Typhi (S.typhi). S.typhi co-evolving with the spread of HIV evolved the ability to spread to the deeper tissues of human, including liver, spleen and bone marrow. S.typhi strain CT18 is resistant to multiple drugs which is a serious emerging threat to the treatment of infectious diseases. Targeting unique effectors of this pathogen can be considered as a powerful strategy for drug design against bacterial variations to drug resistance. In this work we identified the cell invasion protein, SipB and sipD, as potential targets which are known to possess the following functions: host cell entry, transfer of other effector proteins into the host cell, inducing macrophage apoptosis, activating proapoptotic enzyme caspase I for inducing autophagy. Targeting unique effectors of this pathogen can be considered as a powerful strategy for drug design against bacterial variations to drug resistance. Studying the structure of SipB and sipD will help us to understand the mechanisms of the protein function which will pave way to the design of inhibitors. Hence molecular docking studies have been undertaken to optimize novel lead compounds. More than 75 herbal compounds and antibiotics have been docked and the results pave way for design of novel inhibitors. Further investigations into the antipathogenic potential of these compounds may open new avenues for drug development in the control of antibiotic resistant pathogens

Note : This work was partially published at International Conference on Bioinformatics & System Biology; March 20-21, 2019; Singapore City, Singapore