Identification of Lead Compounds againstScm (fms10) in Enterococcus faecium Using Computer Aided Drug Designing

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Abstract

Enterococcus faecium DO is an environmental microbe, which isa mesophilic, facultative, Gram-positive, and multiple habitat microorganism. *Enterococcus faecium* DO is responsible for many diseases in human. The fight against infectious diseases is confronted by the development of multiple drug resistance in *E. faecium*. The focus of this research work is to identify a novel compound against this pathogen by using bioinformatics tools and technology. We screened the proteome (accession No. PRJNA55353) information from the genome database of the National Centre for Biotechnology Information (NCBI) and suggested a potential drug target. I-TASSER was used to predict the three-dimensional structure of the protein, and the structure was optimized and minimized by different tools. PubChem and ChEBI were used to retrieve the inhibitors. Pharmacophore modeling and virtual screening were performed to identify novel compounds. Binding interactions of compounds with target protein were checked using LigPlot. pkCSM, SwissADME, and ProTox-II were used for adsorption, distribution, metabolism, excretion, and toxicity (ADMET) properties. Novel selected compounds have improved absorption and have better ADMET properties. Based on our results, the chemically identified inhibitor ZINC48942 targeted the receptor that can inhibit the activity of infection in *E. faecium*. This research work will be beneficial for the scientific community and could aid in the design of a new drug against *E. faecium* infections. It was observed that novel compounds are potential inhibitors with more efficacy and fewer side effects. This research work will help researchers in testing and identification of these chemicals useful against *E. faecium*.

Biography

Dr. Muhammad Asif Rasheed has his expertise in bioinformatics approaches and passion in improving the health and well being. He recently completed PhD studies from Huazhong Agricultural University, Wuhan, China and applied different bioinformatics approaches against different diseases. Simultaneously he published review and research articles by applying different bioinformatics tools. Recently he is working on In silico approaches to solve issues related to veterinary medicine.

Publications

● Efficacy of brassica, sorghum and sunflower aqueous extracts to control wheat weeds under rainfed conditions of Pothwar, Pakistan

● Immunoproteomic identification of MbovP579, a promising diagnostic biomarker for serological detection of Mycoplasma bovis infection

● Transmission potential and severity of COVID-19 in Pakistan

● Use and impact of insecticides in mealybug control

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[4th International Conference on Pharmaceutics & Advanced Drug Delivery Systems](#) | Frankfurt, Germany | April 05, 2021