Activity of several endophytic fungal extracts from Sri Lanka against *Staphylococcus aureus*; an *in-silico* Assessment

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Staphylococcus aureus is a gram positive pathogen which commonly infects humans. It has evolved as a drug resistant species partuclularly against Methicillin. Methicillin resistant *Staphyloccus aureus* (MRSA) is unresponsive to many current antibiotics. It is of great importance to develop sustainable antibacterial drugs. In this study we used *in-silico* methods to analyse the action of ten endophytic fungal extracts, which were experimentally known to act against gram positive bacteria, including *S .aureus*. 3D structures of the fungal compounds were generated and they were screened against currently used drug targets in *S. aureus* using molecular docking. For the purpose, drug targets and the respective drugs were obtained from DrugBank, an online database of drugs. To compare and evaluate docking scores, currently used drugs were used as reference ligands. The 'fungal molecule-target' complexes that have better scores than the relevant 'reference ligand-target' complexes were subjected for further analysis under molecular dynamics studies. According to the studies done so far, some of our query ligands showed better interactions with Penicillin binding proteins 2 and 4, Dihydrofolate reductase and Isoleucine tRNA ligase in comparison to the relevant drugs used as references. Hence, theoretically, the respective molecules extracted from fungi shows disruption of cell wall synthesis, inhibition of DNA synthesis and inhibition of protein synthesis in *S. aureus* suggesting potential antibiotic applicability against the bacterium. Out of them, Chaetoglobosin A and C promise the most potent antibacterial action due to the predicted synergistic inhibitory activity against *S. aureus*e enzymes.

Keywords: *Staphylococcus aureus*, *In-silico*, molecular docking, molecular dynamics