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In silico identification and structural bioinformatics of druggable protein targets in Schistosoma Species

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Schistosomiasis is a debilitating disease caused by a parasitic flatworm found in freshwater. After malaria, this disease is the second most prevalent disease in Africa and is endemic in the tropical and subtropical regions of the world. Morbidity and mortality attributed to this infection are very high with about 240 million people infected, 800 million persons at risk of the infection and at least 280,000 deaths annually. With the exponential increase in prevalence, Praziquantel (PZQ) remains the only effective drug in the antischistosomal arsenal, which is effective, but ineffective against the juvenile worm. More so, resistance to PZQ has been widely reported of late. Therefore, it is of paramount importance to develop effective alternative antischistosomal compounds using bioinformatics based tools utilizing the broad-spectrum therapeutic capabilities of Antimicrobial Peptides (AMPs). These AMPs are essential components of the innate immune system and are responsible for the complete destruction and immunomodulatory effects in the host defence against pathogenic organisms. Twenty putative antischistosomal AMPs were identified using an in silico mathematical algorithm, Hidden Markov Models (HMMER) but of which six were selected based on their E-values for further exploration. Physicochemical parameters of these six AMPs were computed and their 3D structures were determined using the Iterative Threading ASSEmbly Refinement (I-TASSER) server. Subsequently, the STITCH database was queried to retrieve novel Schistosoma proteins that can potentially serve as targets for the identified AMPs. Glycosyltransferase and Axonemal dynein intermediate chain protein were identified as the novel druggable target proteins. Thereafter, the physicochemical characterization and prediction of the 3D structural elements of the aforementioned proteins were carried out as well. Finally, PatchDock was used to dock the 3D structures of the putative antischistosomal AMPs against the 3D structures of the druggable proteins. Overall, TAK3 showed a good binding affinity with glycosyltransferase and TAK6 displayed the highest binding affinity with axonemal dynein intermediate chain.*emphasized text*

HPC content

This research work was carried out using various bioinformatics software that requires high performance computers with high speed processors. Various tools and servers employed in this study used are Ubuntu (LINUX kernel), Hidden Markov Model, Stitch database, ExPASy, I-TASSER and PatchDock.

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