Contribution ID: **76** Type: **Poster (sponsored)**

Hidden Markov Model, site-directed mutagenesis and molecular docking of antimicrobial peptides towards discovery of potent Schistosome inhibitors

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 both tropical and sub-tropical regions of the world. Morbidity and mortality attributed to this disease are very high with about 240 million people infected, 800 million persons at risk of the infection and an approximately 280,000 deaths occurring annually. With the exponential increase in morbidity and mortality resulting from Schistosomiasis, there is an urgent need for the development of new drug since studies have shown that schistosomes are becoming resistant to the widely accepted first-line drug-of-choice Praziquantel. Therefore, the present study describes the exploration of broad-spectrum therapeutic potentials of Antimicrobial peptides (AMPs) in the design of alternative anti-schistosomal treatment regimen. AMPs are natural antibiotics produced by all living species; they have multifunctional properties and are currently explored as a vital source for the development of new drugs. In this study, six putative AMPs (TAK1-TAK6) were identified to possess very strong anti-schistosomal capabilities using Hidden Markov Model. Added to this, glycosyltransferase and axonemal dynein intermediate chain schistosomal proteins were identified using in silico methods as vital proteins for the survival of the parasite in the host. Site-directed mutagenesis studies based on the putative anti-schistosomal AMPs was carried out to increase their biological activities; homology modelling of the mutated AMPs using I-TASSER showed they are identical to the parental AMPs. More so, results from molecular docking using PatchDock showed that these mutated AMPs are capable of interacting with the schistosome proteins. In conclusion, based on the strong interactions between the mutated AMPs and the schistosomal proteins, we propose that these peptides maybe potential "drug leads" in the design and development of alternative schistosomal therapy and could as well prove effective against PZQ-resistant schistosome strains.

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.

Presenter Biography

Raphael Aruleba, an advocator for human and render selfless service most especially in the field of science to humanity. I have always had passion to learn more, to know a little about everything and more importantly in assisting people achieve their desired goals. Growing up I envisioned making positive impact on many people as possible, which ultimately led me to discovery of anti-microbial peptides that can be used in tackling Schistosomiasis using various bioinformatics techniques. I have also used ULBP2 to study cancer cells and Ganoderma lucidum to inhibit the growth of Plasmodium berghei in mice.

Primary author: Mr ARULEBA, Raphael Taiwo (University of Zululand)

Co-authors: Dr TINCHO, Marius (University of the Western Cape); Dr OYINLOYE, Babatunji Emmaunel (Afe Babalola University, Ado-Ekiti, Nigeria); Dr PRETORIUS, Ashley (University of the Western Cape); Prof. KAPPO, Abidemi Paul (University of Zululand)

Presenter: Mr ARULEBA, Raphael Taiwo (University of Zululand)

Session Classification: Poster session

Track Classification: Bioinformatics and Biological Sciences