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Investigation of the interaction between selected divalent cations and the novel Schistosoma mansoni Universal stress protein G4LZI3.

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Schistosomiasis, despite several eradication and elimination attempts, still represents one of the most debilitating parasitic diseases of poverty amongst all the Neglected Tropical Diseases. Economically challenged countries bear the full brunt of the disease, coupled with those of other diseases of public health importance such as malaria, HIV/AIDS and tuberculosis. Praziquantel (PZQ), a first-line treatment drug has been in use for the last three decades, but has recently showed traces of drug resistance, hence alternative treatment regimen becomes a priority. Universal stress proteins have been postulated to be upregulated in the Schistosoma worm in response to hazardous environmental conditions. More so, three divalent cations have been postulated to play a role in the mechanism of action of PZQ in bringing about therapeutic response against schistosomiasis. Therefore, this study was aimed at investigating the interaction between these divalent cations and a novel Usp G4LZI3 protein that has been hypothesized as a possible vaccine candidate. Bioinformatics was used to predict the secondary structure of the protein, and to generate a 3D model of the protein before the cations were docked against the G4LZI3 protein. These in silico results were then validated using Isothermal Titration Calorimetry, by titrating the divalent cations against purified and concentrated fractions of the protein. Preliminary results confirmed Ca2+, Mg2+ and Zn2+ as putative ligands and additionally identified ATP and AMP as possible interacting molecules. However, biophysical studies only showed interaction between Mg2+ and the novel G4LZI3 protein. These results provide prospects for future studies towards anti-schistosomal drug development.

HPC content

This study makes use of various computer programs in modelling protein structure and docking studies of protein-protein and protein-ligand studies. Various computational and mathematical models employed required high performance computing to achieve results. Computers with high speed processing capacity were used in this study and further study in the design of anti-schistosomal drugs will require high speed computers.

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