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Interaction between S. mansoni Universal stress G4LZI3 protein and selected polyphenols: a bioinformatics investigation.

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For decades, Praziquantel has been the undisputed drug of choice against schistosomiasis; a disease that affects more than 200 million people in over 78 countries and responsible for over 280 000 lives lost per annum, predominantly in sub-Saharan Africa. Rising concerns have been raised due to the unknown mechanism of action of the drug and unavoidable reports of the emergence of drug resistant strains. Moreover, current apprehension has been reinforced by the total dependence on a single drug for treatment. Therefore, the search for novel and effective anti-schistosomal drugs become imperative. This study made use of bioinformatics tools to determine the binding properties of a selective range of polyphenols docked onto the Universal stress G4LZI3 protein, a recently identified 'lead' molecule in the design of alternative treatment drug against schistosomiasis. Schistosomes have over several years, evolved mechanisms that include the presence of USPs, to counter biotic and abiotic stress. Up-regulation of the G4LZI3 protein throughout the multifaceted developmental cycle of the schistosome worm sparks interest in this protein, whose function is currently unknown. Ten polyphenols were docked onto the G4LZI3 protein; the best five complexes were selected for post-molecular dynamics analyses and binding free energy calculations. The strongest binding interactions were observed between the G4LZI3 protein with curcumin and catechin respectively. The major interacting residues conserved in all the complexes provides basis for further structure-based drug design of new compounds, with enhanced inhibitory potency and toxicity against G4LZI3. This study suggests an alternative approach for the development of anti-schistosomal drugs using natural compounds.

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