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Molecular simulations of the interaction between Schistosoma mansoni axonemal dynein intermediate chain protein and dynarrestin

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Praziquantel (PZQ) has been the drug of choice for the treatment of schistosomiasis for more than 30 years. Resistance to this drug, however, has been documented severally in recent years, hence the need for effective alternatives. This study investigated the effect of an inhibitor (dynarrestin) on the identified Schistosoma mansoni axonemal dynein intermediate protein (SmAxDynIC), a potential schistosome drug target. The protein functions in schistosome cilia and flagella beating; therefore inhibiting this protein could lead to the immobility of the worm and disrupt its developmental cycle. Molecular dynamic simulations and post-MD analyses were conducted to ascertain the various characteristics of the inhibitor and its interaction with the SmAxDynIC. This was followed by the screening for a pharmacophore of the inhibitor to discover 'lead' compounds against schistosomiasis. Concluding findings of this study indicated that dynarrestin exhibits ample inhibitory characteristics against the SmAxDynIC, as well as a very strong binding affinity for the active site of the modelled axonemal dynein protein. Three additional ligands were identified using the pharmacophore and it is suggested that these will be employed for in vivo testing on various schistosomal cell lines in future interaction studies.

Keywords: Praziquantel; Schistosomiasis; Schistosoma mansoni; dynarrestin; SmAxDynIC

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