

Comparative Analysis of Selected Anticestodal Drugs Against the Fatty Acid-Binding Protein of the Zoonotic Cestode *Echinococcus Granulosus* Using Molecular Docking

Garg Saumya¹, Deepika Km², Chaudhary Anshu³ and Sharma Bindu^{4*}

Department of Zoology, Chaudhary Charan Singh University, Meerut, India 250004

*Corresponding author: Bindu Sharma
Email Id: dr.bindusharmazooology@gmail.com

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ABSTRACT

Cystic echinococcosis is a medically and economically important zoonotic disease caused predominantly by the larval stage of *Echinococcus granulosus*. The development of new or repurposed therapeutic strategies requires identification of parasite proteins that are essential for nutrient acquisition and survival. Fatty acid-binding proteins are attractive molecular targets because cestodes have limited capacity for de novo fatty-acid synthesis and depend substantially on host-derived lipids. In the present in silico study, the interaction of two established anticestodal drugs, albendazole and praziquantel, with the fatty acid-binding protein of *E. granulosus* was investigated using molecular docking. The experimentally determined protein structure with PDB identifier 1O8V was retrieved from the Protein Data Bank, while ligand structures were obtained from PubChem. Docking was performed using the SwissDock web server, and the resulting complexes were inspected in PyMOL. Both compounds occupied the predicted FABP binding cavity. Albendazole produced the more favorable docking score of -6.456 kcal/mol, whereas praziquantel produced a score of -4.988 kcal/mol. The difference between the best scores was 1.468 kcal/mol in favor of albendazole. These findings indicate a stronger predicted interaction between albendazole and FABP under the computational conditions used in this study. However, docking scores are estimates rather than direct measurements of inhibition, and they do not account fully for protein flexibility, solvation, metabolism, bioavailability, or host-parasite pharmacology. Therefore, albendazole should be considered a promising preliminary candidate for further FABP-focused investigation, rather than a confirmed FABP inhibitor.

Keywords: *Echinococcus granulosus*, cystic echinococcosis, fatty acid-binding protein, molecular docking, Swiss Dock.

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INTRODUCTION

Parasitic helminths continue to represent a major challenge to global public health and livestock production, particularly those with zoonotic transmission cycles involving domestic animals and humans. Among these parasites, *Echinococcus granulosus* is the etiological agent of cystic echinococcosis (CE), a neglected tropical disease that causes significant morbidity, mortality, and economic losses worldwide (Ammann & Eckert, 1996; Thompson, 2023; Staudacher et al., 2026). The parasite is maintained through a dog-livestock transmission cycle, with canids serving as definitive hosts and herbivorous animals such as sheep, goats, cattle, and camels acting as intermediate hosts. Humans acquire infection accidentally by ingesting eggs shed in the feces of infected dogs, resulting in the formation of hydatid cysts, primarily in the liver and lungs (Bowman et al., 2006; Craig et al., 2015).

Cystic echinococcosis (CE), commonly known as hydatid disease, is a neglected zoonotic infection caused

predominantly by the larval stages of the *Echinococcus granulosus* species complex. The disease has a worldwide distribution and is particularly associated with pastoral and livestock-rearing communities where close contact between dogs and domestic herbivores facilitates transmission. Human infection occurs accidentally through ingestion of infective eggs released in the faeces of definitive hosts, principally dogs. Following ingestion, the oncospheres penetrate the intestinal wall, enter the circulation and develop predominantly into hydatid cysts in the liver and lungs, although other organs may also be affected. The prolonged and frequently asymptomatic development of these cysts can delay diagnosis and allow considerable pathological changes before clinical disease becomes apparent (Thompson, 2023; WHO, 2021, 2025).

The epidemiology of CE is closely linked to the complex life cycle of *E. granulosus*. Adult parasites inhabit the small intestine of definitive canid hosts, whereas larval development occurs in suitable intermediate hosts such as

*Author for Correspondence: dr.bindusharmazooology@gmail.com

sheep, goats, cattle and other livestock. Humans function as accidental intermediate hosts and generally represent a dead-end host in the transmission cycle. The maintenance of this parasite between domestic animals and dogs makes CE not only a medical problem but also an important veterinary and socioeconomic concern. Recent epidemiological analyses continue to demonstrate a substantial global burden, with considerable variation among geographical regions and a particularly persistent impact in resource-limited and endemic settings (Craig et al., 2015; Wang et al., 2025; Staudacher et al., 2026). The World Health Organization estimates that more than one million people are affected by echinococcosis at any given time, while the disease is associated with substantial healthcare expenditure and losses to livestock production (WHO, 2021).

The clinical manifestation of CE depends largely on the location, size and developmental stage of the hydatid cyst. The liver is the most frequently affected organ, followed by the lungs, while cysts may occasionally occur in the spleen, kidneys, bones, muscles and central nervous system. Because cyst development can remain clinically silent for several years, patients may present only after the cyst has enlarged sufficiently to cause pressure-related or organ-specific symptoms. Complications may include cyst rupture, secondary infection, allergic reactions and recurrence following treatment. Consequently, the management of CE requires careful assessment of cyst characteristics and disease stage rather than reliance on a single therapeutic approach (WHO, 2021; Kuehn et al., 2024; Staudacher et al., 2026).

Current management of CE includes surgical intervention, percutaneous procedures, pharmacological therapy and, in selected patients, a watch-and-wait strategy. Treatment selection depends on cyst stage, anatomical location, size, complications and available clinical expertise. Benzimidazole compounds, particularly albendazole, constitute an important component of pharmacological management and are also used in association with invasive procedures. Praziquantel is another established antiparasitic compound with activity against cestodes and may be used as an adjunct in selected clinical settings. Nevertheless, chemotherapy does not always result in complete elimination of the parasite, and prolonged administration can be associated with adverse effects and variable therapeutic responses. The continuing need for stage-specific and effective treatment strategies highlights the importance of identifying additional molecular vulnerabilities in *E. granulosus* (Craig et al., 2015; Kuehn et al., 2024; WHO, 2025).

An important characteristic of cestode biology is their dependence on host-derived nutrients. Unlike many free-living organisms, cestodes have a highly specialized metabolism and rely extensively on the host for essential metabolites, including lipids. Fatty acids are required for membrane formation, energy metabolism, cellular signaling and maintenance of parasite tissues. The limited capacity of cestodes for endogenous fatty-acid synthesis therefore

makes the acquisition, transport and utilization of host lipids particularly important for parasite survival and development. This metabolic dependence provides an opportunity to investigate lipid-associated proteins as potential molecular targets for antiparasitic drug development (Alvite et al., 2001; Esteves & Paulino Zunini, 2013; Pórfido et al., 2020).

Fatty acid-binding proteins (FABPs) constitute a family of relatively small intracellular lipid-binding proteins that participate in the binding, intracellular transport and intracellular distribution of fatty acids and other hydrophobic molecules. In parasitic helminths, FABPs have attracted considerable attention because of their association with lipid acquisition and metabolism in organisms that depend strongly on host-derived lipids. *E. granulosus* possesses multiple FABP-related proteins, reflecting the importance and diversification of this protein family within the parasite. Among these proteins, *E. granulosus* fatty acid-binding protein 1 (EgFABP1) has been structurally and biochemically characterized and has demonstrated the ability to bind fatty-acid ligands. The presence of a hydrophobic ligand-binding cavity and its involvement in lipid handling make EgFABP1 an attractive candidate for structure-based investigation (Alvite et al., 2001; Jakobsson et al., 2003; Pórfido et al., 2020).

The structural characterization of EgFABP1 has further strengthened the possibility of investigating this protein through computational approaches. The experimentally determined three-dimensional structure of *E. granulosus* FABP1 is available in the Protein Data Bank under PDB accession 1O8V. Structural information of this type provides an opportunity to examine the spatial characteristics of the ligand-binding cavity and to investigate whether pharmacologically relevant small molecules can theoretically be accommodated within the protein. Such structural approaches are particularly useful for parasite targets for which experimental screening may be technically demanding or resource intensive (Jakobsson et al., 2003; Burley et al., 2017).

The study by Jakobsson et al. (2003) provided important structural insights into the fatty-acid-binding protein 1 (EgFABP1) of *Echinococcus granulosus*. The experimentally determined crystal structure revealed a characteristic β -barrel architecture containing an internal ligand-binding cavity capable of accommodating fatty acids such as palmitic acid. The presence of a defined binding pocket and conserved residues involved in ligand recognition highlights the functional importance of EgFABP1 in the parasite's lipid metabolism. These structural features provide a valuable basis for investigating EgFABP1 as a potential molecular target. In the present study, this experimentally resolved structure was therefore utilized for molecular docking analysis to explore its interactions with selected anthelmintic compounds and to assess their potential binding within the protein's ligand-binding cavity (Jakobsson et al., 2003).

Molecular docking is a widely used structure-based computational technique for investigating the possible interaction of small molecules with biological macromolecules. The method evaluates different orientations and conformations of a ligand within a predicted binding region and uses scoring functions to estimate the relative favorability of the resulting complexes. Although docking scores cannot directly establish biochemical inhibition or clinical efficacy, comparative docking can be useful for prioritizing compounds and generating testable hypotheses for subsequent experimental studies. Web-based platforms such as SwissDock have facilitated the application of molecular docking in biological and pharmaceutical research by providing computational workflows for protein–small-molecule interaction analysis (Grosdidier et al., 2011; Morris & Lim-Wilby, 2008; Bugnon et al., 2024).

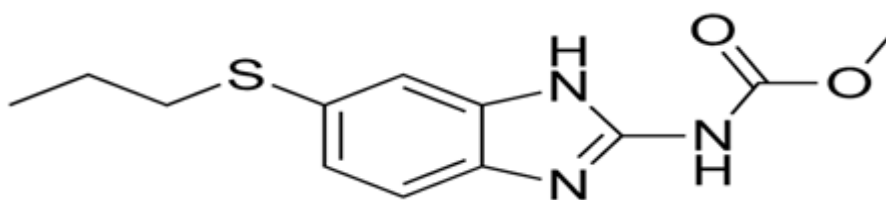
Computational investigation of established antiparasitic drugs against previously characterized parasite proteins may also provide a preliminary framework for drug repurposing. Albendazole and praziquantel are already recognized as important antiparasitic compounds, but their principal pharmacological actions involve molecular targets other than FABP. Albendazole is primarily associated with disruption of parasite microtubule formation through interaction with β -tubulin, whereas praziquantel produces characteristic effects on parasite calcium homeostasis and neuromuscular function. Investigating whether these compounds can additionally interact with a lipid-binding protein such as EgFABP1 may therefore provide insights into possible secondary molecular interactions or previously unexplored target associations (Chambers et al., 2010; Nogueira et al., 2022).

Despite the recognized importance of lipid metabolism in cestodes and the availability of a solved structure for *E. granulosus* FABP1, comparative assessment of established anticestodal drugs against this specific protein remains relatively limited. In particular, the relative docking behaviour of albendazole and praziquantel toward

EgFABP1 has not been sufficiently explored as a preliminary target-based comparison. Such an analysis may help determine whether these compounds can be accommodated within the FABP binding cavity and whether their predicted interaction scores differ under comparable computational conditions. Importantly, a docking-based comparison should be interpreted as a hypothesis-generating approach rather than direct evidence of target inhibition.

Despite considerable advances in diagnosis and clinical management, cystic echinococcosis remains difficult to control because of its chronic nature, complex life cycle, and dependence on both veterinary and public health interventions. Current treatment strategies include surgery, percutaneous techniques, and chemotherapy using benzimidazole derivatives such as albendazole, while praziquantel is commonly administered as an adjunct antiparasitic drug (Figure 1) (Kuehn et al., 2024; WHO, 2025). However, prolonged treatment, drug-associated adverse effects, incomplete parasite elimination, and recurrence continue to limit therapeutic success, emphasizing the need to identify novel molecular targets for improved intervention (Buttenschoen & Carli Buttenschoen, 2003; Craig et al., 2015).

Therefore, the present study was designed to investigate the predicted interaction of two established anticestodal drugs, albendazole and praziquantel, with the fatty acid-binding protein of *E. granulosus* using molecular docking. The experimentally determined EgFABP1 structure (PDB ID: 1O8V) was used as the receptor, while the selected drugs were evaluated under comparable computational conditions using SwissDock. The resulting ligand–protein complexes were subsequently visualized using PyMOL. By comparing the predicted docking scores and binding orientations of the two compounds, this study aims to provide a preliminary structural assessment of their potential interaction with EgFABP1 and to identify a candidate for further FABP-focused biochemical and parasite-based investigation.



Albendazole

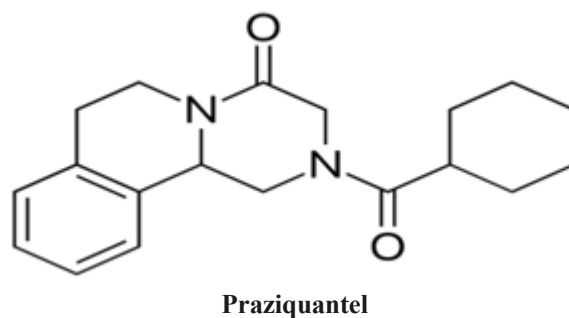


Figure 1: Chemotherapeutics for clinical management of cystic echinococcosis.

Cestodes lack the ability to synthesize fatty acids *de novo* and therefore rely extensively on host-derived lipids for their survival and development. Fatty acid-binding proteins (FABPs) are small intracellular lipid-binding proteins responsible for the uptake, transport, storage, and intracellular trafficking of long-chain fatty acids and other hydrophobic ligands. Among them, *E. granulosus* fatty acid-binding protein-1 (EgFABP1) has been identified as a highly conserved protein with strong affinity for fatty acids, suggesting an essential role in parasite metabolism and making it an attractive candidate for therapeutic targeting (Alvite et al., 2001; Jakobsson et al., 2003; Pórfido et al., 2020).

Recent developments in structural bioinformatics have made structure-based drug discovery an effective approach for identifying potential drug–target interactions. Molecular docking enables the prediction of ligand binding orientation and affinity within a target protein, thereby facilitating the

rapid screening and comparison of candidate compounds before experimental validation (Xia, 2017; Morris & Lim-Wilby, 2008). The availability of experimentally determined three-dimensional protein structures in the Protein Data Bank (PDB) has further strengthened the application of computational approaches in antiparasitic drug research (Burley et al., 2017).

MATERIALS AND METHODS

Retrieval of the target protein

The three-dimensional crystal structure of the *E. granulosus* fatty acid-binding protein was retrieved from the RCSB Protein Data Bank using PDB identifier 1O8V (Figure 2). The structure was downloaded in PDB format and used as the receptor for docking. The target belongs to the lipid-binding protein family and was selected because of its established role in fatty-acid binding and its relevance to parasite metabolism.

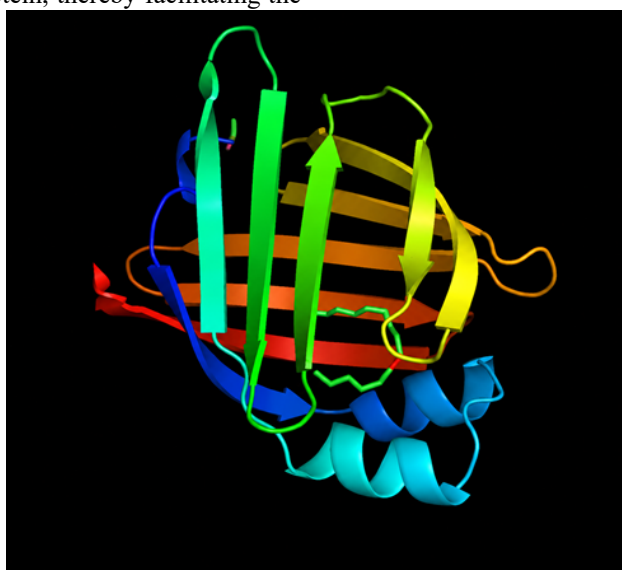


Figure 2: Three-dimensional structure of *Echinococcus granulosus* fatty acid-binding protein (FABP) shown in cartoon representation using PyMOL.

Selection and retrieval of ligands

Albendazole and praziquantel were selected as representative anticestodal drugs. Albendazole is a benzimidazole-derived anthelmintic widely used to manage cystic echinococcosis. Praziquantel is an established cestocidal drug used against a broad range of tapeworm

infections. The molecular structures of the compounds were retrieved from PubChem and prepared in formats compatible with the docking workflow.

Receptor and ligand preparation

The retrieved protein structure was inspected before docking. Ligand structures were checked and converted as required by the docking platform. The receptor and ligand files were then uploaded separately for docking. In the present project, docking was conducted using the standard settings available through SwissDock. The analysis therefore represents a comparative screening experiment performed under the same general computational conditions for both compounds.

Molecular docking using SwissDock

Molecular docking was performed with SwissDock, a web-based protein–small-molecule docking service that uses an AutoDock-based search and scoring workflow (Grosdidier et al., 2011; Bugnon et al., 2024). Multiple ligand poses were generated for each compound. The best-ranked pose was selected according to the reported calculated affinity. The principal comparison was based on the most negative docking score obtained for each drug. The best score was treated as the most favorable predicted interaction among the poses generated for that ligand.

Visualization and interpretation

The docked complexes were visualized in PyMOL using cartoon representation. Visualization was used to confirm that each ligand was positioned within the protein cavity and to inspect its spatial orientation relative to the receptor. The interpretation focused on comparative docking score and overall accommodation of the ligands. No claim of experimentally verified hydrogen-bonding, inhibition, or parasite killing was made solely from the visualization.

RESULTS

Docking scores

Both selected drugs generated docked complexes with the FABP receptor. Albendazole showed the most favorable calculated affinity, with a best docking score of -6.456 kcal/mol. Praziquantel also docked successfully, but its best score was less negative at -4.988 kcal/mol. The difference between the two best scores was 1.468 kcal/mol, indicating a stronger predicted interaction for albendazole under the scoring conditions used.

Table 1. Comparison of the best Swiss Dock docking scores obtained for the two selected drugs against *E. granulosus* FABP.

Drug	Best Docking Score (kcal/mol)	Relative Interpretation
Albendazole	-6.456	More favorable predicted binding
Praziquantel	-4.988	Less favorable predicted binding

Structural visualization of the complexes

The docked complexes of Fatty Acid Binding Protein (FABP) with Albendazole and Praziquantel were visualized using PyMOL Molecular Graphics System. The protein structure was displayed in cartoon representation, while the docked ligand was represented as a stick model to illustrate

its binding orientation within the predicted binding pocket. The final images were generated in PyMOL for graphical representation of the docking results (Figure 3 and Figure 4). However, the less negative score obtained for praziquantel suggests that the predicted interaction was weaker than the albendazole–FABP interaction under the same computational comparison (Figure 5).

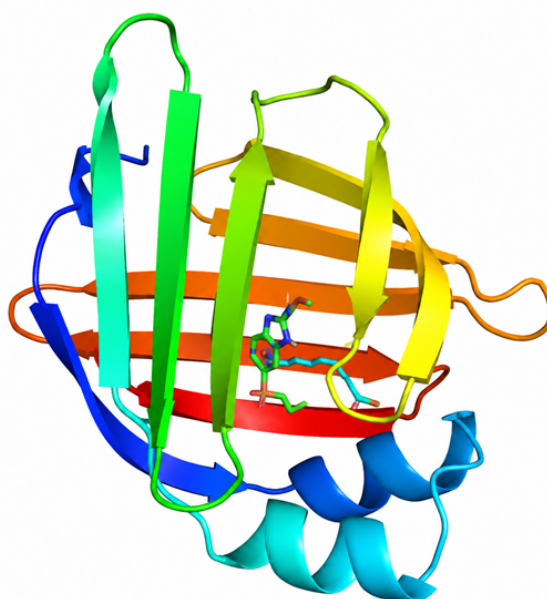


Figure 3: Cartoon representation of the Albendazole–FABP docked complex visualized using PyMOL. Albendazole is shown in stick representation within the predicted binding pocket.

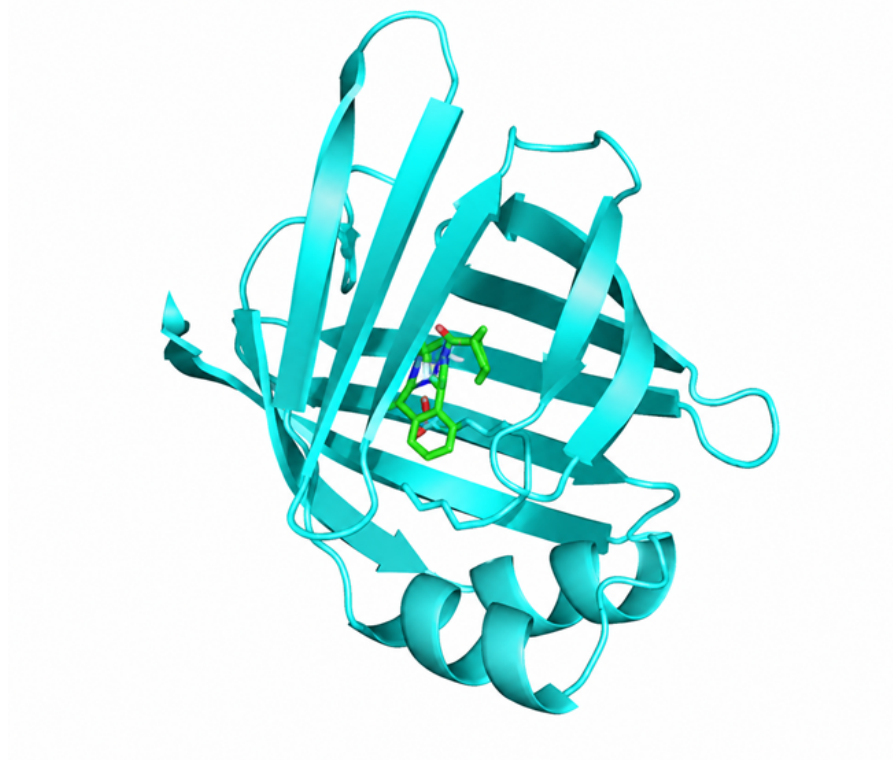


Figure 4: Molecular docking pose of Praziquantel within the predicted binding pocket of FABP visualized using PyMOL. The protein is shown as a cartoon model and the ligand as a stick model.

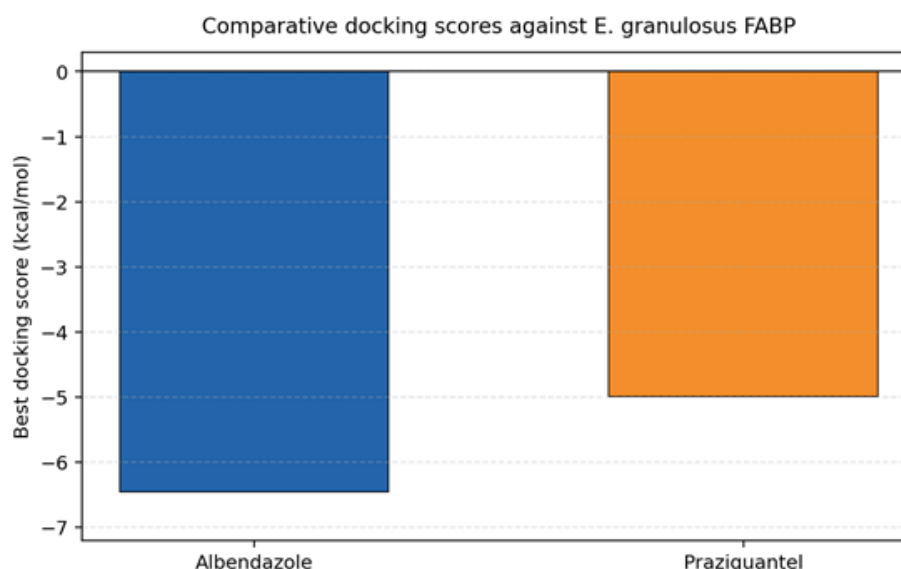


Figure 5. Comparative visualization of the reported best docking scores. More negative values indicate more favorable predicted binding in the docking score model.

DISCUSSION

This study compared two established anticestodal drugs against a parasite lipid-binding protein using molecular docking. Among these selected drugs, albendazole has a well-established activity by selective binding to the beta-tubulin subunit of the microtubules in parasites. It blocks the assembly of tubulin dimers into microtubules, disrupts

the structure of the cell, inhibits cell division and blocks absorption of glucose. Thus, depleted adenosine triphosphate causes death of the parasite (Chambers et al., 2010; Jacob et al., 2022). Praziquantel antagonizes voltage-gated Ca^{2+} channels, causing uncontrolled influx of Ca^{2+} ions, leading to uncontrolled muscle contraction and paralysis. Some studies also suggest role of myosin

regulatory light chains, glutathione-S-transferase, transient receptor potential channels and promoting immunoregulatory pathways (Thomas and Timson, 2020; Nogueira et al., 2022). Here molecular docking against parasitic FABPs will help to derive its potential to interact or inhibit FABPs as parasites are reliable on host fatty acids and to understand their spectrum of efficacy. The central result was that both compounds were predicted to interact with the *E. granulosus* FABP, but albendazole produced the more favorable best docking score. Albendazole scored -6.456 kcal/mol, compared with -4.988 kcal/mol for praziquantel. Within the limits of the scoring function, this difference supports the prioritization of albendazole for further investigation against FABP.

The biological rationale for selecting FABP is based on the nutritional physiology of cestodes. *E. granulosus* develops in a host environment and depends on uptake and utilization of host-derived nutrients. FABPs may help distribute fatty acids to membranes, metabolic enzymes, and signaling pathways. Disruption of this process could influence parasite growth and survival. The presence of a defined hydrophobic cavity also makes FABP suitable for structure-based screening of small molecules.

The stronger predicted interaction of albendazole may reflect a more favorable fit between the ligand and the physicochemical environment of the FABP cavity. Albendazole contains a benzimidazole ring system and polar functional groups that may support a combination of hydrophobic and polar contacts. Praziquantel has a different, more conformationally complex scaffold and may adopt an orientation that is less favorable according to the docking score. These explanations are hypotheses based on the computational result and should not be interpreted as a definitive mechanism without residue-level interaction analysis and experimental testing.

The result is also relevant to drug repurposing. Both albendazole and praziquantel are already associated with antiparasitic treatment, but their primary pharmacological targets are not necessarily FABP. A docking signal against FABP could therefore indicate an additional interaction, a possible off-target effect, or simply a favorable fit that does not translate into functional inhibition. The present study cannot distinguish between these possibilities. It only establishes a comparative structural hypothesis that can guide subsequent experiments.

Several limitations should be considered. First, molecular docking commonly treats the receptor as relatively rigid, whereas proteins are dynamic and may undergo induced-fit movements. Second, docking scores approximate binding free energy and may not reproduce the effects of solvent, entropy, metal ions, protonation states, or alternative protein conformations. Third, the study used one target structure and one principal score for each drug. Re-docking with alternative receptor conformations, consensus scoring, molecular dynamics simulations, and free-energy calculations would provide a more robust assessment. Fourth, the analysis did not evaluate absorption,

distribution, metabolism, excretion, toxicity, or drug concentration at the parasite site.

The biological significance of the docking result must therefore be tested experimentally. Recombinant EgFABP1 binding assays could determine whether albendazole and praziquantel bind directly to the purified protein. Competitive fluorescence assays using a fatty-acid probe could assess whether either drug displaces a native ligand. Enzyme-like functional assays, although FABP is a carrier rather than a classical enzyme, could examine effects on fatty-acid transfer. In vitro assays with protoscoleces or cultured parasite material could then determine whether the compounds alter viability or development at pharmacologically relevant concentrations. Finally, in vivo studies would be required to establish therapeutic relevance.

CONCLUSION

The present molecular docking study provides a comparative assessment of albendazole and praziquantel against the fatty acid-binding protein of *E. granulosus*. Both drugs were successfully accommodated in the predicted FABP binding cavity. Albendazole showed the more favorable docking score of -6.456 kcal/mol, while praziquantel showed a score of -4.988 kcal/mol. The 1.468 kcal/mol difference favors albendazole and identifies it as the stronger preliminary candidate for FABP-focused follow-up studies. These results are computational predictions and should not be equated with confirmed inhibition or superior clinical efficacy. Biochemical binding studies, molecular dynamics, parasite-based assays, and in vivo validation are required before drawing therapeutic conclusions.

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Competing interests

The author declares no competing interests.

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