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Molecular docking and i*n silico* assessment of phytochemicals as potential antifilarial agents against *Wuchereria bancrofti*

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Abstract

Wuchereria bancrofti's effects were first mentioned in ancient writings. Elephantiasis is the name given to the disease by ancient Greek and Roman writers because they observed similarities between the thickened, cracked skin and enlarged limbs of infected individuals, similar to those of elephants. The infection may progress to lymphatic filariasis if treatment is not received. Rarely, it can also result in tropical pulmonary eosinophilia. To effectively determine the binding affinities of selected phytochemicals against the proteins of *Wuchereria bancrofti* using molecular docking simuation. We determined the binding affinities of the phytochemicals against the protein of the Wuchereri bancrofti. About 6,500 phytochemicals obtained from Phytochemical databases were screened using DataWarrior based on Lipinski's Rule of Five and predicted toxicity parameters. A total of 1,700 compounds passed preliminary filtering and were prepared for molecular docking using AutoDock Vina. The 3D structure of the target protein with PDB code 84EF was downloaded from the protein data bank, it was prepared using pymol, USCF Chimera 1.10.1 and Autodock tools vs 1.5.6. The Reference ligand was also downloaded. They were prepared for molecular docking using Autodock tools vs 1.5.6. Validation of docking protocol and Molecular docking was done using Autodock vina 4.2.6 on linux operating system (ubuntu)-20.04. After the molecular docking, the front runners showed high binding affinity; swietenolide has the value -11.1 kcal/mol, Beta-methyl oleanate has the value -10.8 kcal/mol, Teucrin G has the value -10.5 kcal/mol, Tingenin B has the value -10.4 etc. Comparing all the phytochemicals, it can be seen that across all the receptors, swietenolide had more binding affinities followed by Beta-methyl oleanate, Teucrin G, Tingenin B and followed by others. Thus, it can be predicted that Swietenolide among others can be used in the treatment of Lymphatic Filariasis caused by *Wuchereria bancrofti*.

Keywords: *Wuchereria bancrofti*; Lymphatic filariasis; Phytochemicals; Molecular docking; *In silico* drug discovery; Drug-likeness

1. Introduction

Lymphatic filariasis is a neglected tropical disease caused by filarial nematodes, among which *Wuchereria bancrofti* remains the predominant etiological agent responsible for the majority of global infections [1]. Alongside *Brugia malayi* and *Brugia timori*, it infects the human lymphatic system and leads to significant morbidity in endemic regions [2]. The

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disease is transmitted through the bites of infected mosquito vectors, including species of *Aedes*, *Culex*, *Anopheles*, and *Mansonia*, making it a vector-borne parasitic infection of major public health concern [3]. It is estimated that over 120 million people are affected worldwide, particularly in tropical and subtropical regions such as sub-Saharan Africa, Asia, the Pacific Islands, and parts of South and Central America [4].

The life cycle of *W. bancrofti* involves both human and mosquito hosts, with humans serving as the definitive host and mosquitoes as intermediate hosts. Adult worms reside in the lymphatic vessels, where they produce microfilariae that circulate in the bloodstream. These microfilariae exhibit nocturnal periodicity, aligning with the feeding behavior of mosquito vectors and facilitating transmission [1, 5]. Following ingestion by a mosquito, the microfilariae develop into infective larvae, which are subsequently transmitted to a new human host during a blood meal. Over time, these larvae mature into adult worms within the lymphatic system, thereby sustaining the infection cycle [6].

Clinically, lymphatic filariasis progresses gradually, often beginning with asymptomatic or mild inflammatory responses before advancing to severe pathological manifestations. Early-stage infection may present with lymphatic inflammation, edema, and impaired circulation. Chronic infection can lead to lymphatic dysfunction, fibrosis, and permanent tissue damage, resulting in conditions such as lymphedema and elephantiasis, which are characterized by extreme swelling and skin thickening [7, 8]. These debilitating conditions significantly impact physical health and contribute to social stigma and reduced quality of life in affected populations.

Despite ongoing global efforts to eliminate lymphatic filariasis as a public health problem, complete eradication has not yet been achieved [3]. Current treatment strategies rely primarily on antifilarial drugs such as diethylcarbamazine and related chemotherapeutic agents, which are effective in reducing microfilarial load but are associated with limitations, including incomplete parasite clearance, potential adverse effects, and the risk of resistance with prolonged use [2, 4]. These challenges highlight the need for the development of safer, more effective, and sustainable therapeutic alternatives.

In recent years, medicinal plants have gained increasing attention as potential sources of novel bioactive compounds for the treatment of parasitic diseases. Phytochemicals, which are naturally occurring secondary metabolites in plants, possess diverse pharmacological properties, including antiparasitic, anti-inflammatory, and immunomodulatory activities [9,10,11]. Several studies have demonstrated the potential of plant-derived compounds in combating lymphatic filariasis, supporting their relevance in drug discovery [12].

Advances in computational approaches, particularly molecular docking, have significantly enhanced early-stage drug discovery by enabling the prediction of interactions between bioactive compounds and target proteins. Molecular docking provides valuable insights into binding affinity, molecular interactions, and the potential efficacy of candidate compounds, thereby reducing the time and cost associated with conventional experimental methods [13,14,15]. This approach has been widely applied in identifying potential inhibitors against parasitic targets and continues to play a critical role in modern pharmacological research.

Therefore, this study aims to evaluate the potential inhibitory activity of selected phytochemical compounds against *Wuchereria bancrofti* using an *in silico* molecular docking approach, with the objective of identifying promising lead compounds for the development of novel therapeutic agents against lymphatic filariasis.

2. Materials and Methods

2.1. Study Design and Materials

An *in silico* approach was employed to evaluate the interaction between selected phytochemical compounds and *Wuchereria bancrofti* target proteins. The materials and tools used in this study included a personal computer running a Linux operating system (Ubuntu desktop) alongside Windows 10, Open Babel, UCSF Chimera, PyMOL, AutoDockTools (version 1.5.6), AutoDock Vina (version 1.1.2), DataWarrior software, and the Protein Data Bank (PDB) database (http://www.rcsb.org/). Phytochemical compounds were obtained from the Phytochemical database (version 1.4). Additional supporting files used during the docking process included configuration files (conf.txt) and a Bash script (binbash.sh).

2.2. Bioinformatics Mining and Target Identification

Bioinformatics mining was conducted to identify suitable target proteins associated with *Wuchereria bancrofti*. The Protein Data Bank (PDB) was systematically searched using specific selection criteria, including the presence of a co-crystallized organic ligand, structural relevance to *W. bancrofti* pathogenesis, and overall suitability for molecular docking studies. In parallel, chemoinformatic mining was performed to retrieve phytochemical compounds from the Phytochemical database for further screening and analysis.

2.3. Selection and Preparation of Target Protein

Following a comprehensive search of the Protein Data Bank, the protein with PDB ID: 8E4F was selected as the target for this study. The protein has a resolution of 2.47 Å and contains ligands including folic acid (FOL), sodium ion, and nicotinamide adenine dinucleotide phosphate (NADP).

The selected protein structure was downloaded in PDB format and prepared using UCSF Chimera and AutoDockTools. In Chimera, duplicate chains were removed, retaining a single chain for analysis. The processed structure was saved as "Deleted 8E4F." All ligands except the reference ligand (FOL) were removed, and the structure was saved as "Deleted 8E4F + FOL." Subsequently, the reference ligand was separated to obtain the protein backbone, which was saved as "Filtered 8E4F."

The filtered protein structure was then imported into AutoDockTools, where polar hydrogens were added and Kollman charges were assigned. The prepared protein was finally saved in PDBQT format for molecular docking.

2.4. Selection and Preparation of Ligands

Ligand selection was based on specific criteria, including the requirement that compounds must be organic molecules capable of binding to the active site of the target protein. Binding interactions were initially assessed using visualization tools such as PyMOL and Chimera, leading to the selection of folic acid (FOL) as the reference ligand.

The reference ligand was obtained from the Protein Data Bank in Structure Data File (SDF) format. Phytochemical ligands were obtained from the *Phytochemical* database. Ligand preparation was carried out using Open Babel on Ubuntu and AutoDockTools on Windows 10.

All ligands were converted from SDF format to MOL2 format using Open Babel. The converted files were transferred to the Windows environment, where AutoDockTools was used to assign Gasteiger charges and define torsional flexibility by setting bonds as non-rotatable. The prepared ligands were then saved in PDBQT format for docking analysis.

2.5. Validation of Docking Protocol

The docking protocol was validated using AutoDockTools on a Windows 10 platform. The reference ligand, previously separated from the protein using Chimera, was reintroduced alongside the prepared protein structure. A grid box was defined to encompass the active binding site of the protein, ensuring accurate docking simulations.

The center coordinates and dimensions of the grid box were recorded to maintain consistency during docking. This step ensured proper identification of the binding site and confirmed that the docking parameters were suitable for subsequent molecular docking simulations.

Table 1 The Centre and Size of Grid Box used for molecular docking.

Gridbox	Center	Dimension
X	54.291	14
Y	15.762	12
Z	0.44	16

3. Results

A total of approximately 6,500 phytochemicals were retrieved from the phytochemical databases and subjected to preliminary screening using DataWarrior software based on Lipinski's Rule of Five. In addition, toxicity profiling was conducted to evaluate the safety characteristics of the compounds. Following this screening process, only compounds that satisfied the required physicochemical and toxicity criteria were selected for further analysis.

Subsequently, molecular docking was performed using the selected phytochemicals against the target protein (PDB ID: 8E4F). Binding affinities of the ligands were determined, and the results were compared with that of the reference ligand. The top-performing compounds were identified based on their binding energy values.

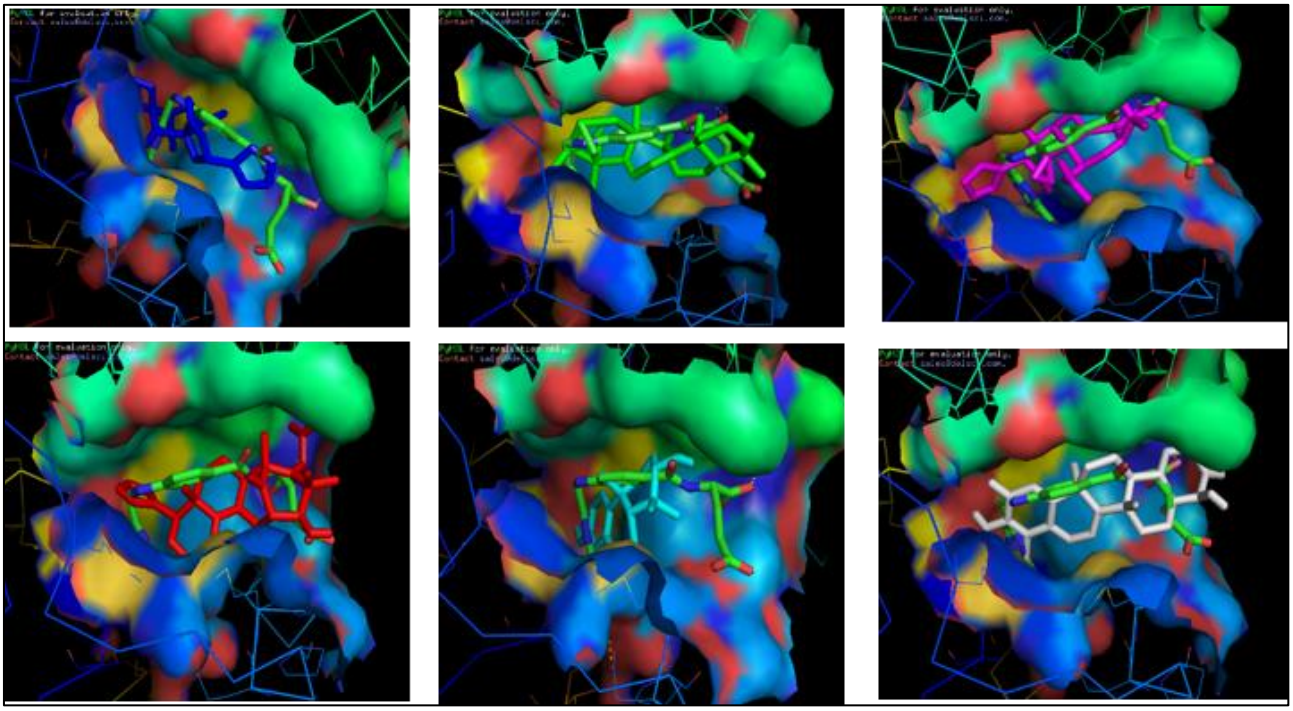
The results obtained after docking analysis are summarized in Table 2, which presents the top 20 phytochemicals with higher binding affinities compared to the reference ligand.

Table 2 Binding affinities of selected phytochemicals in complex with the target protein (8E4F)

S/N	Molecule Name	A1	A2	A3	A4	MEAN	STADV
1	Swietenolide	-11.1	-11.1	-11.2	-11.1	-11.1	0.0
2	beta-methyl oleanate	-10.8	-10.8	-10.8	-10.8	-10.8	0.0
3	teucrin G	-10.5	-10.5	-10.5	-10.5	-10.5	0.0
4	tingenin B	-10.4	-10.5	-10.4	-10.4	-10.4	0.0
5	Uguenensone	-10.4	-10.4	-10.4	-10.4	-10.4	0.0
6	Totaradiol	-10.3	-10.3	-10.4	-10.3	-10.3	0.0
7	abyssinoflavone V	-10.3	-10.3	-10.3	-10.3	-10.3	0.0
8	abyssinone I	-10.3	-10.3	-10.3	-10.3	-10.3	0.0
9	Teferidin	-10.3	-10.3	-10.3	-10.3	-10.3	0.0
10	Uncinatone	-10.3	-10.3	-10.3	-10.3	-10.3	0.0
11	quercetin 5-glucoside	-10.3	-10.2	-10.3	-10.3	-10.3	0.1
12	Foetidin	-10.3	-10.3	-10.2	-10.2	-10.3	0.1
13	farnesiferol A	-10.2	-10.2	-10.2	-10.2	-10.2	0.0
14	Fumariline	-10.2	-10.2	-10.2	-10.2	-10.2	0.0
15	Gummosin	-10.2	-10.2	-10.2	-10.2	-10.2	0.0
16	Rutamontine	-10.2	-10.2	-10.2	-10.2	-10.2	0.0
17	stemmin C	-10.1	-10.1	-10.2	-10.1	-10.1	0.0
18	Taxodione	-10.1	-10.1	-10.2	-10.1	-10.1	0.0
19	Coladonin	-10.1	-10.1	-10.1	-10.1	-10.1	0.0
20	Laudanine	-10.1	-10.1	-10.1	-10.1	-10.1	0.0
536	REFLIGAND	-8.3	-8.1	-8.3	-8.3	-8.3	0.1

The docking results showed that several phytochemicals exhibited strong binding interactions with the target protein, with binding affinity values ranging from -11.1 kcal/mol to -10.1 kcal/mol. The reference ligand demonstrated a comparatively lower binding affinity.

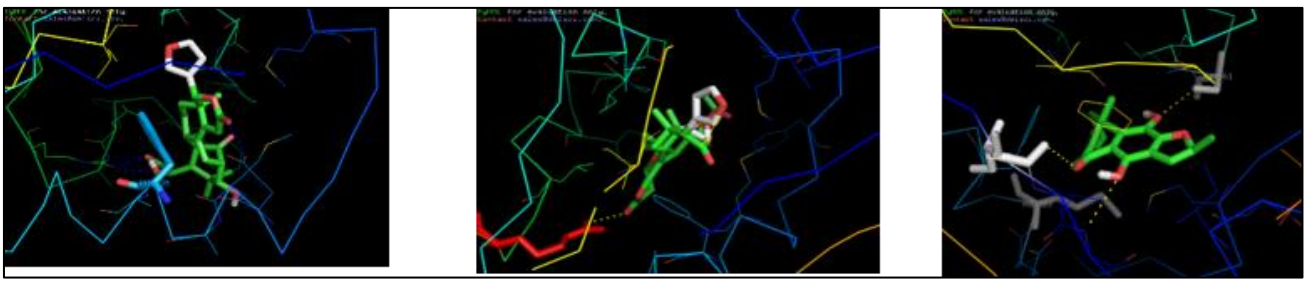
Visualization of ligand binding poses within the active site of the protein receptor is presented in Figure 1, illustrating how the selected phytochemicals interact within the binding pocket of the 8E4F protein.



(A: Beta-methyl oleanate, **B:** Teucrin G, **C:** Uguenensone, **D:** Swietenolide, **E:** Totaradiol **F:** Tingenin B **)**

Figure 1 Binding poses of selected phytochemicals within the active site of the 8E4F protein receptor

Further analysis of ligand–protein interactions revealed the involvement of key amino acid residues within the binding site. The interaction patterns between selected ligands and amino acid residues of the protein are shown in Figure 2.



(**A:** Swietenolide, **B:** Ugenensone, **C:** Uncinatone)

Figure 2 Interaction of selected phytochemicals with amino acid residues of the 8E4F protein

The identified interactions included van der Waals forces and hydrogen bonding with specific amino acid residues. Notably, phenylalanine (PHE-36) was observed to participate in van der Waals interactions, while arginine (ARG-72) formed hydrogen bonds. Additional interactions involved serine (SER-61), isoleucine (ILE-10), and methionine (MET-33), contributing to ligand stabilization within the binding site.

The physicochemical properties of the top-ranking phytochemicals were further analyzed, and the results are presented in Table 3.

Table 3 Molecular descriptors of selected phytochemical compounds

S\N	NAMES OF LIGANDS	CHEMICAL FORMULA	MW	Clogp	HBA	HBD
1	Swietenolide	C27H34O8	486.559	2.0421	8	2
2	beta-methyl oleanate	C30H47O2	439.701	4.8404	2	0
3	teucrin G	C20H22O8	390.387	-0.7429	8	2
4	tingenin B	C28H36O4	436.59	4.4475	4	2
5	Uguenensone	C28H34O8	498.57	2.2768	8	0
6	Totaradiol	C20H30O2	302.456	4.5175	2	2
7	abyssinoflavone V	C2OH18O5	338.358	3.5281	5	2
8	abyssinone I	C2OH18O4	322.358	3.8738	4	1
9	Teferidin	C22H30O3	342.477	4.6726	3	1
10	Uncinatone	C20H22O4	326.391	3.7363	4	2
11	quercetin 5-glucoside	C15H18O3	246.305	1.9554	3	0
12	Foetidin	C24H30O4	382.498	4.5462	4	1
13	farnesiferol A	C24H30O4	382.498	4.4305	4	1
14	Fumariline	C20H17NO5	351.357	3.4324	6	0
15	Gummosin	C24H30O4	382.498	4.4305	4	1
16	Rutamontine	C19H12O7	352.297	2.3651	7	1
17	stemmin C	C21H32O3	332.482	3.3965	3	2
18	Taxodione	C20H26O3	314.423	3.555	3	1
19	Coladonin	C24H30O4	382.489	4.4305	4	1
20	Laudanine	C20H25NO4	343.421	3.0988	5	1

The molecular descriptor analysis showed that the selected compounds possessed acceptable physicochemical properties, including molecular weight, lipophilicity (cLogP), hydrogen bond acceptors (HBA), and hydrogen bond donors (HBD).

In addition, toxicity profiling of the selected phytochemicals was conducted, and the results are summarized in Table 4.

Table 4 Toxicity profile of selected phytochemical compounds

S\n	Names of ligands	Mutagenicity	Tumogenicity	Effect on reproduction	Irritant effect	Nasty functions
1	swietenolide	None	None	None	None	None
2	beta-methyl oleanate	None	None	None	None	None
3	teucrin G	None	None	None	None	None
4	tingenin B	None	None	None	None	None
5	uguenensone	None	None	None	None	None
6	totaradiol	None	None	None	None	None

7	abyssinoflavone V	None	None	None	None	None
8	abyssinone I	None	None	None	None	None
9	teferidin	None	None	None	None	None
10	uncinatone	None	None	None	None	None
11	quercetin 5-glucoside	None	None	None	None	None
12	Foetidin	None	None	None	None	None
13	farnesiferol A	None	None	None	None	None
14	fumariline	None	None	None	None	None
15	gummosin	None	None	None	None	None
16	rutamontine	None	None	None	None	None
17	stemmin C	None	None	None	None	None
18	taxodione	None	None	None	None	None
19	coladonin	None	None	None	None	None
20	laudanine	None	None	None	None	None

The toxicity analysis indicated that all selected phytochemicals were predicted to be non-mutagenic, non-tumorigenic, non-irritant, and showed no adverse effects on reproduction.

4. Discussion

The identification of bioactive compounds with strong binding affinity and favorable drug-like properties is a fundamental step in the development of new therapeutic agents against parasitic infections such as lymphatic filariasis. *Wuchereria bancrofti*, the primary causative agent of this disease, continues to pose a significant public health challenge in endemic regions, largely due to its complex life cycle and long survival within the human host [1,4,7].

In the present study, approximately 6,500 phytochemicals retrieved from the Phytochemical databases were subjected to screening using Lipinski's Rule of Five to evaluate their suitability for oral drug development. Lipinski's criteria remain a widely accepted standard in predicting drug-likeness, particularly in relation to absorption and permeability. Compounds that exceed the thresholds of hydrogen bond donors, hydrogen bond acceptors, molecular weight, and lipophilicity are more likely to exhibit poor pharmacokinetic profiles [16,17]. The results obtained in Table 3 indicate that the selected front-runner compounds largely conform to these criteria, suggesting favorable physicochemical characteristics consistent with previously reported drug-like molecules.

The role of phytochemicals in drug discovery has gained considerable attention due to their structural diversity and biological activity. Natural products have historically contributed significantly to the development of antiparasitic drugs, and several plant-derived compounds have demonstrated promising activity against parasitic infections, including lymphatic filariasis [18,19]. This supports the rationale for exploring phytochemicals as potential inhibitors of *W. bancrofti* target proteins.

Toxicity assessment represents another critical phase in drug discovery, as candidate compounds must demonstrate acceptable safety profiles before advancing to experimental validation. Traditional toxicity testing using animal models is often limited by ethical concerns, high costs, and time constraints. As a result, *in silico* toxicology has emerged as an efficient alternative for early-stage toxicity prediction, enabling the identification and elimination of potentially harmful compounds prior to laboratory testing [20,21]. In this study, approximately 1,700 phytochemicals met the required screening criteria, and the toxicity results presented in Table 4 indicate that all selected front-runner compounds were non-mutagenic, non-tumorigenic, non-irritant, and showed no adverse effects on reproduction.

Molecular docking is a key component of structure-based drug design, allowing for the prediction of ligand–protein interactions and estimation of binding affinity. It provides insight into the stability and orientation of ligand–receptor complexes and plays a crucial role in identifying potential inhibitors [22]. Furthermore, understanding the molecular biology and functional mechanisms of parasitic nematodes enhances the identification of suitable drug targets, thereby improving the efficiency of structure-based drug discovery approaches .

The docking results revealed that the reference ligand exhibited a mean binding affinity of -8.2 kcal/mol. In contrast, the top 20 phytochemicals demonstrated significantly stronger binding affinities, ranging from -11.1 kcal/mol to -10.1 kcal/mol, as presented in Table 2. Binding affinity is commonly used as an indicator of interaction strength, where more negative values correspond to stronger and more stable ligand–protein interactions [22,23,24]. The superior binding energies observed among the selected phytochemicals suggest their potential as effective inhibitors of the target protein.

Visualization of ligand binding within the active site using PyMOL further confirmed that the phytochemicals were appropriately positioned within the binding pocket of the protein. The interaction analysis revealed that key amino acid residues contributed to ligand stabilization through both hydrophobic and polar interactions. Such interactions are essential for maintaining ligand stability within the binding site and enhancing inhibitory potential, which is critical in the development of effective antiparasitic agents.

Persistent transmission of lymphatic filariasis, even after mass drug administration programs, has been attributed to residual infections and the long lifespan of adult worms within the host [25,26]. These challenges further emphasize the need for alternative therapeutic strategies capable of targeting the parasite more effectively.

These findings may contribute to ongoing efforts aimed at identifying safer and more effective therapeutic options for lymphatic filariasis in endemic regions.

Overall, the findings of this study demonstrate that the selected phytochemicals exhibit strong binding affinities, favorable physicochemical properties, and acceptable toxicity profiles. These characteristics highlight their potential as promising lead compounds for the development of novel therapeutic agents against lymphatic filariasis. However, further experimental validation is required to confirm their efficacy and safety.

5. Conclusion

This study demonstrated that several phytochemical compounds exhibit strong binding affinity against the selected *Wuchereria bancrofti* target protein (PDB ID: 8E4F). Among the screened compounds, the top-performing phytochemicals showed significantly higher binding affinities compared to the reference ligand, indicating their potential as effective inhibitors.

In addition to favorable binding interactions, the selected front-runner compounds complied with Lipinski's Rule of Five, suggesting acceptable drug-like properties and potential oral bioavailability. Furthermore, *in silico* toxicity assessment revealed that these compounds were non-mutagenic, non-tumorigenic, non-irritant, and showed no adverse effects on reproduction, indicating promising safety profiles.

These findings highlight the potential of plant-derived phytochemicals as viable lead compounds in the development of novel, cost-effective and accessible therapeutic agents against lymphatic filariasis, particularly in endemic regions. However, since the results are based on computational predictions, further experimental validation through in vitro and in vivo studies is required to confirm their efficacy and safety.

Compliance with ethical standards

Disclosure of conflict of interest

The authors declare that there are no conflicts of interest regarding the publication of this work.

Data availability

No new experimental data were generated. All computational data used in this study are available upon reasonable request.

Statement of ethical approval

This study did not involve human participants or animal experimentation. All analyses were conducted entirely using computational tools and publicly available datasets.

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