WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 4, 1185-1201. Research Article ISSN 2277–7105

IN VITRO ANTHELMINTIC ACTIVITY OF UNRIPE FRUITS AND IN SILICO STUDIES IN LEAF OF *LAWSONIA INERMIS L.*

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Article Received on 15 Jan. 2026,
Article Revised on 05 Feb. 2026,
Article Published on 16 Feb. 2026,

https://doi.org/10.5281/zenodo.18666688

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How to cite this Article: Mrs. Sarala A.1*, Mr. Senthil kumar S.K.2, Ms. Keerthika S.3, Mr. Krishnaraj A.4, Ms. Krishnaveni G.5, Ms. Lokeshwari K.6, Mrs. Madhu Priya V.7. (2026). In Vitro Anthelmintic Activity of Unripe Fruits And In Silico Studies In Leaf of Lawsonia Inermis L.. World Journal of Pharmaceutical Research, 15(4), 1185–1201.

ABSTRACT

Objectives: The present study aimed to evaluate the in vitro anthelmintic activity of unripe fruit extracts of Lawsonia inermis L. and to assess the in silico binding potential of leaf-derived phytochemicals in comparison with the standard anthelmintic drug albendazole. **Methods:** Unripe fruits of Lawsonia inermis L. were extracted using hexane, ethyl acetate, ethanol, and aqueous solvents. Anthelmintic activity was evaluated at concentrations of 5, 10, and 15 mg/mL by recording the time to paralysis and death of worms. Preliminary phytochemical screening was performed to identify major constituents. For computational studies, 20 reported leaf phytoconstituents were screened for ADME properties, and 12 compounds satisfying Lipinski's rule of five were subjected to molecular docking using SwissDock. Albendazole was docked as the standard reference drug. **Results:** The hexane extract exhibited the strongest anthelmintic activity at 15 mg/mL, while other extracts showed moderate, concentration-dependent effects. Phytochemical analysis confirmed the presence of alkaloids, carbohydrates, tannins, flavonoids, and proteins. Docking studies revealed that compound C9 showed the highest binding affinity (−8.414 kcal/mol), which was higher than albendazole (−7.858 kcal/mol), while several other

phytoconstituents showed comparable binding. **Conclusion:** The results indicate that unripe fruits and leaf-derived phytoconstituents of Lawsonia inermis L. possess promising anthelmintic potential. The comparative docking with albendazole supports the potential of selected phytoconstituents as effective β-tubulin inhibitors and prospective plant-based anthelmintic agents.

KEYWORDS: *Lawsonia inermis L.*, In vitro anthelmintic activity, Unripe fruits, Phytochemical screening, Molecular docking, Albendazole, SwissDock.

INTRODUCTION

Anthelmintic activity refers to the ability of a substance to kill (vermicidal) or expel (vermifugal) parasitic worms (helminths) from the body of humans or animals. Helminth infections-caused mainly by nematodes (roundworms), cestodes (tapeworms), and trematodes (flukes) are among the most common chronic infections worldwide, particularly in tropical and subtropical regions. These infections lead to malnutrition, anemia, impaired physical and cognitive development, and reduced productivity, posing a major public health problem.

Anthelmintic agents act through various mechanisms such as inhibition of energy metabolism, paralysis of worm musculature, disruption of microtubule formation, or damage to the parasite's protective tegument. Both synthetic drugs and medicinal plants have shown significant anthelmintic activity, and plant-based anthelmintics are increasingly studied due to rising drug resistance, cost-effectiveness, and better safety profiles. Evaluation of anthelmintic activity is commonly performed using in vitro and in vivo models, such as earthworm or roundworm assays, to assess paralysis and death of worms.

TYPES OF HELMINTICS

- **Roundworms**: These helminths, which have the scientific name nematodes, have a cylindrical body similar to earthworms. They can lead to infection in the intestines or elsewhere in the body.
- **Flukes**: These helminths, or trematodes, have a flat body and leaf-shaped head with a sucker that helps them attach. They generally infect the bile ducts (thin tubes from the liver to the small intestine), liver, or blood.
- **Tapeworms**: Tapeworms, or cestodes, are long, segmented flatworms found in or around the intestines.
- **Thorny-headed worms**: These helminths, or acanthocephalans, have a round body and

barbs around their head. They mainly infect animals, and human infection is very rare.

1. Types of Anthelmintic Agents

➢ Broad-spectrum anthelmintics: These drugs are effective against a wide range of parasitic worms, making them suitable for various infections.

➢ Narrow-spectrum anthelmintics: These drugs are specific to certain types of helminths and may not work against other worm infections.

➢ Natural anthelmintics: Some herbal or natural substances, such as garlic, pumpkin seeds, or neem, have traditionally been used as anthelmintics.

2. Mechanisms of Action

➢ **Paralysis**: Some anthelmintic agents work by paralyzing the muscles of the worms, making them easier to expel from the host's body.

➢ **Disruption of metabolism**: Certain drugs interfere with the worms' metabolism, affecting their ability to survive and reproduce.

➢ **Immobilization**: Anthelmintics may immobilize the worms, preventing their attachment to the host's tissues or causing them to detach.

3. Common Anthelmintic Medications

Albendazole, Mebendazole, Praziquantel, Ivermectin, Niclosamide, Pyrantel pamoate, Levamisole.

BOTANICAL INFORMATION

1. Synonyms

Lawsonia alba Lawsonia spinosa

2. Common Name

Henna Mehandi

Egyptian privet

3. Classification Kingdom : Plantae

Subkingdom : Tracheobionta (Vascular plants)

Division : Magnoliophyta (Angiosperms)

Class : Magnoliopsida (Dicotyledons)

Subclass : Rosidae

Order : Myrtales

Family : Lythraceae

Subfamily : Lythroideae

Genus : *Lawsonia*

Species : *Inermis L.*

4. Category

Medicinal plant Dye-yielding plant Ornamental shrub.

5. Foliage (Leaves)

Leaves are simple

Arrangement : Opposite

Shape : Elliptic to lanceolate

Margin : Entire

Surface : Smooth and glabrous

Colour : Green

Venation : Reticulate venation Leaves contain the dye compound lawsone

6. Flowers (Details)

Flowers are small and fragrant

Colour : White or yellowish-white

Inflorescence : Terminal panicles

Calyx : 4 lobes

Corolla : 4 crumpled petals

Stamens : 8

Ovary : Superior

VERNICULAR NAMES

English	:	Henna, Egyptian Privet
Hindi	:	Mehandi
Urdu	:	Henna, Mehandi
Sanskrit	:	Madayantika, Ranjaka
Tamil	:	Marudhani
Telugu	:	Gorintaaku
Kannada	:	Mendhike
Malayalam	:	Mailanchi
Marathi	:	Mehandi
Gujarati	:	Mehandi

PHARMACOGNOSTICAL STUDIES

Collection and Authentication of plant materials

Lawsonia inermis L. (Family: Lythraceae), commonly known as Henna, is a medicinal plant widely used in traditional systems of medicine. The fruits of *Lawsonia inermis L.* are small, dry capsules that are globose to ovoid in shape, measuring about 4-8 mm in diameter. They are green when immature and turn brown on maturity. The mature fruit is hard and dehiscent, splitting open into four valves to release the seeds. Each capsule contains numerous small, angular, brown seeds with a smooth surface. The fruits contain minor amounts of tannins and phenolic compounds, but they are less medicinally important than the leaves, which are the main source of the active compound lawsone. The fruits are mainly significant for plant propagation and botanical identification.

Fig. 1: Whole plant of *Lawsonia inermis L.* were collected from Tiruvannamalai local areas, Tamil Nadu. They were authenticated by Dr. J. Suresh kumar, M.sc., M.Phil., Ph.D., PGDCA.,

EXTRACTION OF FRUITS

Lawsonia inermis L. unripe fruits were collected and shade dried at room temperature for 3 weeks. The dried fruits were powdered and passed through the sieve no: 22#, 44#.

Requirements

Plant: Dried powder of unripe fruit (*Lawsonia inermis L.)*

Solvent: Aqueous, Ethanol, Ethyl acetate, Hexane

Apparatus: Soxhlet apparatus, beaker, measuring cylinder and weighing balance.

METHOD OF EXTRACTION

1. *Soxhlet process*

35g of dried coarse powder is placed in a porous bag or thimble made of strong filter paper, which is placed in chamber of the Soxhlet apparatus. The extracting solvents in flask is heated and its vapours condense in condenser. The condensed extract, drips into the thimble containing the crude drugs by its contact. When the level of liquid in chamber raises to the top of Siphon tube, the liquid contents of chamber Siphon into flask. This process is continuously carried out until a drop of solvent from the Siphon tube does not leave residue when evaporated.

Fig. 2: Soxhlet Extraction.

2. *Decoction process*

The aqueous decoction of *Lawsonia inermis L.* unripe fruit is prepared by cleaning and coarsely powdering 35g of dried unripe fruits. The powder is boiled with about 350mL of distilled water (10 times the drug weight) on a low flame and simmered for 15–30 minutes

with occasional stirring. The volume is reduced to one-fourth (about 85–90mL), then cooled and filtered through muslin cloth. The collected filtrate is the aqueous decoction of *Lawsonia inermis L.* unripe fruit.

FIG. 3: Decoction.

EVALUATION OF ANTHELMINTIC ACTIVITY

Anthelmintic activity was carried out on Indian adult earthworm (*P.posthuma)* of nearly equal in size, 3 in each group. Each extract was suspended in Tween 80 (3%v/v)with distilled water to obtain concentration of 5,10,15mg/mL. Reference standard drug Albendazole suspension was diluted with the same suspending agent to obtain concentration of 5,10,15mg/mL. Worms were placed in petri dishes containing 10mL of sample solution. Paralyze time was noted either if any movement could not be observed except vigorous shaken. Death was included when the worms lost their motility followed with white discharge on skin and fading away of their body colours.

Table 1: Treatment groups and dosage details.

Drug Administration Groups	Name of The Extracts With Different Doses
Control Group 1	Distilled water
Standard Group 2 Group 3 Group 4	Albendazole (5mg/mL) Albendazole(10mg/mL) Albendazole(15mg/mL)
Test Group 5 Group 6 Group 7	Hexane extract (5mg/mL) Hexane extract (10mg/mL) Hexane extract (15mg/mL)

Test Group 8 Group 9 Group 10	Ethyl acetate extract (5mg/mL) Ethyl acetate extract (10mg/mL) Ethyl acetate extract (15mg/mL)
Test Group 11 Group 12 Group 13	Aqueous extract (5mg/mL) Aqueous extract (10mg/mL) Aqueous extract (15mg/mL)
Test Group 14 Group 15 Group 16	Ethanol extract (5mg/mL) Ethanol extract (10mg/mL) Ethanol extract (15mg/mL)

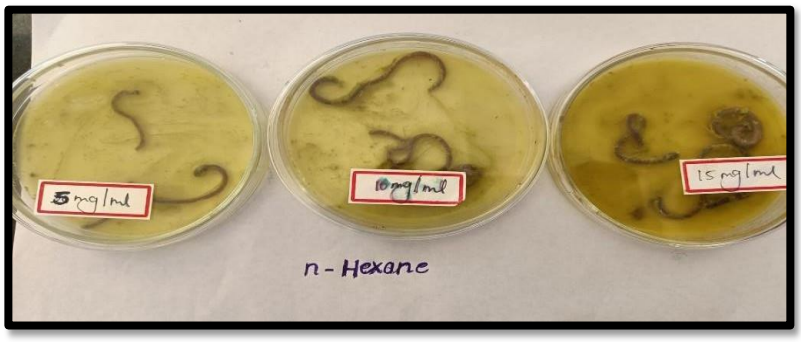


FIG. 4: Anthelmintic Activity of Hexane Extracts.

PHARMACOGNOSICAL STUDIES PRELIMINARY PHYTOCHEMICAL ANALYSIS

All the *Lawsonia inermis L*. (Aqueous, Ethanol, Ethyl acetate, Hexane) extracts were analysed for preliminary phytochemical screening for identification of various phytoconstituents.

TEST FOR ALKALOIDS

DRAGENDORFF'S TEST

To 1mL of the extract, add 1mL of dragendorff's reagent (potassium bismuth iodide solution) An orange red precipitate indicates the presence of alkaloids.

TEST FOR SAPONINS

Take small quantity of alcohol extract and add 20mL of distilled water ad shake in a graduated cylinder for 15min lengthwise. A 1cm layer of foam indicates the presence of saponin.

TEST FOR GLYCOSIDES

LEGAL TEST

Dissolve the extract in pyridine and add sodium nitro prusside solution to make it alkaline,

the formation of pink red colour shows the presence of glycosides.

TEST FOR CARBOHYRATES AND SUGARS

FEHLING'S TEST

To 1mL of the extract, add equal quantities of Fehling's solution A and B. upon heating formation of a brick red precipitate indicates the presence of sugars.

TEST FOR TANNINS

GELATIN TEST

To a few mL of extract, add 1% gelatin solution containing 10% sodium chloride. Formation of white precipitate indicates the presence of tannins.

TEST FOR FLAVONOIDS

SHINODA'S TEST

To the extract solution add few fragments of magnesium ribbon and add concentrated hydrochloric acid drop wise gives cherry red or pink scarlet after few minutes, shows the presence of flavonoids.

TEST FOR STEROIDS

SALKOWSKI TEST

Dissolve the extract in chloroform and add equal volume of concentrated sulphuric acid Formation of bluish red to cherry red colour in chloroform layer and greet fluorescence in the acid layer represents the steroidal components in the tested extract.

TEST PROTEIN FOR AMINO ACIDS

NINHYDRIN TEST

Add 2 drops of freshly prepared 0.2% Ninhydrin reagent (0.1% solution in n-Butanol) to the small quantity of extract solution and heat. Development of blue colour reveals the presence of proteins, peptides or amino acid.

DOCKING STUDIES

FOR SWISSDOCK

1. PREPARATION OF TARGET (PROTEIN):

Download the 2D structure of the protein from the Protein Data Bank (PDB).

2. PREPARATION OF LIGAND

Draw or retrieve ligand structure (e.g., from PubChem).

3. ACCESS SWISSDOCK

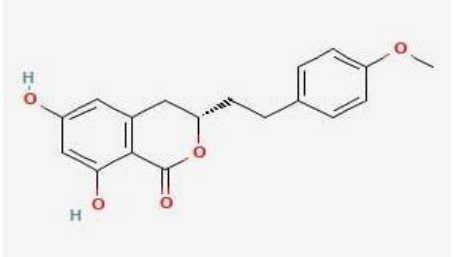
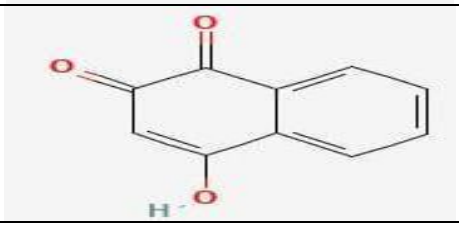
Choose between binding of Ligand (entire protein surface) or targeted Protein(specific binding site.

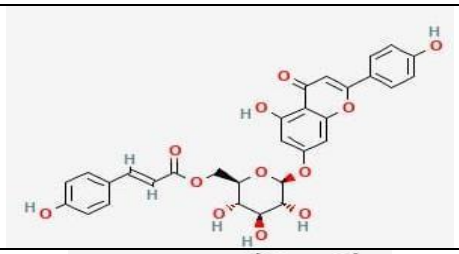
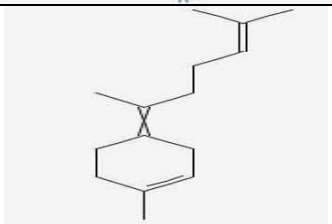
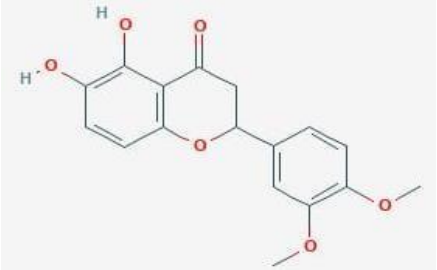
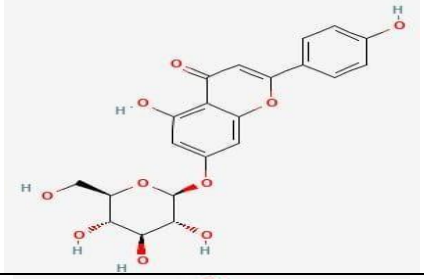
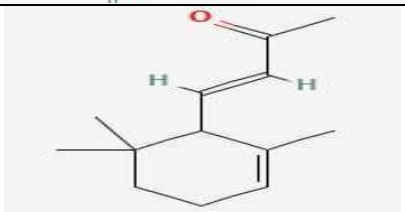
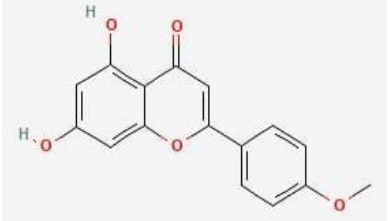
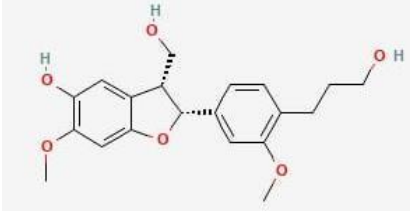
4. ANALYSIS

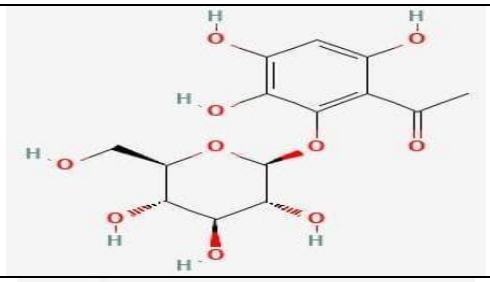
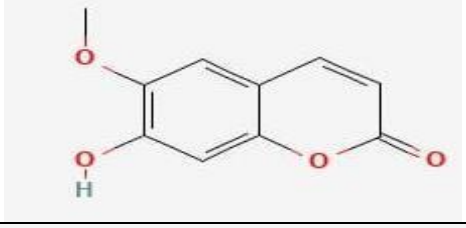
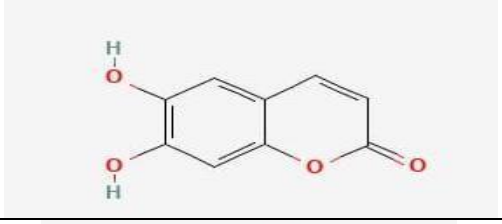
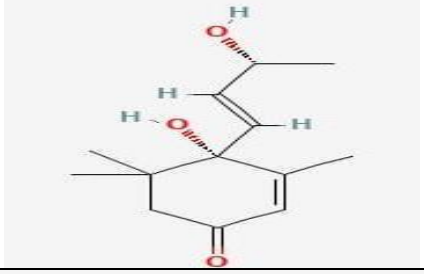
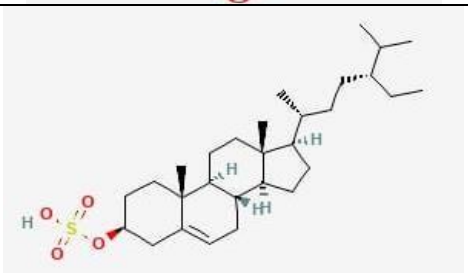
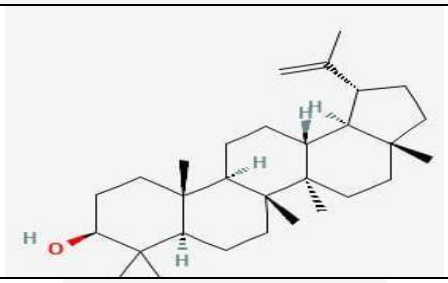
The ADME properties of selected lead molecules were calculated using the ADME and molecular properties module of the SWISSADME. The molinspiration tool in the SWISSADME is used to predict the "drug-likeness" features of various compounds from anthelmintic activity. The physicochemical properties include formula, molecular weight, No. heavy atoms, No. aromatic heavy atoms, fraction Csp3, No. rotatable bonds. No. H-bond acceptors, No. H-bond donors, molar refractivity, TPSA [topological polar surface area]. The lipophilicity includes iLOGP, XLOGP3, WLOGP, SOGP, Silicos-IT Log P, consensus LogP. The predicted water solubility compounds include ESOL log S, ESOL solubility [mg/mL], ESOL solubility[mol/l], ESOL class, Ali log S, Ali solubility[mg/mL], etc.

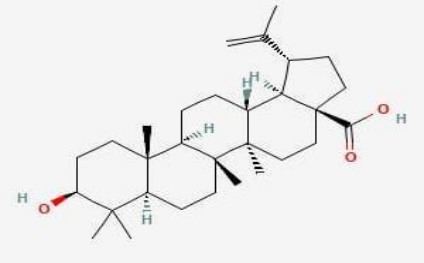
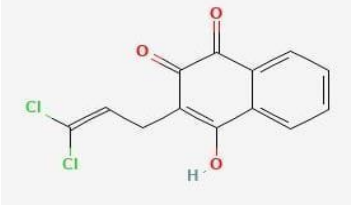
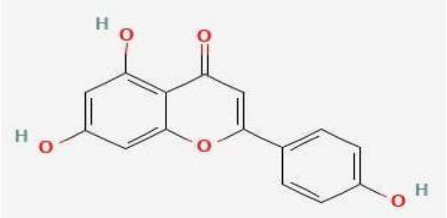
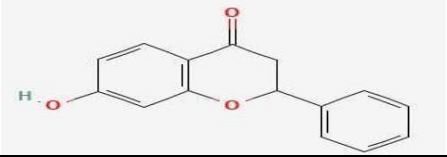
The pharmacokinetics compounds include GI absorption, BBB permeant, Pgp substrate, CYP1A2 inhibitor, CYP2C19 inhibitor, CYP2C9 inhibitor, CYP2D6 inhibitor, CYP3A4 inhibitor, Log Kpa (skin permeation). The predicted drug-likeness compounds include Lipinski, Ghose, Veber, Egan, Muegge, bioavailability, PAINS, Brenk, Lead- likeness, Synthetic accessibility.

Table 2: List of Bioactive compounds with chemical structure.

S.N O	COMPOUND STRUCTURE	NAME OF THE COMPOUNDS
1.		Agrimonolide-6-O-β-D-glucopyranoside
2.		2-Hydroxy-1,4-napthoquinine

3.		Apigenin-7-O-β-D- glucopyranoside
4.		Bisabolene
5.		3,4-dimethoxy flavone
6.		Cosmosiin
7.		α- lonone
8.		Acacetin
9.		Lawsonicin

10.		Lalioside
11.		Scopoletin
12.		Esculetin
13.		Vomifoliol
14.		Beta sitosterol
15.		Lupeol
16.		Betalin

17.		Betulinic acid
18.		Lawsone
19.		Apigenin
20.		7-Hydroxy flavanone

RESULTS AND DISCUSSION

Table 3: Phytochemical screening of various extracts of Unripe fruit of *Lawsonia inermis L.*

S.NO.	PHYTO CONSTITUENTS	HEXANE	ETHYL ACETATE	AQUEOUS	ETHANOL
1.	Alkaloids	+	+	+	+
2.	Saponins	-	-	-	-
3.	Glycosides	-	+	-	+
4.	Carbohydrates/ sugar	+	+	+	+
5.	Tannins	+	+	+	+
6.	Flavonoids	+	+	+	+
7.	Proteins	+	+	+	+

PHARMACOLOGICAL STUDIES

EXTRACTIVE VALUES

Table 4: Determination of Extractive values.

S.No.	EXTRACTS	SAMPLE TAKEN(g)	OBTAINED YIELD(g)	PERCENTAGE YIELD(%)
1.	Aqueous	35	3.96	11.31
2.	Ethanol	35	3.25	9.28
3.	Ethyl Acetate	35	3.56	10.17
4.	Hexane	35	3.06	8.74

Table 5: In vitro anthelmintic activity of unripe fruit extracts of *Lawsonia inermis L.*

S.NO	EXTRACTS	PARALYSIS TIME (MINS) OF VARIOUS CONCENTRATION			DEATH TIME (MINS) OF VARIOUS CONCENTRATION		
		5mg/mL	10mg/mL	15mg/mL	5mg/ml	10mg/ml	15mg/mL
1.	Control (Tween80-3%V/V)	Alive					
2.	Albendazole	9.55	8.43	7.12	11.05	10.45	8.55
3.	Hexane	6.53	5.39	3.46	7.16	6.11	4.17
4.	Ethyl acetate	7.56	6.53	4.16	8.55	7.16	4.53
5.	Aqueous	8.33	6.21	4.23	9.11	6.13	5.39
6.	Ethanol	10.33	9.16	8.33	11.52	9.36	9.01

Data were analysed by ANOVA followed by Dunnet's test. Values are represented as mean ±SEM, (n=3), *P<0.05

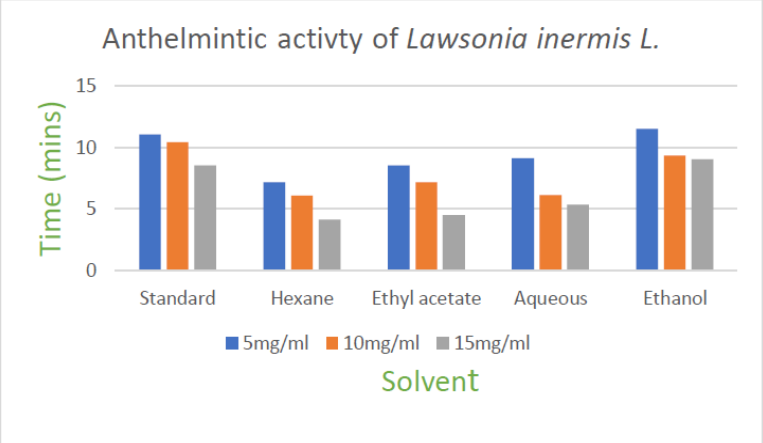


Fig. 5: Paralysis Time.

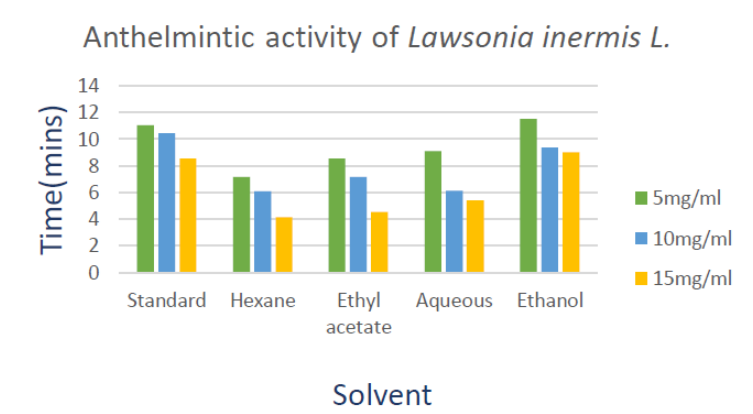


Fig. 6: Death Time.

DOCKING STUDIES

Captured various compounds were then subjected to ADME testing using SWISSADME software. The forecasted ADME property of various compound based on their structure,

functional groups and molecular properties such as Mol/M.W (Molecular weight), BBB permeant (Blood-Brain Barrier parameter of compounds), GI (Gastrointestinal absorption), H-bond acceptors, H-bond donors, Violation and MLogP (Moriguchi octanol-water partition coefficient). Few compounds transgressed druglikeness tests were removed as those compounds have poor ability to cross the biological membrane. The ADME report are mentioned under the following table.

Table 6: ADME Report study.

Cpds No.	M.W g/mol	BBB	GI Absorption	H-bond Acceptor	H-bond Donor	Violation	MLogP
1.	476.47	No	High	10	5	0	0.04
2.	174.15	Yes	High	3	1	0	0.03
3.	432.38	No	Low	10	5	1	-1.61
4.	204.35	No	Low	0	0	1	4.53
5.	282.29	Yes	High	4	0	0	1.57
6.	432.38	No	Low	10	5	1	-1.61
7.	206.28	Yes	High	2	0	0	1.93
8.	284.26	No	High	5	2	0	0.77
9.	360.40	No	High	6	3	0	1.17
10.	346.29	No	Low	10	5	1	-2.84
11.	192.17	Yes	High	4	1	0	0.76
12.	178.14	No	High	4	2	0	0.45
13.	224.30	Yes	High	3	2	0	1.14
14.	414.71	No	Low	1	1	1	6.73
15.	426.72	No	Low	1	1	1	6.92
16.	442.72	No	Low	2	2	1	6.00
17.	458.70	No	Low	3	2	1	5.82
18.	283.11	Yes	High	3	1	0	1.32
19.	270.24	No	High	5	3	0	0.52
20.	240.25	Yes	High	3	1	0	1.85
Limit	**≤500**	**No**	**High**	**≤10**	**≤5**	**0**	**≤4.15**

Table 7: Docking score in SwissDock [Protein id:4DXD].

S.No.	Cpds. No.	Docking score (Kcal/mol)
1.	C9	-8.4103
2.	C1	-8.0612
3.	C8	-7.5374
4.	C19	-7.5265
5.	C5	-7.4777
6.	C11	-7.2662
7.	C18	-7.2179
8.	C17	-7.1020
9.	C20	-7.0710
10.	C7	-6.8050
11.	C2	-6.5383

12.	C12	-6.4845
13.	**Albendazole**	**-7.5851**

The molecular docking study against the β-tubulin protein (PDB ID: 4DXD) demonstrated a clear comparison between the standard drug albendazole and selected phytoconstituents. Albendazole showed a docking score of −7.5851 kcal/mol, which was used as the reference standard. Notably, compounds C9, C1, C8, and C19 exhibited higher binding affinities, with more negative docking scores than albendazole, indicating stronger and more stable interactions with the β-tubulin active site.

Among these, C9 showed the highest binding affinity, followed by C1, C8, and C19, suggesting their enhanced potential to inhibit microtubule polymerization, a key mechanism underlying anthelmintic activity. Since β-tubulin is a validated molecular target for anthelmintic drugs, superior binding affinity implies improved inhibitory effectiveness.

Overall, the comparative docking results highlight C9, C1, C8, and C19 as promising lead phytoconstituents with potential anthelmintic activity, supporting further in vitro and in vivo investigations.

DOCKING IMAGES

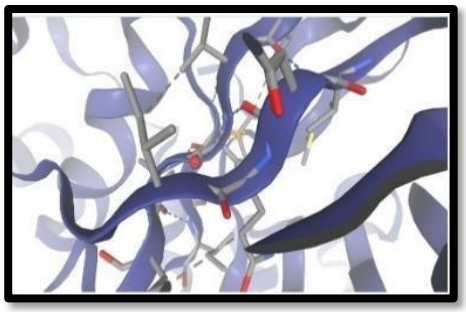


Fig. 7.

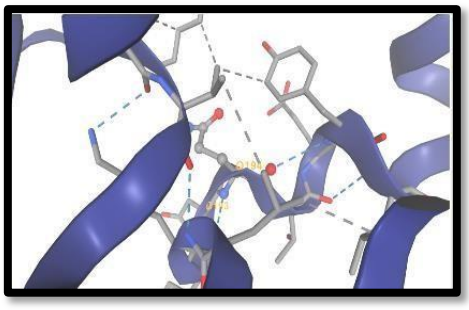


Fig. 8.

CONCLUSION

The present study demonstrates the significant anthelmintic potential of *Lawsonia inermis L*. through an integrated in vitro and in silico approach. Phytochemical screening revealed the presence of important secondary metabolites such as **alkaloids, flavonoids, tannins, terpenoids and phenolic compounds.** These constituents are known to contribute anthelmintic activity by interfering with helminth neuromuscular function and metabolic pathways, thereby supporting the observed experimental results.

In vitro evaluation against *Pheretima posthuma* showed that extracts prepared using solvents of different polarity produced a clear concentration-dependent reduction in paralysis and death times at 5, 10, and 15mg/mL. Among the extracts tested, the hexane extract exhibited the highest anthelmintic activity, producing **the shortest paralysis time (3.46mins) and death time (4.17mins) at 15mg/mL.** The ethyl acetate extract showed moderate activity, followed by the aqueous extract, while the ethanolic extract showed the least activity. The overall order of efficacy was **Hexane > Ethyl acetate > Aqueous > Ethanol,** indicating the importance of non-polar bioactive compounds.

Based on the docking results, compounds **C9, C1, C8, and C19 exhibited higher binding affinity toward the β-tubulin protein (4DXD)** compared to the standard drug **albendazole (−7.5851 kcal/mol).** Their superior docking scores indicate stronger and more stable ligand–protein interactions, suggesting that these phytoconstituents may possess enhanced inhibitory potential against the target protein. This comparative analysis highlights C9, C1, C8, and C19 as promising lead compounds and supports the potential of *Lawsonia inermis L.* as a source of effective natural anthelmintic agents.

Overall, these results suggest that *Lawsonia inermis L*. particularly its hexane extract, is a promising source of natural anthelmintic agents and merits further in vivo investigation.

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