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IN-VITRO AND IN-SILICO ASSESSEMENT OF ANTHELMINITIC ACTIVITY OF FRUIT PEEL FROM *ANNONA SQUAMOSA L.*

Mrs. Sarala A.[1*], Mr. Senthil Kumar S. K.[2], Ms. Kaviya M.[3], Ms. Kaviya Sri A. S.[3], Ms. Kiruthiya S.[3], Mr. Kotteeshwaran S.[3], Ms. Krishna Priya R.[3], Mr. Krishna Raj R.[3], Mr. Kumaravel M.[3]

[1*]Associate Professor, Department of Pharmaceutical Chemistry, Arunai College of Pharmacy, Tiruvannamalai.

[2]Principal Cum Professor, Department of Pharmaceutics, Arunai College of Pharmacy, Tiruvannamalai.

[3]B. Pharmacy Final Year Students, Arunai College of Pharmacy, Tiruvannamalai.

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***Corresponding Author**
Mrs. Sarala A.
Associate Professor, Department of Pharmaceutical Chemistry, Arunai College of Pharmacy, Tiruvannamalai.

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ABSTRACT

Objectives: The aim of the present study was to investigate the anthelmintic activity of the *Annona squamosa L.* (Annonaceae), fruit peel extract using adult earthworm (*Pheretima Posthuma*) and to assess the in-silico binding potential of fruit peel-derived phytochemicals in comparison with the standard anthelmintic drug albendazole. **Methods:** Aqueous, ethanol and ethyl acetate solvents were used to extract the fruit peel *Annona squamosa L.* anthelmintic activity was assessed by timing the worm's paralysis and death at dosages of 20, 40 and 60mg/mL. To determine the main components, a preliminary phytochemical screening was conducted. For computational studies, 63 phytoconsistuents were screened for ADME properties, and 12 compounds were satisfying Lipinski's rule of five were subjected to molecular docking using Swiss Dock. Albendazole was docked as the standard reference drug. **Result:** The anthelmintic activity of the ethanol extract was the highest at 60mg/mL, but effect of the other extracts was moderate and varied on concentration. Phyto chemical analysis confirmed the presence of alkaloids, carbohydrates, tannins, flavonoids, terpenoids, phenolic compounds, steroids, and glycosides. According to

docking studies compound C1 demonstrated the highest binding affinity (-8.2700 kcal/mol) surpassing that of albendazole (-7.1069 kcal/mol) but a few other phytoconstituents displayed similar binding. **Conclusion:** From the work we conclude that traditional usage of *Annona squamosa L*. fruit peel for treating worm infestation has been validated. The comparative docking with albendazole suggests the possibility of some phytoconstituents as possible plant-based anthelmintic medicines and effective β-tubulin inhibitors.

KEYWORDS: *Annona squamosa L.*, In-vitro Anthelmintic activity, Fruit peel, Phytochemical screening, Molecular docking, Albendazole, Swiss Dock.

INTRODUCTION

Helminthiasis is a disease in which a part of the body is infested with worms such as pinworm, roundworm and tapeworm. Typically, the worms reside in the GIT but may also burrow into the liver and other organs. They produce harmful effect on host by depriving him of food, causing blood loss and by secreting toxins.

The parasitic worms are categorized into three groups are tapeworms, roundworms, and flukes. Anthelmintic activity refers to the ability of a substance to destroy or expel parasitic worms, also known as helminths, from the body of a host. These parasitic worms can infect various parts of the human or animal body, causing diseases and health issues, which are specifically designed to target and eliminate the parasitic worms.

Anthelmintic agents act through various mechanisms such as paralysis, disruption of metabolism, inhibition of muscular function, prevention of nutrient uptake, and 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

- **Nematodes** (Roundworms): These helminths resemble earthworms in their cylindrical bodies. Infections in the intestines or other parts of the body may result from them.
- **Cestodes** (Tapeworms): These are long, segmented flatworms that live in or near the intestines.

- **Trematodes** (Flukes): These have a flat body and a leaf-shaped head with a sucker to aid in attachment. They typically infect the liver, blood, or bile ducts, which are tiny tubes that connect the liver to the small intestine.
- **Acanthocephalans** (Thorny-headed worms): These are round-bodied and have barbs on the top of their heads. Human infection is quite uncommon, and they primarily infection in animals.

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 anthelmintic activity.

MECHANISM 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 worm’s 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.

COMMON ANTHELMINITIC DRUG

1. Albendazole
2. Mebendazole
3. Praziquantel
4. Ivermectin
5. Niclosamide
6. Pyrantel pamoate
7. Levamisole

BOTANICAL INFORMATION

1. Synonyms

Annona squamosa L.

2. Classification

Kingdom - Plantae

Division - Magnoliophyta

Class - Magnoliopsia (Dicotyledon)

Subclass - Magnoliidae

Order - Magnoliales

Family - Annonaceae (Custard – apple family)

Sub Family - Maloideae

Tribe - Abreae

Genus - Annona

Species - Squamosa L.

3. Morphological Description

Characters	Seeds	Leaves	Stem	Roots	Fruits
Colour	Black	Green	Green to Brown	Light	Greenish outside
Odour	Odourless	Characteristic odour	Characteristic odour	Odourless	Sweetish
Taste	Tasteless	Bitter	Sight bitter	Bitter	Sweetish

Leaves

Leaves are oblong-lanceolate, 10-15cm long and 3-5cm wide, alternately arranged on short petioles, young leaves are slightly hairy, solitary, and clustered crystals occur in epidermal cells.

Flower

Flower is 2-4cm long and contains three degenerated sepals and six petals. The six petals are arranged into two whorls with three each and the petals of the inner whorl are degenerated into small scales or completely disappear.

Stem

Stems are Irregular branches with thin grey bark.

Fruit

Trees starts to bear fruit when 3-4year-old. The flesh nearest to the rind, tastes like sugar crumbs too. It is usually conical in shape but sometimes, be almost round. The rind is thick with knobby segments but will turn soft and crack open, releasing a sweet aroma when it ripe.

Roots

Branched tap root.

Seeds

Seeds are black or deep brown in colour. There are 30-40 seeds in an average fruit. The *Annona squamosa L.* is a diploid species with 2n=14.

Vernacular name

Tamil - Seethapazham

English - Custard apple, sugar apple, sweetsop

Hindi - Sitafal

Bengali - Ata

Malayalam - Aathappazham, Seetha pazham

Telugu - Seetha pazham

Kannada - Seethaphala

Marathi - Sitaphal

Sanskrit - Sitaphalam

Urudu - Sharifa

COLLECTION AND AUTHENTICATION OF PLANT MATERIALS

Annona squamosa L. (Family: Annonaceae) Trees start to bear fruit when 3-4-year-old. Sugar apple, as the name says it all, is sweet as sugar. The flesh nearest to the rind, tastes like sugar crumbs too. It is usually conical in shape but sometimes, it may be almost round. It is easy to tell when it is ready to eat. The rind is thick with knobby segments but will turn soft and crack open, releasing a sweet aroma when it ripe. Normal ripening occurred at temperature between 15-30 °C.

Fig. 1: *Annona squamosa L.*

The fruit peel of *Annona squamosa L.* were collected from, Thanneerpandhal village, Thandarampet taluk, Tiruvannamalai District. Tamil Nadu which was authenticated by Dr. J. Sureshkumar, M.Sc., M.Phil., Ph.D., PGDCA.

EXTRACTION OF FRUIT

Annona squamosa L. (Fruit peel) were collected and shade dry at room temperature for 3 weeks. The dried fruit peel was powdered and passes through sieve no: 22#, 42#.

Requirements

Plant: Dried powdered of fruit peel (*Annona squamosa L.*)

Solvent: Ethanol, Ethyl acetate, Aqueous.

Apparatus: Soxhlet apparatus, Beaker, Measuring cylinder, Weighing balance and Stirrer.

Fig. 2: Dried fruit peel of *Annona squamosa L*.

METHOD OF EXTRACTION

1. Soxhlet process

60g 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 condensed 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. 3: Soxhlet process.

2. Decoction process

The aqueous decoction of Annona squamosa L. unripe fruit was prepared by first cleaning and coarsely powdering 50 g of dried unripe fruits. The powdered material was then boiled with approximately 350 mL of distilled water (about 10 times the weight of the drug) over a low flame and allowed to simmer for 15-30 minutes with occasional stirring. The volume of the solution was reduced to one-fourth (approximately 85-90 mL). The mixture was then cooled and filtered through muslin cloth. The collected filtrate represents the aqueous decoction of Annona squamosa L. unripe fruit.

Fig. 4: Decoction process.

EVALUATION OF ANTHELMINTIC ACTIVITY

Anthelmintic activity was carried out on Indian adult earthworm(*P.posthuma*) of nearly equal in size, 5 in each group. Each extract was suspended in Tween 80 (3%v/v) with distilled water to obtain concentration of 20, 40, 60mg/mL. Reference standard drug Albendazole suspension was diluted with the same suspending agent to obtain concentration of 20, 40,

60mg/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 GROUP	NAME OF THE EXTRACTS WITH DIFFERENT DOSES
Control Group 1	Distilled water
Standard Group 2 Group 3 Group 4	Albendazole (20mg/mL) Albendazole (40mg/mL) Albendazole (60mg/mL)
Test Group 5 Group 6 Group 7	Ethanol extract (20mg/mL) Ethanol extract (40mg/mL) Ethanol extract (60mg/mL)
Test Group 9 Group 10 Group 11	Ethyl acetae extract (20mg/mL) Ethyl acetae extract (40mg/mL) Ethyl acetae extract (60mg/mL)
Test Group 12 Group 13 Group 14	Aqueous extract (20mg/mL) Aqueous extract (40mg/mL) Aqueous extract (60mg/mL)

Fig. 5: Anthelmintic Activity of Ethanol extract.

PRELIMINARY PHYTOCHEMICAL ANALYSIS

All the *Annona squamosa L*. (Aqueous, Ethanol, and Ethyl acetate) extracts were analysed for preliminary phytochemical screening for identification of various phytoconstituents.

TEST FOR ALKALOIDS

HAGER'S TEST

To 1ml of the extract, add 3ml of Hager's reagent (saturated aqueous solution of picric acid), yellow coloured 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'S TEST

Dissolve the extract in pyridine and add sodium nitroprusside solution to make it alkaline, the formation of pink, red colour shows the presence of glycosides.

TEST FOR CARBOHYRATES AND SUGARS

FEHLING'S TEST

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 sugar.

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

LEAD ACETATE

1mL of plant extract add few drops of 10% lead acetate solution. Formation of yellow precipitate indicates 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 green fluorescence in the acid layer represents the steroidal components in the tested extract.

TEST PROTEIN FOR AMINO ACIDS

MILLON'S TEST

1mL of test solution is made acidic with sulphuric acid and add Million's reagent (Mercuric nitrate in nitric acid) and boils this solution. A yellow precipitate is formed indicates the presence of proteins.

TEST FOR TERPENOIDS

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 indicates presence of terpenoids.

TEST FOR PHENOLIC COMPOUND

FERRIC CHLORIDE TEST

1mL of plant extract add few drops of 5% ferric chloride solution. Formation of dark green / bluish black indicates presence of phenolic compounds.

DOCKING STUDIES

FOR SWISS DOCK

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

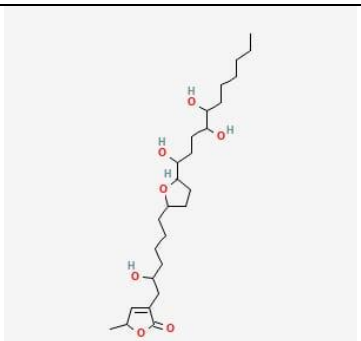
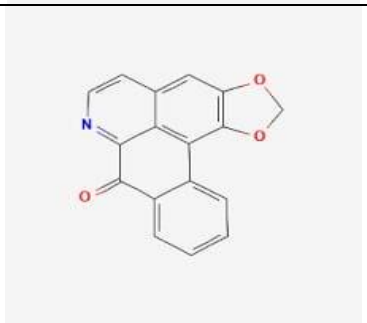
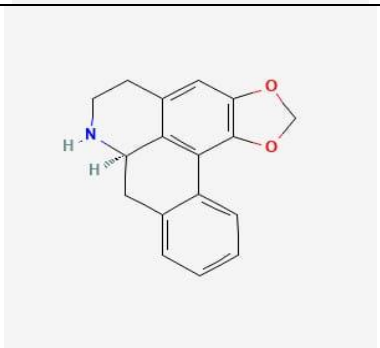
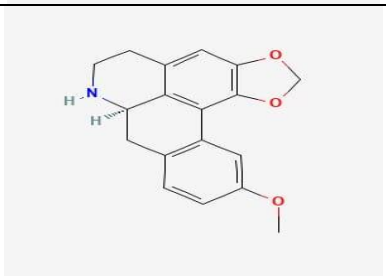
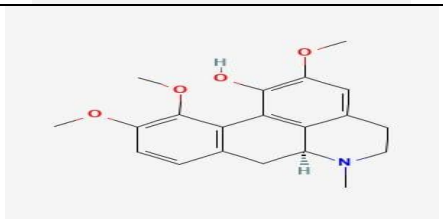
Choose between binding of Ligand (entire protein surface) or targeted Protein (specific binding site).

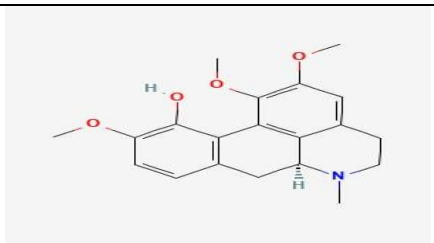
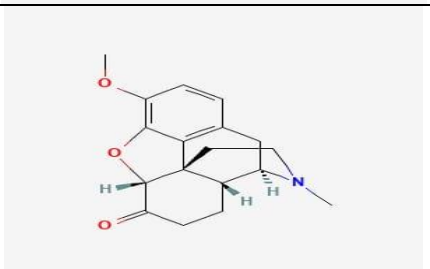
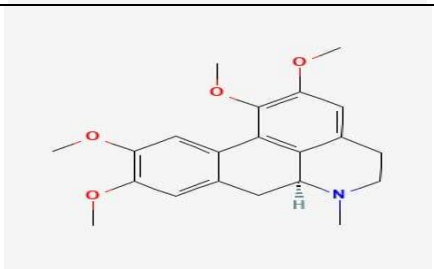
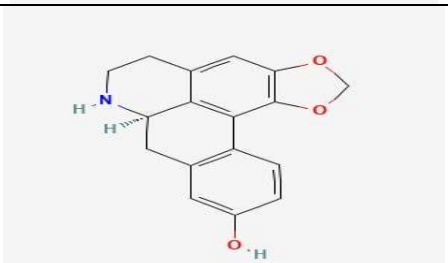
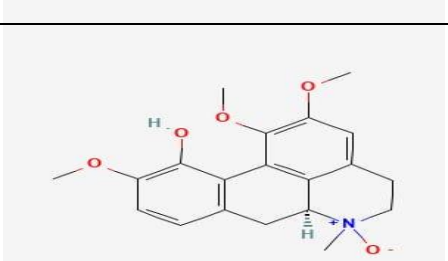
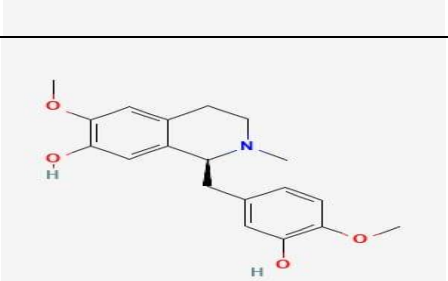
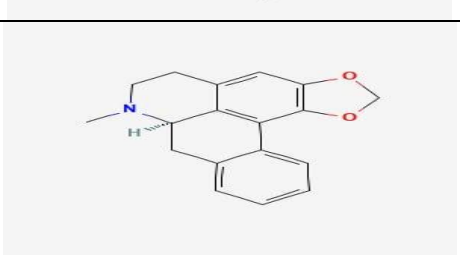
4. ANALYSIS

The ADME properties of selected lead molecules were calculated using the ADME and molecular properties module of the SWISSADME. The mol inspiration 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 iLOG P, XLOGP3, WLOGP, SOGP, Silico-IT Log P, Log P consensus 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. 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.NO	COMPOUND STRUCTURE	COMPOUND NAMES
1.		**Acetogenine**
2.		**Liriodenine**
3.		**Anonine**
4.		**Norlaureline**
5.		**Corydine**

6.		**Isocorydine**
7.		**Norcorydine**
8.		**Glaucine**
9.		**Anolobine**
10.		**Norisocorydine**
11.		**Reticuline**
12.		**Roemerine**

RESULT AND DISCUSSION

Table 3: Phytochemical screening of various extract in fruit peel of *Annona squamosa L.*

S.NO	PHYTO CONSTITUENTS	ETHANOL	ETHYL ACETATE	AQUEOUS
1.	Alkaloids	+	+	+
2.	Carbohydrates	+	+	+
3.	Flavonoids	+	+	+
4.	Tannins	+	-	+
5.	Saponins	+	-	+
6.	Glycosides	+	-	+
7.	Proteins	+	+	+
8.	Phenolic compound	+	+	+
9.	Terpenoids	+	+	+
10.	Steroids	+	+	+

PHARMACOLOGICAL STUIDES

EXTRACTIVE VALUES Table 4: Determination of extractive values

S.NO	EXTRACTS	SAMPLE TAKEN (g)	OBTAINED YIELD (g)	PERCENTAGE YIELD (%)
1.	Ethanol	60	4.69	7.81
2.	Ethyl acetate	60	4.63	7.7
3.	Aqueous	60	5.10	8.5

Table 5: In vitro anthelmintic activity of fruit peel extracts of *Annona squamosa L.*

S.NO	EXTRACTS	PARALYSIS TIME (MINS) OF VARIOUS CONC.			DEATH TIME (MINS) OF VARIOUS CONC.		
		20mg/mL	40mg/mL	60mg/mL	20mg/mL	40mg/mL	60mg/mL
1.	Control (Tween 80-3%V/V)	Alive					
2.	Albendazole	9.32	8.34	7.21	11.25	10.13	8.09
3.	Ethanol	7.35	6.42	5.13	8.31	7.51	6.11
4.	Ethyl acetate	8.54	7.21	6.39	9.11	8.33	7.23
5.	Aqueous	10.36	9.24	7.53	11.55	10.32	8.21

Data were analysed by ANOVA followed by Dunnet's test. Values are represented as mean ±SEM, (n=5) *P<0.05

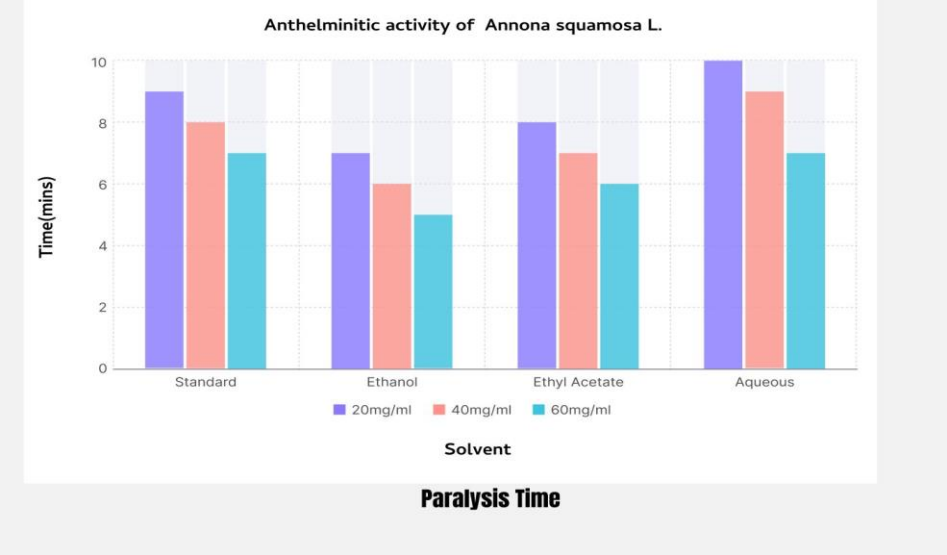


Fig. 6: Paralysis Time.

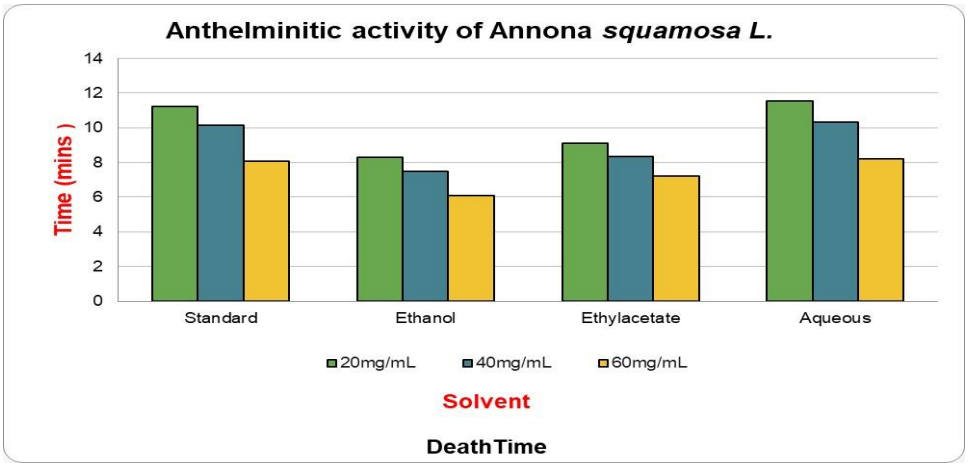


Fig. 7: Death Time.

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/MW (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 drug likeness 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 Donar	Violation	MLogP
1.	470.64	No	High	7	4	0	1.74
2.	275.26	Yes	High	4	0	0	1.71
3.	265.31	Yes	High	3	0	0	2.83
4.	295.33	Yes	High	1	1	0	2.49
5.	341.40	Yes	High	5	1	0	1.98
6.	341.40	Yes	High	5	1	0	1.98
7.	327.37	Yes	High	5	2	0	1.75
8.	355.43	Yes	High	5	0	0	2.20
9.	281.31	Yes	High	4	2	0	2.25
10.	327.37	Yes	High	5	2	0	1.75
11.	329.39	Yes	High	5	2	0	1.75
12.	279.33	Yes	High	3	0	0	3.07
Limit	**≤500**	**No**	**High**	**≤10**	**≤5**	**0**	**≤4.15**

Table 7: Docking score in Swiss Dock (Protein id: 2YLH).

S.NO	Compounds No.	Docking score (Kcal/mol)
1.	C1	-8.2700
2.	C2	-7.1784
3.	C3	-7.0079
4.	C4	-7.4978
5.	C5	-7.2468
6.	C6	-7.3832
7.	C7	-7.4978
8.	C8	-7.5240
9.	C9	-7.1165
10.	C10	-7.6689
11.	C11	-7.3586
12.	C12	-7.2569
13.	**Albendazole**	**-7.1069**

The conventional medication albendazole and a few phytoconstituents were clearly compared in the molecular docking investigation against the β-tubulin protein (PDB ID: 2YLH). The reference standard, albendazole, has a docking score of −7.0093 kcal/mol. Compared to albendazole, compounds C1 showed higher binding affinities and more negative docking scores, suggesting stronger and more stable interactions with the β-tubulin active site, followed by C10, C8, C7, C4, C11, C12, C5, C2, C9 and C3, 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 molecular docking results C1 as promising lead phytoconstituents potential anthelmintic activity, supporting further in vitro and in vivo investigation.

DOCKING IMAGES

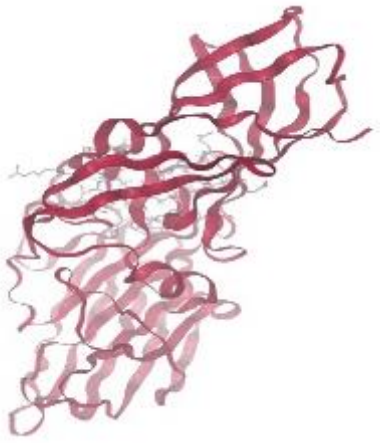


Fig 8: Docking of C1 compound.

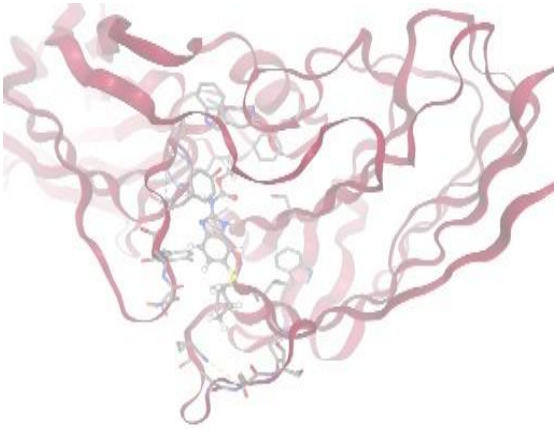


Fig 9: Docking of albendazole.

CONCLUSION

The present study demonstrates the significant anthelmintic potential of *Annona squamosa 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 20, 40, and 60mg/mL. Among the extracts evaluated, the ethanol extract exhibited the highest anthelmintic activity, producing **the shortest paralysis time (5.13mins)** and **death time (6.11mins) at 60mg/mL.** The ethyl acetate extract showed moderate activity, followed by the aqueous extract. The overall order of efficacy was, **Ethanol > Ethyl acetate > Aqueous**

Based on the docking results, compound C1, exhibited higher binding affinity towards the β-tubulin protein (2YLH) compared to the standard drug albendazole (−7.0093 kcal/mol). The

superior dockings score indicates stronger and more stable ligand–protein interactions, suggesting that these phytoconstituents may posses enhanced inhibitory potential against the target protein.

From the work we concluded that traditional usage of *Annona squamosa L*. fruit peel for treating worm infections has been validated.

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