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Antimicrobial and Anthelmintic Potential of *Premna barbata*: *In Vitro* and *In Silico* Insights

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Abstract

Background: *Premna barbata* and other species of the same genus, *Premna* (*Lamiaceae*), have been used in folk medicine for various diseases such as arthritis, dropsy, fever, diarrhoea, *etc*., in the form of powders, juice, paste, and decoctions. These folk uses make *P. barbata* more explorable for different pharmacological activities. **Aim:** This manuscript evaluated ethanolic and aqueous extracts of *P. barbata* with antimicrobial and anthelmintic activities, with *in silico* insights. **Methods:** Both extracts were phytochemically screened, which confirmed the presence of phytoconstituents. Then biologically tested for antimicrobial and anthelmintic activity. Molecular docking analyses were performed using *P. barbata* phytoconstituents with *Staphylococcus hominis* and Anthelmintic receptors. **Results:** *P. barbata* aqueous extract showed stronger and more consistent antimicrobial activity than ethanolic extract, demonstrating a clear dose-dependent inhibition pattern with measurable ZOI at both 100 mg/ml and 50 mg/ml. Ethanolic showed weaker activity, producing inhibition only at the highest concentration (17 mm at 100 mg/ml) and failing to suppress bacterial growth at lower concentrations. Aqueous extract showed dose-dependent anthelmintic activity. Molecular docking analysis data showed that geniposidic acid and epi-alpha-bisabolol observed with good docking scores against 8ZFK and rutin, and geniposidic acid showed good docking scores against 6QP2 receptors. These phytoconstituents may be responsible for the antimicrobial and anthelmintic properties of *P. barbata*. **Conclusion:** These findings confirmed that *P. barbata* showed good potential as an antimicrobial and anthelmintic agent.

Major Findings: *P. barbata* showed significant antimicrobial and anthelmintic properties. Computational investigation confirmed the importance of its phytoconstituents in the treatment of microbial and parasitic infections.

Keywords: Antimicrobial, Anthelmintic, Extraction, Molecular Docking, *Premna barbata*

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1. Introduction

Premna barbata (Aganyo or Bakhara), a deciduous shrub or small tree, has been used in folk and Ayurvedic medicine due to its potent pharmacological activities. It is a member of the genus *Premna* (*Lamiaceae*), which is distributed throughout tropical and subtropical regions of Asia, Africa, Australia, and the Pacific Islands. Since ancient times, it has been used to treat various diseases, including arthritis, dropsy, fever, diarrhoea, and herpes, in the form of powders, juices, pastes, and decoctions.

In recent years, a drive to identify more ecologically safe compounds as therapeutic agents for various diseases has led to increased research on medicinal plants. Medicinal plants contain several secondary metabolites, including flavonoids, alkaloids, steroids, triterpenoids, glycosides, and sesquiterpenes. These metabolites are well known for their pharmacological effects, including antimicrobial and cytotoxic activities[1]. As of date, about 45 constituents have been identified in *P. barbata*, while more than 250 compounds have been isolated from the other *Premna* species, such as the *Premna*

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latifolia and the *Premna tomentosa*, consisting mainly of diterpenoids, iridoid glycosides and flavonoids, which play an important role in its many therapeutic activities, including antimicrobial, antioxidant, anti-inflammatory, immunomodulatory, antihyperglycemic and cytotoxic activities[2]. Hospitalacquired infections caused by *Staphylococcus* species are among the major clinical challenges. *Staphylococcus aureus* has traditionally received the most attention. Focusing on a single strain is not always beneficial when multiple Staphylococcal infections are present, particularly in medical settings. As such, other strains have also attracted increasing attention in recent years. These include multidrug-resistant coagulase-negative Staphylococci (CoNS), such as *S. epidermidis* and *S. hominis*. *S. hominis* (Gram-positive bacteria) is often isolated from patients suffering from blood infections. It is a spherical bacterium (cocci) that forms irregular, grape-like clusters with a size of 1.0-1.5 µm. As a major CoNS species, *S. hominis* is a common cause of infections, particularly in immunocompromised patients and neonates. It has been shown to cause inflammation of the endocardium, peritoneum, bones, joints, and the eye, as well as vulvar infections, and pus-containing inflammation of the skin and subcutaneous connective tissue. CoNS have long been linked with meningitis via foreign body implantation or any type of cerebrospinal fluid conduit, but despite knowledge, bacterial meningitis remains a life-threatening condition in multiple age groups, regardless. *S. hominis* has also been found to cause infections related to the upper respiratory tract and the oropharynx of the human body[3]. During air sampling conducted in a dental clinic to investigate the causes of such infections, it was found that 60-80% of Staphylococcus species were dominated by Staphylococcus hominis (22-24%), making it an abundant pathogenic bacterium. *Staphylococcal infections are most commonly treated with beta-lactam antibiotics*, *which inhibit* cell wall synthesis. However, methicillin-resistant strains, such as S. hominis, are resistant to nearly all β-lactam antibiotics because they carry the mecA gene, which encodes a penicillin-binding protein (PBP2a) with lower affinity for β-lactams. In addition to bacterial infections, parasitic infections contribute to mortality if not properly treated. Most common drugs for treating helminths include benzimidazoles, which, though effective, often cause a lot of side effects such as stomach-ache, liver issues and dizziness[4]. *P. barbata* contains several secondary metabolites that attract more research on their antimicrobial and antiparasitic properties. In this study, we used aqueous and ethanolic extracts of *P. barbata* to evaluate its antimicrobial (against *S. hominis*) and anthelmintic properties[5].

2. Materials and Methods

2.1 Preparation of Sample

Fresh Leaves of *P. barbata* were collected from the upper forests of Nainital district, Uttarakhand, India, and subsequently authenticated. After cleaning, the leaves were shade-dried at temperatures below 40°C and coarsely ground.

2.2 Plant Extraction Process

Premna barbata, dried leaves were defatted using petroleum ether for 24 hours, then they were filtered out and dried in a vacuum desiccator, followed by air drying. Aqueous (sample A) and ethanolic extraction (sample B) of the *P. barbata* leaves were separately extracted using a Soxhlet apparatus. Extractions were dried using a rotatory evaporator. The concentrated yields of the extracts were calculated and stored in amber colored vials[6].

2.3 Phytochemical Screening

Ethanolic and aqueous extracts of *P. barbata* were analysed for glycosides, alkaloids, flavonoids, phenols, tannins, proteins, steroids, and triterpenoids using standard phytochemical screening methods, including Kellar-Killiani, legal, Borntrager's, Modified Borntrager's, Dragendorff's, Mayer's, Wagner's, Shinoda, alkali, concentrated sulfuric acid, lead acetate, Salkowski, Zimmermann, Liebermann–Burchard, ferric chloride, Liebermann's, and phenolphthalein tests[7].

2.4 Antimicrobial Activity of the Extract against *Staphylococcus hominis* (Well Diffusion Assay)

The well diffusion method evaluates antimicrobial activity by measuring the inhibition zone around wells containing the test sample. As the compound diffuses into the agar, it inhibits microbial growth,

forming a clear zone that indicates antimicrobial potency. Mueller-Hinton agar plates and *S. hominis* were used, with vancomycin as a positive control. A fresh *S. hominis* culture was prepared in nutrient broth, incubated at 37°C for 16 to 18 h, and adjusted to a 0.5 McFarland standard (~1×10^8 CFU/mL). Sterilised Mueller-Hinton agar was poured into Petri dishes, solidified, and swabbed with the standardised culture. Wells approximately 6 mm in diameter were created using a sterile cork-borer and labelled as test or control. Stock solutions (100 mg/mL) were prepared in 10% ethanol and sterile distilled water, with 50 mg/mL and 25 mg/mL dilutions prepared as needed. Each well received 100 µL of the appropriate concentration. Vancomycin (1 mg/mL) and negative controls (ethanol and sterile distilled water) were added to separate wells. Plates were incubated at 37°C for 24 h[8].

2.5 Anthelmintic Activity of Aqueous Extract of *P. barbata*

The aqueous extract of *P. barbata* was evaluated for anthelmintic activity in *Metaphire posthuma* (earthworms). Earthworms collected from Premnagar, Dehradun, were washed, acclimatised for 30 min, and divided into seven groups of six. Test samples of the extract were prepared at 15, 25, 35, 45, and 50 mg/mL, with albendazole (20 mg/mL) as the standard and distilled water as the control. Each group was exposed to a different concentration, standard, or control in Petri dishes. Paralysis Time (PT) and Death Time (DT) were recorded, with paralysis defined as no movement except upon vigorous shaking and death confirmed by no movement in warm water (50°C) and fading body colour. The experiment was conducted in triplicate, and results were reported as mean ± standard error[9].

2.6 Molecular Docking Studies of *P. barbata* Phytoconstituents with *Staphylococcus hominis* and Anthelmintic Receptors

Molecular Docking Studies of *P. barbata* phytoconstituents with crystal structure of PLP-bound C-S lyase from *Staphylococcus hominis* (PDB id: 6QP2) and crystal structure of *Caenorhabditis elegans* ACR-23 in betaine and monepantel bound state associated with anthelmintic activity (PDB id: 8ZFK)[10]. As per the literature review, the leaves of *P. barbata* consisted of four main phytoconstituents, such as 1-Octen-3-ol, epi-alpha-bisabolol, rutin, and geniposidic acid[5,11]. 6QP2 receptor is an aminotransferase enzyme with two chains of 421 amino acids, and Pyridoxal-5'-Phosphate is present as a complexed ligand. 6QP2 receptor was developed using *Staphylococcus hominis* as the organism and *Escherichia coli* MC1061 as the expression system with 1.60 Å resolution.

8ZFK receptor is betaine receptor acr-23, soluble cytochrome b562 with five chains of 620 amino acids, and {N}-[(2~{S})-2-cyano-1-[5-cyano-2-(trifluoromethyl) phenoxy]propan-2-yl]-4-(trifluoromethylsulfanyl) benzamide is present as complexed ligand[12]. 8ZFK receptor was developed using *Caenorhabditis elegans*, *Escherichia coli* as the organism and *Spodoptera aff. frugiperda* 1 BOLD-2017 as an expression system with 2.64 Å resolution. The structures of 1-Octen-3-ol, epi-alpha-bisabolol, rutin, and geniposidic acid were drawn and energy minimised by Avogadro software[13]. The ligands and receptors were saved in PDBQT format[14]. The grid box sizes of 6QP2 and 8ZFK receptors were center_x = 3.971, center_y = -16.707, center_z = 27.891 and center_x = 168.083; center_y = 167.23, center_z = 184.285 with size_x = 24, size_y = 24, size_z = 24 and size_x = 40, size_y = 40, size_z = 40, exhaustiveness = 8. Autodock vina 1.2.7, MGLTools 1.5.7, and Drug Discovery Studio visualiser 4.5 were used for a molecular docking study[15].

3. Results and Discussion

3.1 Phytochemical Screening

The phytochemical analysis of both aqueous and ethanolic extracts of *P. barbata* was successfully carried out. Identification tests for fats and proteins were observed to be negative. Phytochemical analysis of both *P. barbata* aqueous and ethanolic extracts was done successfully with good results. Kellar-Kiliani, legal, Borntrager's and modified Borntrager's test for the identification of glycosides showed positive results for both samples. Dragendorff's, Mayer's, and Wagner's tests for alkaloid detection yielded positive results in both samples. The Shinoda test for flavonoids was positive in Sample A but negative in Sample B. The Alkali (alkaline reagent) test was negative for both samples, whereas the concentrated sulfuric acid test and the lead acetate test gave positive results in

both cases. For the identification of steroidal content, the Salkowski test showed positive results for both extracts while, the Zimmermann test and Liebermann-Burchard test were negative for both samples. Ferric chloride and Liebermann's test were observed to be positive (Sample A and Sample B) for the presence of phenol, and the Phenolphthalein test gave negative results for both samples.

3.2 Antimicrobial Activities of Aqueous (Sample A) and Ethanolic (Sample B) Extracts of *P. barbata* against *Staphylococcus hominis*

Both Sample A and Sample B were tested for antimicrobial potential at different concentrations (100mg/ml, 50mg/ml and 25mg/ml) as per standard protocol[16,17]. The antimicrobial activity of Sample A and Sample B was assessed against *Staphylococcus hominis* using the agar well diffusion method. Zones of Inhibition (ZOI) were recorded at concentrations of 100 mg/ml, 50 mg/ml, and 25 mg/ml, with Vancomycin serving as the positive control and sterile water and 10% ethanol as the negative control for sample A and sample B, respectively. All results showed potential to inhibit the growth of microorganisms, as shown in Table 1. Sample A demonstrated a clear dose-dependent antimicrobial effect against *S. hominis*. At 100 mg/ml, a ZOI of 20 mm was observed. At 50 mg/ml, the ZOI reduced to 17 mm; at 25 mg/ml, no inhibition was detected. The decreasing ZOI trend with decreasing concentration indicates that Sample A possesses measurable antibacterial potential, and its effectiveness correlates with concentration. However, its activity remains lower than the positive control (25 mm), suggesting moderate potency. Sample B showed variable antimicrobial performance across concentrations: At 100 mg/ml, Sample B produced a ZOI of 17 mm; at 50 mg/ml, reoccurrence of bacterial growth was observed, indicating loss of inhibitory effect at this dose. At 25 mg/ml, no inhibition was recorded. This indicates weaker activity compared to Sample A at the same concentration. The pattern suggests that Sample B has only mild antimicrobial activity, effective only at the highest concentration tested. While it is active at 100 mg/ml, its ZOI is smaller than the positive control and smaller than that of Sample A at the same concentration. The positive control (Vancomycin, 1 mg/ml) consistently produced a 25 mm inhibition zone, confirming assay reliability[18]. The negative control for both samples exhibited no inhibition, validating that solvent effects did not influence results. Based on the well diffusion assay results, both samples displayed antimicrobial activity against *Staphylococcus hominis*, but with distinct differences in potency and consistency; Sample A showed stronger and more consistent antimicrobial activity than Sample B, demonstrating a clear dose-dependent inhibition pattern with measurable ZOI at both 100 mg/ml and 50 mg/ml. Sample B showed weaker activity, producing inhibition only at the highest concentration (17 mm at 100 mg/ml) and failing to suppress bacterial growth at lower concentrations.

3.3 Anthelmintic Activity of *P. barbata* Aqueous Extract

In this study, the anthelmintic activity of *P. barbata* aqueous leaf extract was performed on *M. posthuma* earthworm. Different concentrations (15, 25, 35, 45, and 50) mg/mL of extract showed paralysis in the

Table 1. Zone of inhibition of aqueous (Sample A) and ethanolic (Sample B) extracts of *P. barbata* against *Staphylococcus hominis*

S. No.	Concentration	Zone of Inhibition (mm)	
		Aqueous extract of *P. barbata* (Sample A)	Ethanolic extract of *P. barbata* (Sample B)
1	100 mg/ml	20	17
2	50 mg/ml	17	Recurrence
3	25 mg/ml	NA	NA
4	Positive control (1.0 mg/ml)	25	25
5	Negative control	Sterile water	10% ethanol

NA: Not Available

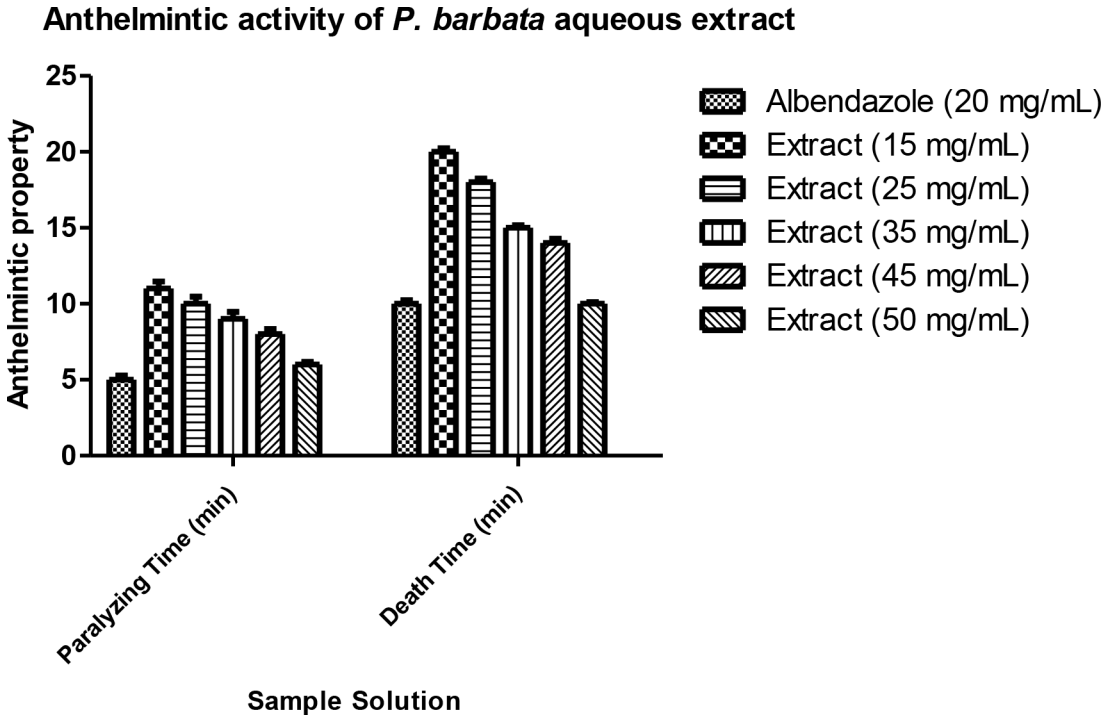


Figure 1. Anthelmintic activity of *P. barbata* aqueous extract with albendazole as reference.

Table 2. Molecular docking interaction data of *P. barbata* phytoconstituents with *Staphylococcus hominis* and Anthelmintic receptors

S. No.	Name of the compound	Receptor	Dock score (kcal/mol)	Interacting residues	Receptor	Dock score (kcal/mol)	Interacting residues
1	1-Octen-3-ol	8ZFK	-4.8	Pro 300[b], Leu 161[b], Leu 247[b], Tyr 244[b], Pro 307[b], Met 299[c], Ser 301[c], Val 306[c], Ser 303[c], Cys 305[c]	6QP2	-4.4	Ile 107[b], Val 108[b], Tyr 132[b], Ile 214[b], Phe 274[b], Lys 246[c], Tyr 72[c], Ser 245[c], Thr 276[c], Asp 212[c], Gly 106[c], Ala 109[c]
2	Rutin	8ZFK	-6.5	Val 246[b], Leu 243[b], Pro 242[c], Trp 590[c], Asn 583[c], Ala 251[c], Trp 587[c], Phe 166[c], Leu 584[c], Ser 303[c]	6QP2	-8.5	Tyr 72[a], His 105[a], Ala 109[a], Tyr 132[a], Glu 365[a], Gln 366[a], Val 108[b], Phe 274[b], Met 137[b], Ala 107[c], Gly 106[c], Gly 133[c], Pro 134[c], Ala 47[c], Val 46[c]
3	Geniposidic acid	8ZFK	-8.9	Asn 248[a], Thr 314[a], Thr 302[a], Cys 305[a], Ile 292[b], Ala 310[b], Ser 296[c], Ile 309[c], Tyr 244[c], Met 299[c], Pro 300[c], Ser 301[c]	6QP2	-7.6	Ala 47[a], Arg 376[a], Glu 362[a], Val 108[b], Pro 134[b], Phe 274[b], Met 137[c], Thr 276[c], Tyr 132[c], Asn 184[c], Phe 367[c], Tyr 72[c], Gly 133[c], Gln 366[c], Phe 367[c], Ile 107[c], Ala 109[c], Gly 106[c]
4	Epi-alpha-bisabolol	8ZFK	-6.7	Ile 292[b], Tyr 313[b], Val 295[b], Leu 247[b], Ala 310[b], Pro 307[b], Tyr 244[b], Val 306[b], Asn 248[c], Ser 296[c], Cys 305[c]	6QP2	-5.9	Ala 47[a], Glu 362[a], Met 17[b], Val 46[b], Tyr 72[b], Tyr 132[b], Tyr 246[c], Arg 376[c]

a: hydrogen bond interaction; b: hydrophobic interaction; c: van der Waals interaction

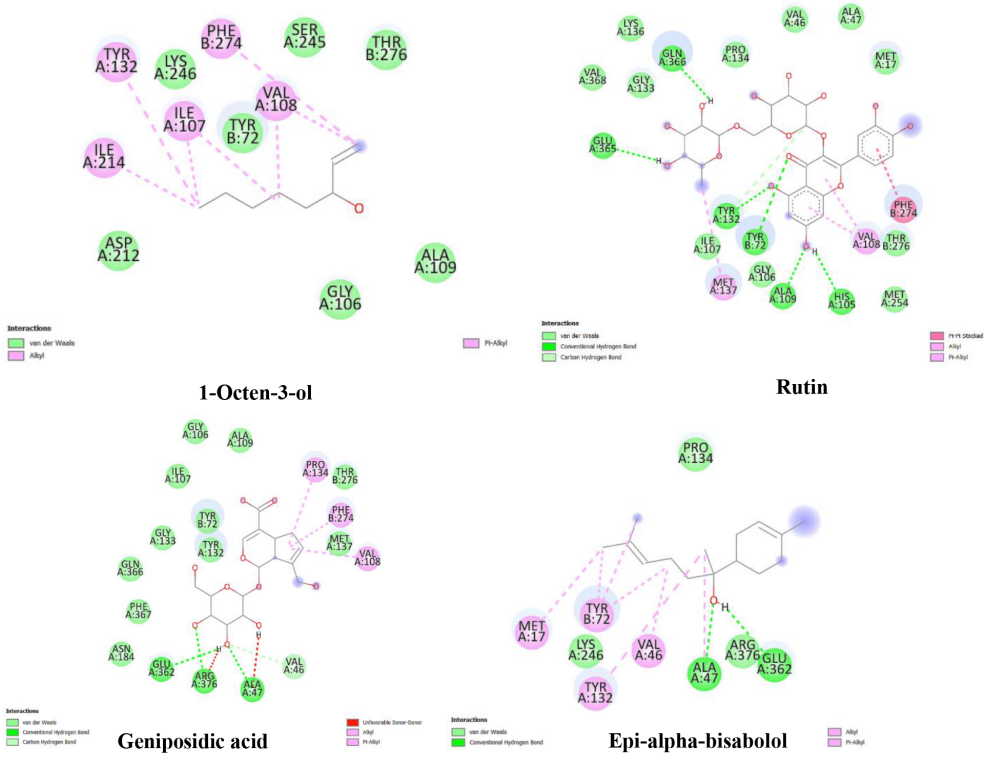


Figure 2. Molecular docking interaction data of *P. barbata* phytoconstituents with *Staphylococcus hominis* and Anthelmintic receptors.

earthworms at 11 min, 10 min, 9 min, 8 min, and 6 min, respectively. Also, earthworms died in the presence of different concentrations of *P. barbata* aqueous leaf extract at 20 min, 18 min, 15 min, 14 min, and 10 min, respectively. Aqueous extracts of *P. barbata* showed dose-dependent anthelmintic activity. The standard albendazole at 20 mg/mL concentration showed good anthelmintic activity, as paralysing and death times were 5 min and 10 min, respectively[19]. All the results were shown in Figure 1. GraphPad Prism 7.0 was used to plot the data in a graph.

3.4 Molecular Docking Interaction Data of *P. barbata* Phytoconstituents with *Staphylococcus hominis* and Anthelmintic Receptors

Molecular docking analysis data of *P. barbata* phytoconstituents with *Staphylococcus hominis* (PDB id: 6QP2) and anthelmintic receptor (PDB id: 8ZFK) showed that dock scores of 1-Octen-3-ol (-4.4 kcal/ mol), epi-alpha-bisabolol (-5.9 kcal/ mol), rutin (-8.5 kcal/ mol), geniposidic acid (-7.6 kcal/ mol), and 1-Octen-3-ol (-4.8 kcal/ mol), epi-alpha-bisabolol (-6.7 kcal/ mol), rutin (-6.5 kcal/ mol), geniposidic acid (-8.9 kcal/ mol), respectively[20,21]. In case of molecular docking interaction of best docked molecule rutin with *Staphylococcus hominis* (PDB id: 6QP2) showed hydrogen bond, hydrophobic, and van der Waals interactions with Tyr 72, His 105, Ala 109, Tyr 132, Glu 365, Gln 366; Val 108, Phe 274, Met 137; and Ala 107, Gly 106, Gly 133, Pro 134, Ala 47, Val 46, respectively[22]. In case of molecular docking interaction of best docked molecule geniposidic acid with anthelmintic receptor (PDB id: 8ZFK) showed hydrogen bond, hydrophobic, and van der Waals interactions with Asn 248, Thr 314, Thr 302, Cys 305; Ile 292, Ala 310; and Ser 296, Ile 309, Tyr 244, Met 299, Pro 300, Ser 301, respectively (Table 2 and Figure 2).

4. Conclusion

In this manuscript, the extraction of *P. barbata* was performed using aqueous and ethanol, along with antibacterial activity against *Staphylococcus hominis* and anthelmintic activity against *M. posthuma*. Aqueous extract of *P. barbata* showed good antibacterial and anthelmintic activities. As per *in silico* study data, rutin and geniposidic acid may be responsible for antibacterial activity against *Staphylococcus hominis* and anthelmintic activity, respectively. These findings highlighted the antibacterial activity against *Staphylococcus hominis* and anthelmintic activity against *M. posthuma* potentials of *P. barbata*.

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7. References

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Author Contribution

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