Original Article

In vitro Anthelmintic Impact of Various Extracts of *Pavetta tomentosa* Root on *Pheretima posthuma* and *in-silico* Molecular Docking Evaluation of some Isolated Phytoconstituents

Dintakurthi Sree Naga Bala Krishna Prasanth[1,*], Siva Prasad Panda[2], Atmakuri Lakshmana Rao[3], Nayudu Teja[4], Veenam Bhavya Naga Vani[3], Tera Sandhya[5], Pathange Bharghava Bhushan Rao[4]

[1]Pharmacognosy Research Division, K L College of Pharmacy, Koneru Lakshmaiah Education Foundation, Vaddeswaram, Guntur, Andhra Pradesh, INDIA.
[2]Pharmacology Research Division, K L College of Pharmacy, Koneru Lakshmaiah Education Foundation, Vaddeswaram, Guntur, Andhra Pradesh, INDIA
[3]Department of Pharmaceutical Analysis, V. V. Institute of Pharmaceutical Sciences, Gudlavalleru, Krishna, Andhra Pradesh, INDIA.
[4]Department of Pharmaceutics, V. V. Institute of Pharmaceutical Sciences, Gudlavalleru, Krishna, Andhra Pradesh, INDIA.
[5]Department of Pharmacology, Institute of Pharmaceutical technology, Sri Padmavati Manila Visvavidyalayam, Tirupati, Andhra Pradesh, INDIA.

ABSTRACT

Background: The current study assesses the anthelmintic impact of root extracts of *Pavetta tomentosa* on *Pheretima posthuma* compiled by molecular docking analysis of phytocompounds steemed from the plant with the β-Tubulin (PDB ID: 1SA0). **Methods:** In this study, *P. tomentosa* root was subjected to extraction using methanol and water. *In vitro,* anthelmintic activity was assessed by utilizing the *Pheretima posthuma* and *in silico* molecular docking was executed making use of Autodock 4.0. **Results:** The outcomes revealed that the methanolic extract has the most significant dose-dependent anthelmintic activity at various doses, followed by aqueous extracts of root. Amongst all the substances, β-eudesmol revealed the most effective docking rating of -6.53, which is nearer to Albendazole, i.e., -6.79, ensuring that β-eudesmol has a strong binding fondness in between protein and ligand. **Conclusion:** From the examinations, a conclusion can be drawn that the anthelmintic activity of *P. tomentosa* root in both *in vitro* and *insilico* assays. The information sustains β-eudesmol to be a useful anthelmintic compound beneficial to future clinical examinations.

Key words: *In-silico*, Autodock 4.0, *Pavetta tomentosa,* β-eudesmol, Albendazole, ADME/T.

INTRODUCTION

Considering that the beginning of the human world, alternative medicine with healing has been made use of in the therapy of numerous disorders.[1] According to the WHO, eighty percentile of the populace of a few Asian countries rely on conventional medicine in their day-to-day elements of healthcare.[2] About twenty-five percentile of the arbitrary drugs consist of plant-derived components and also about 120 active constituents are presently made use of in pharmaceutical products.[3]

The last fifty years of research study has offered a couple of medications made use of to treat human helminthiases infection; nevertheless, in lasting usage, lots of parasites are revealing resistance to these medications. The factor given for the reduced activity can be either due to the heritable changes (epigenetic or genetic) lack of ability of anthelmintic versus a populace of parasites or decrease in time to which medical therapy uses its impact. The usage of the plant can play an essential function in antihelmintic drug-target recognition.[4,5]

Submission Date: 04-01-2020;
Revision Date: 26-02-2020;
Accepted Date: 30-04-2020

DOI: 10.5530/ijper.54.2s.81

Correspondence:
Dr. Dintakurthi Sree Naga Bala Krishna Prasanth
Associate Professor, Department of Pharmacognosy, K L College of Pharmacy, Koneru Lakshmaiah Education Foundation, Vaddeswaram -522 502, Guntur, Andhra Pradesh, INDIA.
Phone: +91 7382027437
E-mail: dsnbkprasanth@kluniversity.in

www.ijper.org

Pavetta tomentosa Roxb. ex Smith., a therapeutic and consumable herb of the family Rubiaceae, is a plant having an elevation of 3 m high,[6] which extensively disburse in India and Indo-China in deciduous forests and scrub jungles long hill slopes.[7,8] *Pavetta tomentosa* continues to be presented the usage of the whole plant as Conventional Medication intended for the several treating illnesses. Cooked fruits are taken to eliminate intestinal worms, for a similar purpose recommended the flower extract. The stem bark extract of the plant has orally intended for liver disorders, like the hepatic stimulant and hepatoprotective.[9,10] Here, this study is performed to assess the possible anthelmintic activity of various portions of the *P. tomentosa* root and also its phytoconstituents. However, their anthelmintic activity is not well recorded, via researching their binding possibilities with β-Tubulin.

In the age of modern innovations, the analog system based technique is made use of in the evaluation of phytoconstituents of therapeutic plant essences with the help of molecular docking as well as likewise molecular attributes, which are essential devices in biology in addition to computer-assisted medication design.[11] In docking, the goal is to anticipate the primary binding site in betwixt a ligand and a protein of 3D structure, as well as individual ligand confirmation in the dynamic scoring of the protein, is placed using racking up feature.[12] In the 1990s, inadequate pharmacokinetic, as well as toxicity properties, triggers pricey last phase failings in drug development. So, *in silico*, ADMET modeling obtained a substantial interest in reasonable drug-design layout. Promising substances are explored for their pharmacokinetic properties, metabolic process, possible toxicity and also unfavorable results.

The chemical constituents and efficiency of extracts from genus Pavetta had been intensively explored in earlier research. The genus *Pavetta* has been reported to contain several phytoconstituents including linoleic acid, (9z,12z,15z)-octadecyl- 9,12,15-trienoic acid, proanthocyanidin, epicatechin and ferulic acid,[13] palmitic acid, stearic acid, myristic acid, capric acid, adipic acid, β-eudesmol, β-pinene, tetracontane, 3- methyl-4-heptanone, n-hexadecane, ethyl phthalate, tartronic acid,[14] epicatechin, (+)-catechin, ent-epicatechin, proanthocyanidin A_2 and proanthocyanidin A_4,[15] trans and cis octadecanoyl ferulate,[16] Pavetannins B7 and B8[17] and possess antiprotozoal, antimicrobial, antitumor,[18] anticonvulsant,[19] hepatoprotective,[20] and against *Schistosoma mansoni* infection.[21]

Our research study intended to assess the anti-helminthic potency of various portions of *P. tomentosa* extract as well as identify the molecular interactions existing between various phytoconstituents with the beta-tubulin enzyme.

MATERIALS AND METHODS

Collection and identification of plant material

Fresh plants of *P. tomentosa*, Rubiaceae, was gathered from Tirumala, Tirupati, Andhra Pradesh (13° 37' 44.6340" N and also 79° 25' 28.0056" E), acknowledged and also confirmed by Prof. K. Madhava Chetty, Plant Taxonomist, Assistant Professor, Department of Botany, Sri Venkateswara University, Tirupati, Andhra Pradesh, India.

Reagents and chemicals

All chemicals were of analytical grade (E. Merck, Darmstadt, Germany), except the methanol used for the preparation of extracts, which was of high-performance liquid chromatography grade (J.T. Baker, Center Valley, PA, USA). Albendazole (100% purity) was obtained from Sigma- Aldrich (#A0325100) bearing CAS number: 54965-21-8.

Preparation of extracts

About 1000 g of powdered drug of the root of *P. tomentosa* was extracted by Soxhelation with 5000 mL of petroleum ether, ethyl acetate, chloroform and methanol, for 18 hr. The aqueous extract was prepared by cold maceration method. The extracts were concentrated by distilling off the solvent and then evaporating to dryness on the water bath and stored in the refrigerator for future use.[22]

Preliminary phytochemical Screening

The root extract of *P. tomentosa* underwent initial phytochemical testing for the recognition of chemical components according to the standard operating procedures.[23-26]

Experimental Model

Adult Indian earthworms, *Pheretima posthuma* (*P. posthuma*) having anatomical as well as physiological resemblance with intestinal roundworm parasite of the person was made use of to assess anthelmintic activity. These were collected from moistened soil and washed with tap water to get rid of all fecal matter.

Collection of worms

The Indian earthworms, *Pheretima posthuma* (Annelida) utilized in today's research study, were gathered from damp soil of Vaddeswaram Village, Guntur District Andhra Pradesh, India.

Anthelmintic activity

A total of 72 earthworms were collected and divided into 12 groups, each of 6 worms. Various concentrations (25, 50, 75 and 100 mg/ml) of the extracts (PTME and also PTAQ) and standard (Albendazole), were prepared in distilled water of 10 ml. The earthworms have been formerly washed in tapped water, were launched into 10 ml of the corresponding Petri dish. Promptly after releasing the earthworms in the concerned Petri dishes, the time of launching was recorded and also consequently, the motility of the earthworms was observed. The time of paralysis was seen when the worms showed no movement except when worms were shaken vigorously. Also, the time of death was noted after determining that worms neither moved when shaken vigorously nor when dipped in warm water(40-50°C).[27,28]

Molecular Docking

The docking studies of compounds Albendazole, Adipic acid, β-eudesmol, β-pinene and tricyclene were carried out using Autodock 4.0 and Discovery studio Biovia 2017 software to find out the interaction between ligand and the target protein (Figure 1). The crystal structure of β-tubulin (1SA0) (Figure 2), was derived from the protein data bank. Physicochemical abilities of the ligands satisfied the standards of Lipinski's guideline of five or else understood as Lipinski's guideline of drug-likeness (Table 1).[29-32]

ADMET Analysis

ADMET of the ligands is their pharmacokinetic properties that are required to be examined to establish their function inside the body. The ADMET inheritance of the ligands was studied, making use of admetSAR.

Statistical Analysis

All information was revealed as the mean ± S.D; information went through one-way ANOVA adhered to by Tukey examination. The analytical evaluation executed with Graphpad Prism (Version 3, U.S.A.) software program. $P < 0.05$ was taken into consideration statistically considerable.

RESULTS

Phytochemical Screening of the extract

Initial phytochemical testing of *P. tomentosa* root exposed different phytoconstituents detailed in Table 2.

Anthelmintic activity

The extract displayed substantial dose-dependent anthelmintic activity in concentration as contrasted to standard, Albendazole (Table 3). At higher concentration, loss of mobility and also death was noticeable against *P. posthuma*. The time needed for triggering paralysis was (2.18±0.63) min and also fatality (4.55±0.09) min at 100 mg/ml by the extract, which was practically equivalent to the outcomes acquired with Albendazole (Figure 7 and 8).

Table 1: Physico-chemical properties of current ligands.

Physicochemical properties	Ligands				
	Albendazole	Adipic acid	β-Eudesmol	β-pinene	Tricyclene
Pubchem ID	2082	196	91457	14896	79035
Smiles	CCCSC1=CC2=C(C=C1)N=C(N2)NC(=O)OC	C(CCC(=O)O)CC(=O)O	CC12CCCC(=C)C1CC(CC2)C(C)(C)O	CC1(C2CCC(=C)C1C2)C	CC1(C2CC3C1(C3C2)C)C
Molecular Formula	$C_{12}H_{15}N_3O_2$	$C_6H_{10}O_4$	$C_{15}H_{26}O$	$C_{10}H_{16}$	$C_{10}H_{16}$
Molecular weight (g/mol)	265.33	146.14	222.37	136.23	136.23
Hydrogen-bond Donor Count	2	2	1	0	0
Hydrogen-bond Acceptor Count	4	4	1	0	0
Rotatable bond count	5	5	1	0	0
XLogP3	2.9	0.1	3.7	3.1	3.2
Molar Refractivity	73.22	34.5	70.46	45.22	43.32
NO. of Deviations	0	1	0	0	0

Table 2: Phytochemical analysis of various extracts of the root of *P. tomentosa*.

Phytoconstituents	Method	Aqueous Extract	Alcohol Extract	Chloroform Extract	Ethyl acetate Extract	Pet. Ether Extract
Flavonoids	Shinoda Test	+	+	-	+	-
	Zn. Hydrochloride test	+	+	-	+	-
	Lead acetate Test	+	+	-	+	-
Volatile oil	Stain test	+	+	-	-	-
Alkaloids	Wagner Test	+	+	+	-	-
	Hager's Test	+	+	+	-	-
Tannins and Phenols	$FeCl_3$ Test	+	+	-	+	-
	Potassium dichromate test	+	+	-	+	-
Saponins	Foaming Test	+	+	-	-	-
Steroids	Salkowski test	+	+	+	-	+
Carbohydrates	Molish test	+	+	-	-	-
Acid compounds	Litmus test	-	-	-	-	-
Glycoside	Keller-Killani Test	+	+	-	-	-
Amino acids	Ninhydrin test	+	+	-	-	-
Proteins	Biuret test	+	+	-	-	-

"+" – Present; "-"- Absent

Table 3: Anthelmintic activity of aqueous and methanolic root extract of *Pavetta tomentosa* against *Pheretima posthuma*.

Conc. (mg/ml)	Paralysis Time (min)		Death Time (min)		Albendazole		
	PTME	PTAE	PTME	PTAE	Conc. (mg/ml)	Paralysis Time (min)	Death Time (min)
Control	---	---	---	---	---	---	---
25	15.45±2.52*	18.85±3.53*	22.86±1.85*	26.12±2.63*	25	10.86±1.25	16.52±0.86
50	9.75±1.15#	13.58±1.25#	18.52±2.02#	23.85±2.85#	50	6.8±0.75	11.86±0.36
75	6.58±1.87*	11.23±2.55*	10.56±2.18*	14.48±1.88*	75	3.6±0.51	7.22±0.65
100	2.18±0.63$	8.32±1.33$	4.55±0.09$	12.22±2.13$	100	2.2±0.06	4.15±0.21

Values are expressed as mean±S.D (n=6), *, p<0.05, #, p<0.01 and $, p<0.001 versus Standard. PTME=Crude Methanolic extract of *Pavetta tomentosa*; PTAE= Crude Aqueous extract of *Pavetta tomentosa*.

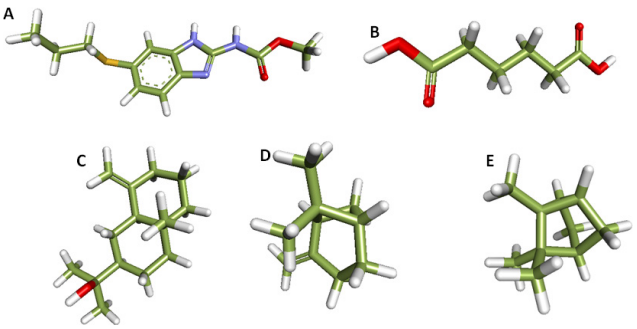


Figure 1: The Three Dimensional structures of ligands. (a) Albendazole (b) Adipic acid (c) β-eudesmol (d) β-pinene (e) Tricyclene.

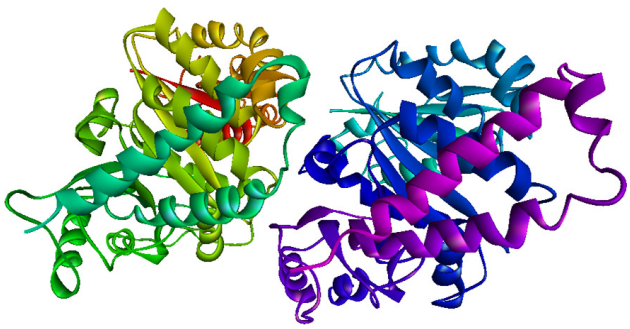


Figure 2: Three Dimensional Structure of the molecular target, Tubulin-Colchicine: Stathmin-Like Domain Complex (1SA0).

Table 4: Binding affinites of isolated compounds at the active site of β-Tubulin.

Ligands	Highest to Lowest mode of conformation with corresponding RMS binding affinities in ΔG (Kcal/mol)								
	1	2	3	4	5	6	7	8	9
Albendazole	-6.79	-6.27	-5.9	-5.89	-5.84	-5.74	-5.65	-5.54	-5.31
Adipic acid	-1.56	-1.19	-1.03	-1.03	-1	-0.59	-0.55	-0.33	-0.33
β-Eudesmol	-6.53	-6.51	-6.47	-6.3	-6.15	-5.94	-5.93	-5.77	5.75
β-pinene	-5.24	-5.22	-5.21	-5.21	-5.2	-5.2	-5.19	-5.18	-5.11
Tricyclene	-5.05	-5.05	-5.04	-5.04	5.02	-4.38	-4.23	-4.23	-4.23

Table 5: Interactions of β-Tubulin amino acid residues with ligands at receptor sites.

Ligands	Binding Affinity, ΔG (Kcal/mol)	Amino acids involved and Distance (A°)		
		Hydrogen Binding Interactions	Hydrophobic Interactions	Electrostatic Interactions
Albendazole	-6.79	Gly142 (3.75), Glu183 (4.94), Ser178 (5.25), Ala174 (4.06)	Pro173(4.48)	Ala12 (4.69), Ser140(4.47)
Adipic acid	-1.56	Lys254 (4.45), Asn249 (3.23)	-	-
β-Eudesmol	-6.53	Ala174 (4.11), Val177 (4.42)	Pro173 (4.39)	Ala12 (5.05)
β-pinene	-5.24	-	-	Ala12 (5.04), Ile171 (4.97), Pro173 (4.35)
Tricyclene	-5.05	-	-	Ala12 (4.77), Ile171 (4.42), Pro173 (4.18)

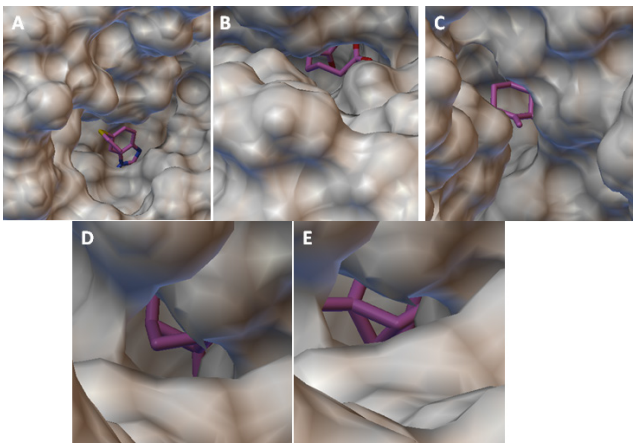


Figure 3: *In silico* Docked complexes of Ligand (Ball and Stick representation) with Tubulin-Colchicine: Stathmin-Like Domain Complex (1SA0) (Molecular representation) by Autodock 4.0. (a) Albendazole (b) Adipic acid (c) β-eudesmol (d) β-pinene (e) Tricyclene.

Computational Study

In today's examination, to evaluate the possibility of substances accountable for anthelmintic activity, the docking score was made use of to verify the prospective binding energy. The molecules were additionally based on iLOG predictors utilizing online tools to identify their ADME/T properties.

Docking researches revealed that out of the five substances consisted of in the study, β-eudesmol had the most excellent docking rating of -6.53, which showed both hydrogen bond interactions (Ala174, Val177) and also hydrophobic interactions (Pro173) with the β-tubulin enzyme. β-pinene and also tricyclene revealed no hydrogen bonding and even hydrophobic interactions with the amino acids of the β-tubulin, however, had significant electrostatic communications. The standard Albendazole revealed the highest possible docking rating of - 6.79. The outcomes gotten by the autodock 4.0 are shown in Table 3, as well as the protein-ligand interactions revealing hydrogen bonding and also binding settings are additionally published in Tables 4 and 5 (Figure 3-6).

ADME/T evaluation by using admetSAR

The ADMET properties of the ligands were assessed, making use of admetSAR. ADMET properties for the substances in the research study were evaluated, making use of admetSAR. All the substances revealed excellent human intestinal solubility (HIA), blood-brain barrier (B.B.B.) infiltration. No medication was cancer-causing. All the compounds were AMES negative. The results of HIA, B.B.B., LD_{50} values for the compounds are listed in Table 6.

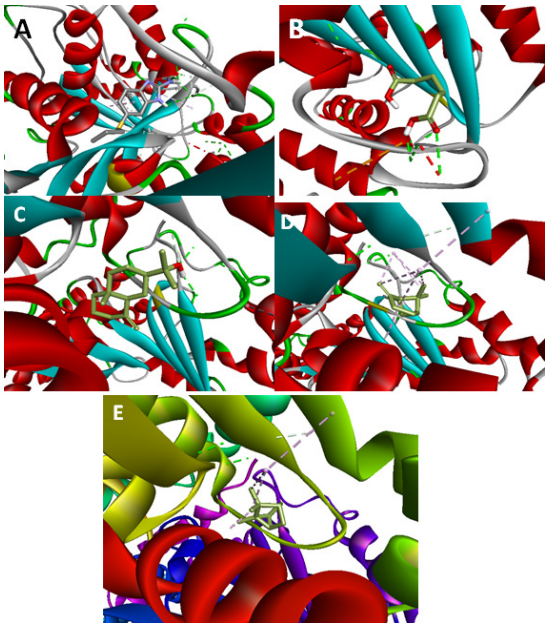


Figure 4: The ligands (Ball and Stick) are docked into the binding cavity of the receptor (Cartoon), and the putative conformations are explored by using Discovery Studio Visualizer 2017. (a) Albendazole (b) Adipic acid (c) β-eudesmol (d) β-pinene (e) Tricyclene.

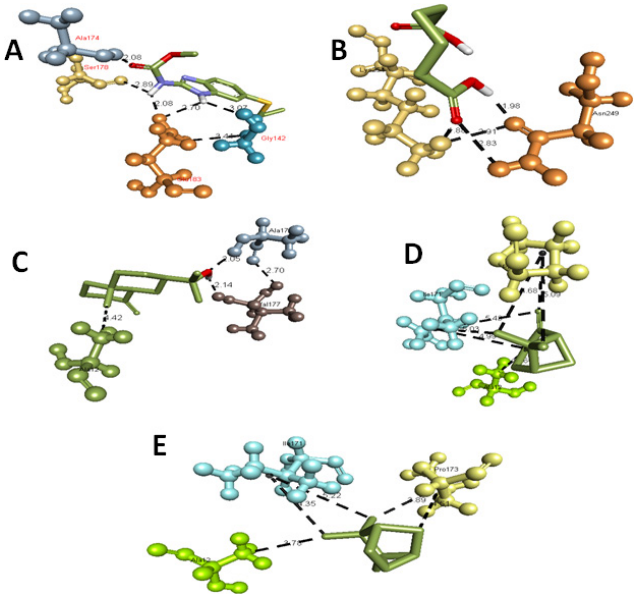


Figure 6: Various three dimensional Interactions of ligands with Tubulin-Colchicine: Stathmin-Like Domain Complex (1SA0). a) Albendazole (b) Adipic acid (c) β-eudesmol (d) β-pinene (e) Tricyclene.

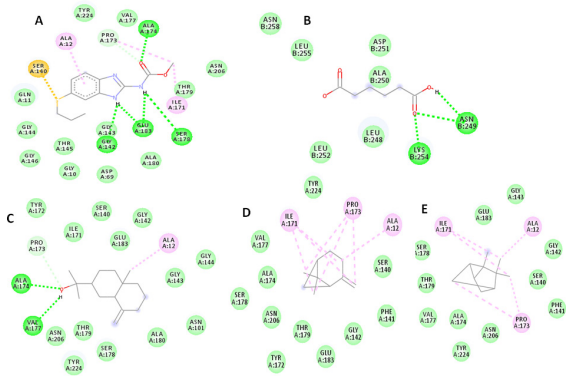


Figure 5: Various Two dimensional Interactions of ligands with Tubulin-Colchicine: Stathmin-Like Domain Complex (1SA0). a) Albendazole (b) Adipic acid (c) β-eudesmol (d) β-pinene (e) Tricyclene.

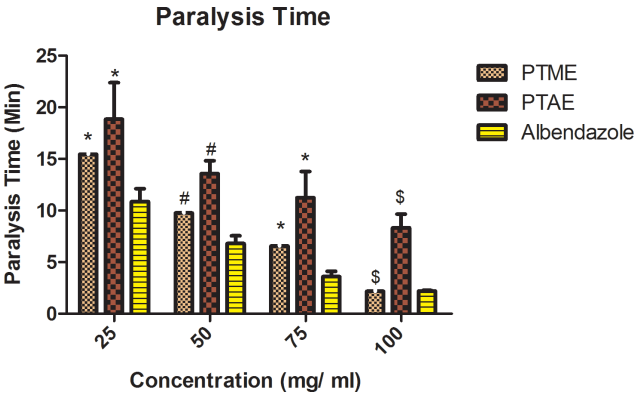


Figure 7: Paralysis Time for Aqueous and Methanolic Extracts of *Pavettta tomentosa* concerning Albendazole.

Table 6: ADME/T Properties of different compounds from *Pavetta tomentosa*.

Compound	HIA	BBB	AMES Toxicity	Carcino-genicity	LD_{50} in rat (mol/kg)
Albendazole	0.9944	0.9381	Non-toxic	Non-carcinogenic	2.0752
Adipic acid	0.5319	0.8236	Non-toxic	Non-carcinogenic	1.4221
β-Eudesmol	0.995	0.9596	Non-toxic	Non-carcinogenic	1.8911
β-pinene	0.9834	0.9229	Non-toxic	Non-carcinogenic	1.4934
Tricyclene	0.9956	0.9827	Non-toxic	Non-carcinogenic	2.0257

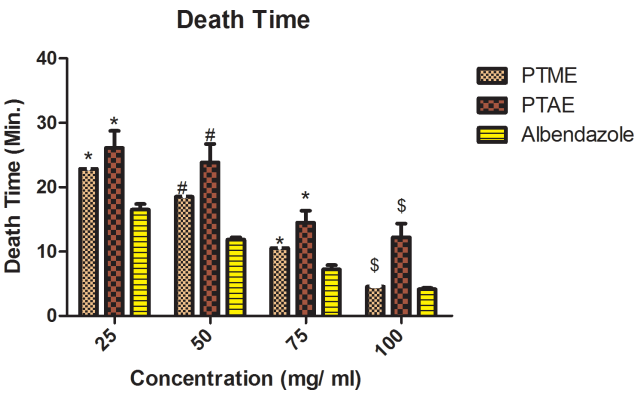


Figure 8: Death Time for Aqueous and Methanolic Extracts of *Pavettta tomentosa* concerning Albendazole.

DISCUSSION

Phyto-compounds have gotten interested as a possible resource of new healing representatives. Many of the scientifically active medications are from natural resources, which show the significance of medicines having all-natural remedies in medicine exploration procedure. In this view, *P. tomentosa* has been checked out for the assessment of anti-helminthic task utilizing earthworm complied with by molecular docking research study as well as ADMET evaluation.[33]

Helminths infection is thought about to be an essential issue in humans and also pets that bring about a disastrous as well as a persistent illness, which inevitably results in a fatality as well as likewise triggers drug resistance to various other conditions. To avoid an epidemic of helminths, there is a requirement for researches concentrating on all-natural products such as medicinal plants which provide new bioactive substances having no or less unwanted effects, conveniently readily available to individuals of establishing nations as well as even more significantly, they have the best compatibility with human physiology than traditional medications.[34,35] Several bioactive phytoconstituents such as alkaloids, flavonoids, saponins, as well as tannins were discovered primarily throughout the phytochemical evaluation of the PTME and PTAE which have been related to anti-helminthic activity.[36]

Our current research study wraps up that PTME and PTAE have been located to have a considerable anthelmintic capacity in a dose-dependent way. A few of these phytoconstituents such as alkaloids, tannins, phenols and so on might be accountable for the substantial anthelmintic task. Alkaloids can create paralysis by acting upon the C.N.S. In contrast, polyphenols and also tannins uniquely bind to complementary proteins existing in the G.I. system and, even at some point, create fatality. On the various other hands, the anthelmintic effectiveness of saponins is because of its membrane layer permeabilizing properties.

On the other hand, organic medications that have been utilized given that the old times keep reduced toxicity, have far better absorption, as well as abundant. Scientists around the world remain in search of plants that have such biological activities, which will undoubtedly aid in the improvement of the existing clinical system, making less expensive as well as reliable therapy.

Online testing, utilizing molecular docking programs, has ended up being a significantly prominent method to the advancement of new medicines, partly due to the desired time and also budgeting prices of *in silico* medication testing compared to standard lab experiments. In this research, we used a docking method making use of open software programs as well as virtualized. Interactions of the ligands adipic acid. β-eudesmol, β-pinene, tricyclene and standard, Albendazole with the anti-helminthic protein β-Tubulin.

ΔG indicates informative of ligand docking in the active site of a protein, kind of molecular communications, such as hydrogen bond, hydrophobic, as well as likewise electrostatic interactions, with necessary amino acid, which is a step of ligand docking in favorable conformations. Hydrophobic synergy is the main aspect of the firmness of proteins. Hydrogen bonding furthermore maintains protein firmness, yet to a minimized degree than hydrophobic synergy.

Our results disclose that electrostatic, hydrophobic and hydrophilic communications are regulated by numerous amino acid deposits in each ligand-protein communication. Specifically, Ala12 was determined in all electrostatic interactions of all ligands with β-tubulin other than for adipic acid. No hydrophobic interactions were existing in adipic acid, β-pinene and also tricyclene with β-tubulin. Even no hydrogen bonds were living in β-pinene and also tricyclene.

CONCLUSION

The outcomes confirm the ethnomedicinal use of *P. tomentosa* to anthelmintic activity, which recommends that this plant might be a possible resource for the growth of a new anthelmintic representative. The here and now molecular docking experiments suggest that adipic acid. β-eudesmol, Tricyclene as well as β-pinene are prospect ligands for anthelmintic activity as well as act with interactions with β-Tubulin. High-throughput evaluating making use of molecular docking evaluation brought about the final thought that eudesmol revealed ideal fitness score as well as appropriates for personal usage, specifically. Even more, intricate measurable S.A.R. is needed to guarantee its safety and also bioefficacy. Additionally, *in vivo* experiments are required to verify these *in silico* outcomes.

ACKNOWLEDGEMENT

The authors thank Dr. K. Madhavachetty, plant taxonomist, Department of Botany, Sri Venkateswara University, Tirupati, Andhra Pradesh, for identifying and authenticating the plant material and also thank Management of K L College of Pharmacy, Vaddeswaram, Guntur (Dt.), Andhra Pradesh for providing the research facilities.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

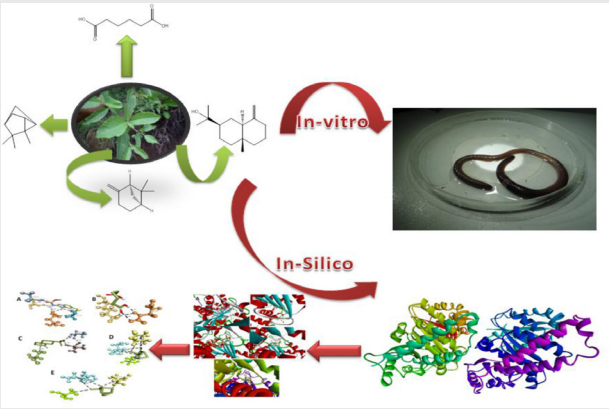
ABBREVIATIONS

HIA: Human Intestinal Absorption; **B.B.B.:** Blood-Brain Barrier; **LD_{50}:** Lethal Dose 50%; **RMSD:** Root mean square deviation; **PTME:** Crude Methanolic extract of *Pavetta tomentosa;* **PTAE:** Crude Aqueous extract of *Pavetta tomentosa*.

REFERENCES

1. Mohamed I, Shuid A, Borhanuddin B, Fozi N. The application of phytomedicine in modern drug development. The Internet Journal of Herbal and Plant Medicine. 2012;1(2):1-9.
2. Robinson MM, Zhang X. The world medicines situation 2011, traditional medicines: Global situation, issues and challenges. World Health Organization, Geneva. 2011;1-12.
3. Rates SMK. Plants as source of drugs. Toxicon. 2001;39(5):603-13.
4. Shalaby HA. Anthelmintics resistance: How to overcome it?. Iranian Journal of Parasitology. 2013;8(1):18.
5. Geerts S, Gryseels B. Drug resistance in human helminths: Current situation and lessons from livestock. Clin Microbiol Rev. 2000;13(2):207-22.
6. Pullaiah T, Mohammed MS. Flora of Ranga Reddi District Andhra Pradesh, India: Daya Books. 2000.
7. Sivarajan V, Balachandran I. Ayurvedic drugs and their plant sources: Oxford and I.B.H. publishing. 1994.
8. Balfour E. The Cyclopaedia of India and of Eastern and Southern Asia: Akademische Druck-u. Verlagsanstalt. 1885.
9. Quattrocchi U. C.R.C. world dictionary of medicinal and poisonous plants: common names, scientific names, eponyms, synonyms and etymology. C.R.C. Press. 2016;5.
10. Khare CP. Ayurvedic pharmacopoeial plant drugs: Expanded therapeutics. Routledge. 2015.
11. Sørensen J, Demir Ö, Swift RV, Feher VA, Amaro RE. Molecular docking to flexible targets. Molecular Modeling of Proteins: Springer. 2015;445-69.
12. Meng XY, Zhang HX, Mezei M, Cui M. Molecular docking: A powerful approach for structure-based drug discovery. Curr Comput Aided Drug Des. 2011;7(2):146-57.
13. Raama MJ, Venkataraman S, Meera R, Prasad S, Devi P. Phytochemical Investigation Of *Pavetta indica*. International Journal of Chemical Sciences. 2010;8(3):1517-22.
14. Suresh S, Pradheesh G, Alex RV. Phytochemical Screening and GCMS Studies of the Medicinal Plant *Pavetta indica* Linn. American Journal of Ethnomedicine. 2015;2(6):347-55.
15. Baldé AM, Pieters LA, Gergely A, Kolodziej H, Claeys M, Vlietinck AJ. A-type Proanthocyanidins from stem-bark of *Pavetta owariensis*. Phytochemistry. 1991;30(1):337-42.
16. Baldé AM, Claeys M, Pieters LA, Wray V, Vlietinck AJ. Ferulic acid esters from stem bark of *Pavetta owariensis*. Phytochemistry. 1991;30(3):1024-6.
17. Balde AM, DeBruyne T, Pieters L, Kolodziej H, Vanden BD, Claeys M, *et al*. Oligomeric proanthocyanidins possessing a doubly linked structure from *Pavetta owariensis*. Phytochemistry. 1995;38(3):719-23.
18. Baldé ES, Megalizzi V, Traoré MS, Cos P, Maes L, Decaestecker C, *et al*. *In vitro* antiprotozoal, antimicrobial and antitumor activity of *Pavetta crassipes* K. Schum leaf extracts. Journal of Ethnopharmacology. 2010;130(3):529-35.
19. Sharma J, Gairola S, Gaur RD, Painuli RM, Siddiqi TO. Ethnomedicinal plants used for treating epilepsy by indigenous communities of sub-Himalayan region of Uttarakhand, India. Journal of Ethnopharmacology. 2013;150(1):353-70.
20. Jyothi RG, Prasanth RV, Sreepavani M, Rajaram C, Nelson KS, Kanhere RS. Evaluation of hepatoprotective potential of ethanolic extract of *Ixora pavetta* against isoniazid and rifampicin induced hepatotoxicity in rats. Drug Invention Today. 2013;5(3):201-6.
21. BaldÉ AM, Marck EV, Vanhaelen M. *In vivo* activity of an extract of *Pavetta owariensis* bark on experimental *Schistosoma mansoni* infection in mice. Journal of Ethnopharmacology. 1986;18(2):187-92.
22. Chander PA, Sri HY, Sravanthi NB, Susmitha UV. *In vitro* anthelmintic activity of *Barleria buxifolia* on Indian adult earthworms and estimation of total flavonoid content. Asian Pacific Journal of Tropical Disease. 2014;4:S233-5.
23. Kokate C. Practical pharmacognosy. Vallabh Prakashan, New Delhi. 1986;111.
24. Raaman N. Phytochemical techniques. Pitam Pura, New Delhi: New India Publ. Agency. 2006.
25. Wallis TE. Textbook of pharmacognosy. 1955;3.
26. Khandelwal KR. Practical pharmacognosy: Techniques and experiments. Maharashtra: Niral Prakashan. 2008.
27. Chander PA, Sri HY, Sravanthi NB, Susmitha UV. *In vitro* anthelmintic activity of *Barleria buxifolia* on Indian adult earthworms and estimation of total flavonoid content. Asian Pacific Journal of Tropical Disease. 2014;4:S233-5.
28. Mahato K, Kakoti BB, Borah S, Kumar M. Evaluation of *in-vitro* anthelmintic activity of *Heliotropium indicum* Linn. leaves in Indian adult earthworm. Asian Pacific Journal of Tropical Disease. 2014;4:S259-62.
29. Trott O, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading. J Comput Chem. 2010;31(2):455-61.
30. Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, *et al*. Auto Dock 4 and Auto Dock Tools 4: Automated docking with selective receptor flexibility. J Comput Chem. 2009;30(16):2785-91.
31. Lim SV, Rahman MB, Tejo BA. Structure-based and ligand-based virtual Screening of novel methyltransferase inhibitors of the dengue virus. BMC Bioinformatics: Bio Med Central. 2011;12(13):S24.
32. Jaghoori MM, Bleijlevens B, Olabarriaga SD. 1001 Ways to run Auto Dock Vina for virtual Screening. J Comput Aided Mol Des. 2016;30(3):237-49.
33. Saleh-e-In MM, Sultana N, Hossain MN, Hasan S, Islam MR. Pharmacological effects of the phytochemicals of *Anethum sowa* L. root extracts. BMC Complement Altern Med. 2016;16(1):464.
34. Sreejith M, Kannappan N, Santhiagu A, Mathew AP. Phytochemical, Anti-oxidant and Anthelmintic activities of various leaf extracts of *Flacourtia sepiaria* Roxb. Asian Pac J Trop Biomed. 2013;3(12):947-53.
35. Maisale A, Attimarad S, Haradagatti D, Karigar A. Anthelmintic activity of fruit pulp of Cordia dichotoma. International Journal of Research in Ayurveda and Pharmacy. 2010;1(2):597-600.
36. Jamkhande PG, Barde SR. Evaluation of anthelmintic activity and *in silico* PASS assisted prediction of *Cordia dichotoma* (Forst.) root extract. Ancient Science of Life. 2014;34(1):39.

PICTORIAL ABSTRACT



SUMMARY

- The methanolic extract of *Pavetta tomentosa* has significant anthelmintic activity in comparison with aqueous extract.
- All the isolated constituents showed good docking scores in comparison with standard Albendazole.
- Amongst the isolated compounds, β-eudesmol has potent efficacy as an anthelmintic drug, with a docking score of -6.53.
- All the isolated compounds have no toxicity and are non-carcinogenic.

About Authors

Dr. D.S.N.B.K. Prasanth is working as an Associate Professor at K L College of Pharmacy, Koneru Lakshmaiah Education Foundation, Vaddeswaram, Guntur, Andhra Pradesh, INDIA. He is having 8 years of Teaching and Research experience. He guiding 1 Ph.D. Scholars and 20 B.Pharm Candidates. He published 25 papers in various International and National Journals. He is Reviewer and Editorial Board Member for some reputed International and National journals. He is having memberships in 2 professional societies.

Dr. Siva Prasad Panda is working as an Associate Professor at K L College of Pharmacy, Koneru Lakshmaiah Education Foundation, Vaddeswaram, Guntur, Andhra Pradesh, INDIA. He is having 15 years of Teaching and Research experience. He guiding 5 Ph.D. Scholars and 35 B.Pharm Candidates. He published 20 papers in various International and National Journals. He is Reviewer and Editorial Board Member for some reputed International and National journals.

Dr. A. Lakshmana Rao is working as a Professor and Principal of V. V. Institute of Pharmaceutical Sciences, Gudlavalleru, A.P. He is having 20 years of Teaching, Research and Administrative experience. He guided 9 Ph.D. Scholars and 50 M.Pharm. Candidates. He received many awards and prizes from various organizations. He received Dr.APJ Abdul Kalam Award for Teaching Excellence from Marina Labs, Chennai; Noble Principal of the Year Award from Operant Pharmacy Federation, Rajasthan and Principal of the Year Award from Association of Pharmacy Professionals, Bhopal. He conferred with Meritorious University Best Teacher Award from Jawaharlal Nehru Technological University Kakinada, Kakinada. He is given 10 Guest Lectures in different universities and colleges. He published 295 papers in various International and National Journals. He published 1 Text Book and 2 E-Books. He is Editor-in-Chief, Reviewer and Editorial Board Member for 109 reputed International and National journals. He organized 25 Seminars, Conferences and Workshops. He participated 89 Seminars, Conferences and Workshops. He presented 32 scientific papers in various Seminars and Conferences and received 12 prizes. He is having 1 Indian Patent in his credit. He received Grants from AICTE and PCI. He is having memberships in various professional societies like IPA, APTI, ABAP, APP, ISTE etc.

Mr. N. Teja, is currently pursuing M. Pharm of Pharmaceutics at V. V. Institute of Pharmaceutical Sciences, Seshadri Rao Knowledge Village, Gudlavalleru, Andhra Pradesh, INDIA.

About Authors

Veenam Bhavya Naga Vani, is currently pursuing M.Pharm of Pharmaceutical Analysis at V. V. Institute of Pharmaceutical Sciences, Seshadri Rao Knowledge Village, Gudlavalleru, Andhra Pradesh, INDIA

Ms. T.Sandhya, is currently pursuing M.Pharm of Pharmacology at Sri Padmavathi School of pharmacy, Tirupati, Andhra Pradesh, INDIA.

Dr. P. Bhargava Bhushan Rao is working as an Associate Professor at V. V. Institute of Pharmaceutical Sciences, Seshadri Rao Knowledge Village, Gudlavalleru, Krishna, Andhra Pradesh, INDIA. He is having 11 years of Teaching and Research experience. He guided 40 B. Pharm Candidates. He published more than 15 papers in various International and National Journals. He is Reviewer and Editorial Board Member for some reputed International and National journals.

Cite this article: Prasanth DSNBK, Panda SP, Rao AL, Teja N, Vani VBN, Sandhya T, Rao PBB. *In vitro* Anthelmintic Impact of Various Extracts of *Pavetta tomentosa* Root on *Pheretima posthuma* and *in-silico* Molecular Docking Evaluation of some Isolated Phytoconstituents. Indian J of Pharmaceutical Education and Research. 2020;54(2s):s251-s260.