

# A Theoretical Review and Molecular Docking Study of *Sphaeranthus amaranthoides*

Yuvraj M Katu, Richa Jain\*

Department of Biotechnology and Microbiology, CSRD, People's University Bhopal, Madhya Pradesh, India.

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## ABSTRACT

*Sphaeranthus amaranthoides* Linn is a tiny, procumbent herb that grows in a semiaquatic habitat and has spreading branches. It is a member of the Asteraceae family. In the practice of siddha, it serves as an energizing aid. A wide variety of ailments, including eczema, blood ailments, stomach worms, filaria, fever, skin illnesses, anti-helminthes, and jaundice, were alleviated with the help of this herb. Wound healing, antidiarrheal, antibacterial, analgesic, anti-inflammatory, hepatoprotective, anti-diabetic, anti-mutagenic and antioxidant effects were among the observed benefits. The current article summarizes the many plant-related activities that have been documented.

**Keywords:** *Sphaeranthus amaranthoides*, Asteraceae, Ailments, Hepatoprotective.

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## INTRODUCTION

People have been using herbal remedies since the beginning of time. According to Ayurveda, India's oldest traditional system, ancient Indians knew a great deal about the healing properties of various plants. Because of its vastly different climates and topographies, India boasts an exceptionally diverse floral kingdom. Many of the crude medications utilized in ancient systems have been scientifically explored since the birth of science.<sup>1,2</sup> Figure 1 displayed an image of *Sphaeranthus amaranthoides* plant.

The little procumbent herb *S. amaranthoides* Burm (Asteraceae) has a stem rooting system, and its leaves are palmately 3-foliolate and covered in appressed hair. It thrives in the paddy fields of India, especially in the southern regions of Tirunelveli, Thanjur, and Travancore. *S. amaranthoides* is also rich in alkaloids, steroids, phenolics, sugars, saponins, amino acids, flavonoids, and tannins, as shown by a phytochemical examination of crude extracts.<sup>3,4</sup> Traditional Indian medicine makes extensive use of *S. amaranthoides*, a medicinal herb. It is endemic to India's tropical regions' rice paddies, dry waste areas, and cultivated plains.<sup>5</sup> This little procumbent herb, *S. amaranthoides* Linn. thrives in a semi-aquatic setting. The stems root and are glabrous with appressed hairs; the leaves are palmately trifoliolate. It is a member of the Asteraceae family. Eczema, blood diseases, stomach worms, filarial, and fever are just few of the conditions that this plant can alleviate. It's effective against kapha, vata, and piles, too. Used for

the treatment of skin disorders.<sup>6</sup> The plant's blossoms have cleansing, refreshing, and strengthening properties. Both the seeds and the root are employed as anti-helminthic and stomachic.<sup>7</sup> Powdered leaves can be applied topically for the treatment of jaundice, urethral discharges, and persistent skin conditions.<sup>8</sup> Many different species of this plant can be found in the tropical regions of Asia, Africa, and Australia. It is a common weed in rice fields in the southern Indian states of Tanjore, Thirunelveli, Southern Mysore, and Travancore.<sup>9</sup> *Sphaeranthus indicus*, a closely similar species, has been linked to a variety of interesting phenomena.<sup>10</sup>

## Therapeutic Effects of Plant<sup>11,12</sup>

### Wound healing

Wounded tissue breaks down. Wound healing involves various biochemical and cellular processes. Coagulation stops blood vessel bleeding. Analgesics to expensive chemotherapeutics are utilized to treat wounds. The plant reported wound healing properties earlier.

### To treat diarrhea

The WHO has launched a diarrhoeal ailment regulator campaign to eliminate the death rate caused by diarrhea in developing countries. The use of traditional medicine is recognized as a valid complement to Western treatment.

### Antibacterial effect

It has been proved as an antibacterial against various bacterial strains.



Figure 1: *S. amaranthoides* plant

- Hypoglycemic effect
- Antipyretic effect
- Hepatoprotective effect
- Nephroprotective effect
- Antioxidant effect
- Antiviral effect

### Microscopy of Plant

Lamina cross-sections showed the leaf's dorsoventrally. The epidermis has roughly barrel-shaped cells, followed by a palisade mesophyll layer and a spongy layer with somewhat lobed, closely isodiametric globular cells. Trichomes are club-shaped glandules. The palisade-spongy mesophyll interstice occasionally showed vascular bundles. Cell size distinguishes the upper and lower epidermis. The abaxial side of the midrib has 1 to 3 resin canals and arcuate collateral vascular bundles. Adaxial foliar epidermis cells exhibit uneven contours. Both sides had ranunculaceous and cruciferous stomata. Confirmation then contamination for standardization of *S. amaranthoides* may benefit from the pharmacognostic investigation, physicochemical characteristics, and preliminary phytochemical analyses provided here. It contains phenolics, alkaloids, steroids, saponins, tannins and flavonoids per diverse grade.<sup>13-15</sup>

### Phytoconstituents of Plant

*S. amaranthoides* extract described as highly antibacterial in contradiction of equally gram-positive and gram-negative bacteria. Steroids, triterpenoids, phenolic compounds, flavonoids, tannins, and glycosides were all identified in the

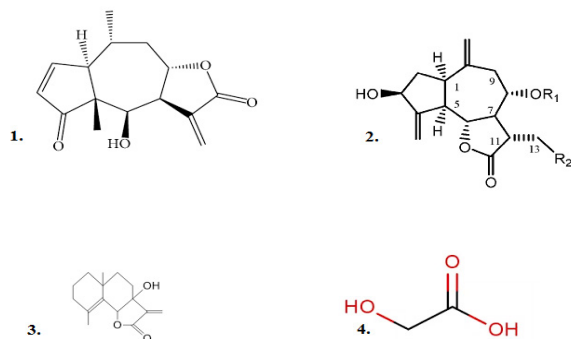


Figure 2: Phytoconstituents 1. sesquiterpene lactone, 2. 7-hydroxyeudesm-4-en-6,12-olide, 3. sesquiterpene acid & 4. 2-hydroxycostic acid

plant's phytochemical examination.<sup>15,16</sup> Some of the examples of phytoconstituents of this plant are mentioned below in Figure 2.

### Pharmacological Activities

#### Anti-diarrhoeal outcome

World Health Organization (WHO) initiated a diarrheal disease control program to eradicate the mortality rate associated with diarrhea in developing countries. Diarrhea was induced in wistar albino rats using castor oil. The ethanolic extract of *S. amaranthoides* demonstrated a notable reduction in diarrhea in rats at two distinct doses: 200 to 400 mg/kg body weight. The 400 mg/kg dosage exhibited a comparable efficacy to that of 5 mg/kg diphenoxylate, a standard medication for diarrhea.<sup>17</sup>

#### Antimicrobial activity

In light of the escalating microbial resistance to existing antibiotics, investigations into the antimicrobial properties were conducted. The methanolic extract of the entire plant of *S. amaranthoides* Linn was evaluated for its antibacterial effects in contrast to gram-positive and gram-negative bacteria, with *Escherichia coli* exhibiting the highest susceptibility. The antibacterial efficacy was quantified in terms of the zone of inhibition, revealing significant growth suppression across various tested organisms, notably *Bacillus subtilis* being the most susceptible, followed by *E. coli* and *Pseudomonas aeruginosa*, with inhibition zones ranging from 32 to 9 mm.<sup>17</sup>

#### Anti-inflammatory activity

This activity was assessed using the carrageenan-induced acute hind paw edema technique in wistar albino rats. A concentration of 1000 mg/kg orally led to 95% inhibition during the second phase of acute inflammation, attributed to the suppression of the cyclooxygenase enzyme and succeeding prostaglandin synthesis, indicating hindered anti-inflammatory effects.<sup>18</sup>

#### Hepatoprotective activity

The ethanolic extract of the plant's aerial parts was investigated for hepatoprotective activity on the drug-metabolizing microsomal enzyme system. In rats injected with  $\beta$ -D-GalN, a significant reduction in enzyme actions of cytochrome P450, cytb5, and NADPH cytp450 reductase was perceived. However, administration of the ethanolic extract restored enzyme levels to normal, suggesting potential protection against drug-induced liver toxicity.<sup>19</sup>

#### Anti-diabetic activity

Evaluation of anti-diabetic activity involved ethanol extraction of the whole plant, followed by preparation and characterization of silver nanoparticles. The anti-diabetic efficacy was assessed by observing the inhibition of  $\alpha$ -amylase enzyme action, with an  $IC_{50}$  value of 0.28  $\mu$ g/mL compared to the standard acarbose.<sup>19-21</sup>

#### Antioxidant activity

Regarding antioxidant activity, the methanolic extract demonstrated substantial free radical scavenging capacity

**Table 1:** Molecular docking studies of plant

Ligand	Target	2D Image	3D image	Energy (Kcal/mol)	H-bond
3,4-xylyl- 3,5-di-tert- butylbenzoate	Human estrogen receptor alpha (ER $\alpha$ )			-10.1	H-bond: 2 CYS A:530 THR A:347
	Human epidermal growth factor receptor 4 (HER4)			-9.3	H-bond: 2 ASN D:797 ASN D:830
9-octadecenoic acid	Mammalian target of rapamycin (mTOR)			-6.2	H-bond: 2 LYS A:52 GLN A:85
	Human estrogen receptor alpha (ER $\alpha$ )			-5.2	H-bond: 2 PRO A:325 LEU A:327
	Human epidermal growth factor receptor 4 (HER4)			-5.2	H-bond: 1 ASN D:797
n-hexadecanoic acid	Human estrogen receptor alpha (ER $\alpha$ )			5.5	H-bond: 1 THR A:347
	Human epidermal growth factor receptor 4 (HER4)			-5.2	H-bond: 2 THR A:347 CYS A:530
	Mammalian target of rapamycin (mTOR)			-5.5	H-bond: 1 LYS A:52

comparable to butylated hydroxyl anisole, with higher phenolic content compared to chloroform and acetone extracts. Additionally, the methanolic extract exhibited superior antioxidant potential compared to ethanolic and aqueous extracts, akin to ascorbic acid. Molecular docking studies of the plant are detailed in Table 1.<sup>20-22</sup>

## CONCLUSION

The *S. amaranthoides* located in a moist, semiaquatic environment. The small, procumbent herb spreads its branches outward. This plant goes in the direction of the Asteraceae family. This herb has been used to treat various conditions, from jaundice and helminth infections to eczema and blood abnormalities.

The docking study result concludes that chemical compounds having lower docking score of bonds are more stable and better for drug design because of higher binding affinity. In this articles phytoconstituents present in *S. amaranthoides* like a sesquiterpene lactone, 7-hydroxyeudesm-4-en-6,12-olide, sesquiterpene acid & 2-hydroxycostic acid have lower docking score and better potential activity against receptors 4 (HER4) and mamalian target of rapamycin (mTOR).

In these phytoconstituents, sesquiterpene lactone shows high binding affinity of (-10) at human estrogen receptor alpha protein molecules. Thus, based on the *in-silico* evaluation and molecular docking, it can be concluded that, phytoconstituents of *S. amaranthoides* could be used in different formulations. This review briefly summarizes the diverse array of documented activities and descriptions provided for *S. amaranthoides*.

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