

# Sapindus mukorossi Bio actives: Ethnomedicinal Importance, Pharmacological Potential and Molecular Docking Analysis

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## ABSTRACT

*Sapindus mukorossi* (soapberry) is a deciduous tree widely distributed across Asia and extensively used in Ayurvedic, Chinese and folk medicine for managing diverse ailments. Its pericarp, seeds, leaves, roots and galls have historically been employed as expectorants, contraceptives, anti-inflammatory and antimicrobial agents. This review aims to consolidate current knowledge on the ethnomedicinal relevance, phytochemical composition, pharmacological properties and molecular docking studies of *S. mukorossi*, highlighting its potential as a lead source of bioactive compounds. Published literature on *S. mukorossi* was reviewed with emphasis on phytochemistry, pharmacological studies (*in vitro* and *in vivo*) and *in silico* molecular docking analyses of triterpenoid saponins and other key phytoconstituents. The plant is a rich source of structurally diverse triterpenoid saponins (oleanane, dammarane, tirucallane and lupane types), flavonoids, fatty acids and sesquiterpenoidal glycosides. Experimental studies demonstrate broad-spectrum biological activities including spermicidal, anti-inflammatory, antioxidant, antimicrobial, anticancer, hepatoprotective, hypoglycemic, and insecticidal effects. *Sapindus mukorossi* represents a promising medicinal resource with multiple pharmacological effects validated by experimental and computational approaches. Molecular docking studies revealed strong binding affinities of selected saponins with therapeutic targets such as COX-2, DNA gyrase, lanosterol 14 $\alpha$ -demethylase, Keap1-Nrf2 complex and EGFR, supporting their proposed mechanisms of action. However, further mechanistic, toxicological and clinical investigations are required to translate these findings into standardized therapeutic applications.

**Keywords:** Ethnomedicine, Pharmacological activities, Phytochemistry, *Sapindus mukorossi*, Triterpenoid saponins.

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## INTRODUCTION

*Sapindus mukorossi*, belonging to the *Sapindaceae* family goes by multiple regional names such as soapnut, soapberry, reetha, aritha, dodan and dodani Table 1 (Genus species). This deciduous species is predominantly found across India's upper Sub-Himalayan zones, the Shivalik hills and the Ganges plains (Upadhyay *et al.*, 2012; Suhagia *et al.*, 2011; Kirtikar *et al.*, 1918; Trease *et al.*, 1989). It possesses a various pharmacological profile and has been extensively utilized in Indigenous medicine systems. It exhibits multiple therapeutic properties, functioning as an expectorant, emetic and contraceptive agent. Additionally, it has been employed in the management of neurological and

dermatological conditions, including migraine, hypersalivation, epilepsy, psoriasis and freckles. Its historical use is well documented in traditional Chinese and Japanese medicine, where it has served as a component in various formulations. In the Ayurvedic system, *S. mukorossi* is recognized for its capacity to pacify the Kapha dosha, as described in the classical text Aryabhishak. Furthermore, its application in treating respiratory disorders, notably Dam (a term associated with dyspnea or breathlessness), is referenced in the compendium Ayurvedic Jadi-Buti Rahasya - 2 (Shastri *et al.*, 2018; India Vegan *et al.*, 2013; Kasai *et al.*, 1986; Acharya *et al.*, 2014).

## Morphological characteristics

Soapberry is a medium- to large-sized deciduous tree reaching 12-20 m in height and up to 1.8 m in girth, characterized by a straight bowl and dense summer foliage that is shed in winter Table 2 (Taxonomy), Table 3 (Phytoconstituents). The species exhibits rapid growth, strong root establishment and pronounced coppicing potential, producing annual shoots of 41-59 cm in length and <14 mm in diameter (Goyal *et al.*, 2014). Bark



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morphology varies ontogenetically: young stems possess smooth grey bark, whereas mature trunks develop dark grey fissured bark with vertical lenticels and woody flakes; the inner bark (0.8-1.3 cm) is brittle, granular and pale orange-brown. The crown assumes a rounded canopy with leathery foliage. Leaves are alternate, paripinnate (30-50 cm), bearing 14-30 lanceolate leaflets (5-18 × 2.5-5 cm) with entire margins, acuminate apices and short petioles (2-5 mm); the rachis is glabrous and narrowly margined. Inflorescences occur as large terminal panicles (>30 cm) with pubescent axes, bearing numerous greenish-white subsessile flowers (~5 mm). Flowers are predominantly bisexual, though functional staminate forms anthes earlier. Floral morphology includes five unequal ciliate sepals (~2 mm), five clawed petals (~3 mm) with woolly scales, eight free stamens with pubescent filaments and a sessile, three-locular ovary with a trilobed stigma (Orwa et al., 2009). Fruits are globose drupes (1.8-2.5 cm), initially green and smooth, becoming yellowish-brown at maturity with a saponin-rich pericarp enclosing a solitary, black, smooth globose seed (2-2.5 cm) (Figure 1). The deep taproot system facilitates subsurface water and nutrient acquisition, conferring adaptability to nutrient-poor or arid soils.

Reproductively, the species reaches maturity 4-5 years post-germination. Flowering occurs during May-June (~25 days), fruit initiation in July-August, and maturation in October-November, with drupes often persisting until January (Rastogi et al., 1999). Phenological events include leaf senescence (December), defoliation (December-January), and flushing of new foliage (March-April). In the cultivar 'Yue Shuo Bodhi', bud burst occurs in early March, fruit development spans ~130 days and leaf fall is delayed to December (Zhao et al., 2019). Pollination is entomophilous, mediated primarily by bees, flies, and butterflies attracted by nectar and perianth coloration. Cytogenetically, *S. mukorossi* is an auto-diploid ( $2n=28$ ) as confirmed by molecular karyotyping and K-mer analysis, a chromosome counts distinct from related Sapindaceae taxa (Xue et al., 2022).

Botanical description of plant, The Sapindaceae is an important family that includes 2000 plant species in 150 genera.

## METHODOLOGY/SEARCH STRATEGY

Published literature on *S. mukorossi* was reviewed with an emphasis on phytochemistry, pharmacological studies (*in vitro* and *in vivo*), and *in silico* molecular docking analyses of triterpenoid saponins and other key phytoconstituents. Molecular docking was executed using Auto Dock Vina in PyRx version 0.8, with protein structures obtained from the RCSB Protein Data Bank and ligands prepared using published phytochemical data.

## Phytochemistry

Sapindaceae plants contain cyclitols, glycosides and saponins. Different sections of *S. mukorossi* have yielded different

compounds. The plant produces a lot of saponins in its fruits. The fruit contains 11.5% saponins and 10% sugars. The crude protein content of *S. mukorossi* seeds is approximately 21.6% (Singh et al., 2021). Above 103 active constituents mentioned as flavonoids, triterpenoids, carbohydrates, fatty acids, phenols, fatty oils and saponins are found in *Sapindus mukorossi's* fruit, seeds, roots and leaves (Zikova et al., 1970). The ovules of *S. mukorossi* have 23% oil and 92% triglycerides. The oil portion of triglycerides contains glycerides, dioleo-palmitin, dioleostearin and dioleo-arachidine (Saxena et al., 2004). Seed oils also contain cyanolipid, a non-glyceride component (1-cyano-2-hydroxymethylprop-1-en-3-ol). Diolein-type glycerides (56.7%), oleo-palmitoarachidine glycerides (30%) and oleo-diarachidine glycerides (13%). *Sapindus mukorossi* leaves include flavonoids as an apigenin, kaempferol, rutin and quercetin (Hu et al., 2018). The fruits of *S. mukorossi* contain six distinct fatty acid esters of tetracyclic triterpenoids as well as sesquiterpenoid glycosides. It has been discovered that *S. mukorossi* galls, fruits and roots contain a range of triterpenes, such as tricullane saponins, dammarane and oleanane in addition to the newly identified lupane-type in the plant pulp (Francis et al., 2002)

Most of the phytoconstituents found in *S. mukorossi* (10%-11.5%) are saponins, which are mainly responsible for a variety of pharmacological actions. Glycosidic bonds bind saponins to one or more oligosaccharide units. The term "sapogenins" refers to a broad family of structurally similar steroidal or triterpenoid aglycone chemicals. Aglycones or sapogenins may have more than unsaturated carbon-carbon bonds. The phytoconstituent A variety of solvents such as water, ethanol, methanol, acetone and n-hexane can be used to separate the bioactive molecules based on the characteristics of the active ingredient (Sengupta et al., 1975).

**Table 1: The genus Sapindaceae is composed of three main species (Kirtikar et al., 2004).**

Sl. No.	Different Species	Species Name
1	American species	<i>Sapindus Saponaria</i>
2	Asian species	<i>Sapindus mukorossi</i> , <i>Sapindus trifoliate</i>
3	Other <i>Sapindus</i> species	<i>Sapindus delayaye</i> <i>Sapindus detergens</i> <i>Sapindus emarginates</i> <i>Sapindus laurifolia</i> <i>Sapindus marginatus</i> <i>Sapindus vitiensis</i> <i>Sapindus tomentosus</i> <i>Sapindus oahuensis</i> <i>Sapindus rarak</i>

**Table 2: Taxonomical classification (Sharma et al., 2011).**

Kingdom	Plantae (Plants)
Sub-kingdom	Tracheobionta (Vascular plants)
Super-division	Spermatophyta (Seed plants)
Division	Magnoliophyta (Flowering plants)
Class	Magnoliopsida (Dicotyledons)
Sub-class	Rosidae
Order	Sapindales
Family	Sapindaceae
Genus	<i>Sapindus</i> L (soapberry)
Species	<i>Sapindus mukorossi</i> geartn (Chinese soapberry)

**Table 3: Major phytoconstituent compounds present in different plant parts of *Sapindus mukorossi*.**

Sl. No.	Chemical constituent	Part of the plant
1	Triglyceride (Guha et al., 1979) Oleo-palmito-arachidin glyceride Oleo-di-arachidin glyceride Di-olein	Kernel
2	Lipid (Azhar et al., 1994)	Kernel
3	Sesquiterpeneoidal glycosides (Wei et al., 2021)	Drupe
4	Flavonoids (Francis et al., 2002) Quercetin, Apigenin, Kaempferol Rutin	Leaves
5	Saponin (Nakayama et al., 1986) Triterpenes	Gall, Drupe and root
6	Oleanane (sapidoside A and B) (Pelegriani et al., 2008)	Fruit gall
7	Dammarane (sapinmusaponin A-E) (Ni et al., 2006) Tricullane (sapinmusaponin F-K) (Adetunji et al., 2021)	Gall and root

### Phytochemical characterisation

Soapberry is a rich reservoir of structurally diverse triterpenoid saponins, extracted from distinct anatomical parts of the plant including the drupe, galls, pericarp and roots. These saponins are predominantly classified into three major structural types: oleanane, dammarane and tirucallane, each contributing to the plant's broad pharmacological profile (Huang et al., 2008). The fruits and galls have yielded numerous oleanane-type triterpenoid saponins such as Sapindosides A and B. Previous studies have

identified additional variants, including Sapindosides C-E with Sapindosides D and E being hexaoside and nonaoside derivatives of hederagenin respectively (Pooja et al., 2022). Dammarane-type saponins Sapinmusaponins A-E (Figure 4) (Table 4) and tirucallane-type Sapinmusaponins F-J (Figure 5) were reported from the tissue outgrowths of the plant species, whose molecular configurations were shown via 1D and 2D NMR spectroscopy (Kalinowska et al., 2005). Further investigations also revealed Sapinmusaponins O and P (Figure 3) (dammarane type) (Table 5) and Sapinmusaponins K-N (oleanane type) (Table 6), alongside Mukorozisaponins G and E1 (Table 7) and Sapindosides A and B from fruits and galls (Ni et al., (2006). Mukorozisaponins X, Y1 and Y2 were isolated from the pericarp. Additionally, Sapinmusaponins Q and R (tirucallane type) (Table 8) and three oleanane-type saponins-including a complex hederagenin-based trisaccharide-were obtained from ethanolic extracts of galls (Figures 1-6) (Ni et al., 2004).

The roots of *S. mukorossi* have also been studied extensively. Tirucallane-type saponins Sapimukosides A-D (Table 9) were initially isolated and this series was later expanded to include Sapimukosides E-J (Ling Y et al., 2020). These ten root-derived compounds (Sapimukosides A-J) (Figure 2) (Table 10). Complementing these findings, LC-MS analysis to identify six saponins from the fruit: Mukorozisaponins E1 and Y1 (Figure 6) and Sapindosides A-D (Table 11). This analytical confirmation highlights the extensive chemical diversity of *S. mukorossi* supporting its significance in natural product research and pharmaceutical applications (Rosa et al., 1971).

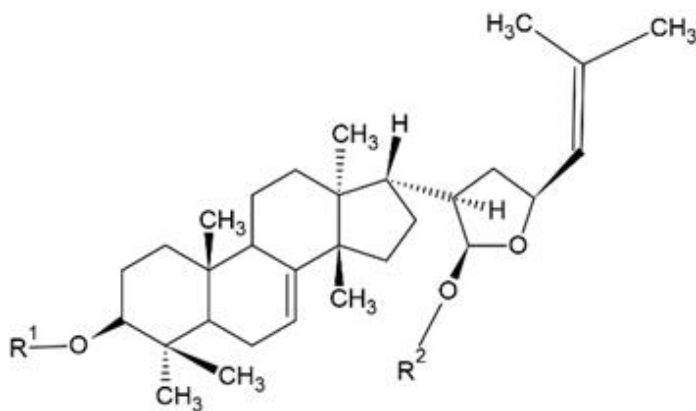
### Classical uses of soapberry

Since antiquity, medicinal plants have served as a primary origin of therapeutic agents for the treatment of multiple ailments and functional disorders. The Chinese, Unani and Ayurvedic medicinal systems all make extensive use of herbal products. *Sapindus mukorossi* is widely recognized for its application in traditional medicine. *Sapindus mukorossi* pericarp has been employed in traditional medicine for its expectorant properties and is recognized as a natural surfactant owing to its rich saponin composition. Soapnuts have been traditionally employed in the management of head lice infestations due to the presence of saponins-natural glycosides recognized for their potent cleansing action and insecticidal properties (El Aziz et al., 2021)

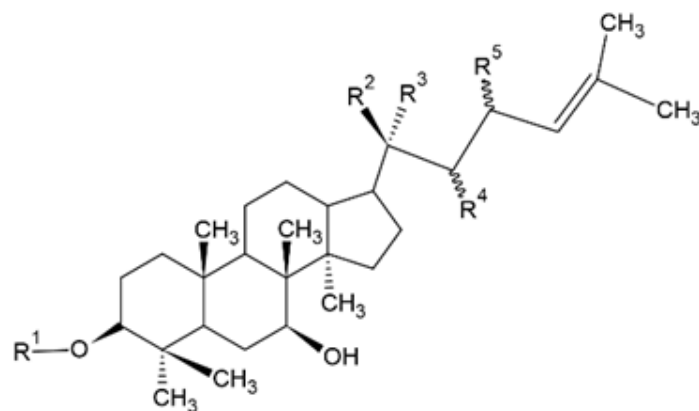
Its fruit paste is used as a febrifuge or fever-lowering medication. The ground kernels are used to treat colds, constipation, rheumatoid arthritis, tooth decay and nausea. Its seeds are used in Ayurveda to treat skin freckles and sunburn. Its effectiveness in removing oily secretions and generating a foamy lather makes it a popular choice for use as a hair-cleansing agent. Its fruits were used by Indian jewellers to polish tarnished gold, silver and other precious metal jewellery. Fruit foam is used to treat burns. The leaves are added to bath water to ease arthralgia and the roots are



**Figure 1:** *S. mukorossi* (A) Tree (B) Leaves (C) Seed (D) Flowers.



**Figure 2:** Structural Framework of Sapimukosides A-J.



**Figure 3:** Structural framework of Sapinmusaponins A-B and O-P.

utilised to treat rheumatism and gouty arthritis (Maikhuri *et al.*, 2003).

### Pharmacological effects of *S. mukorossi*

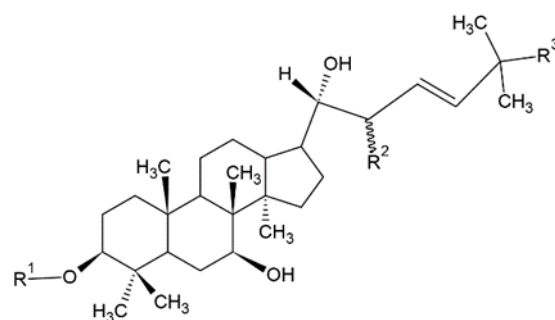
Studies have shown that extracts and phytoconstituents derived from *S. mukorossi* possess multiple pharmacological properties such as Anti-cancer, Anti-microbial, Anti-oxidant, Tissue regeneration, Anti-gonococcal potential, Sperm-inhibiting, Anti-thrombotic activity, Hypoglycemic activity, Liver-protecting, Inflammation-modulating activity, Anti-protozoal, and Anti-lipid peroxidation activities Table 12 (Pharmaceutical activities).

### Antibacterial activity

At low concentrations, ethanol and chloroform extracts of *Sapindus mukorossi* demonstrated significant Anti-*Helicobacter pylori* activity. Oral dosing of these extracts to male Wistar rats for 1 week effectively suppressed the growth of both susceptible and resistant *H. pylori* strains. *In vitro* assays discovered a broad region of restriction at dosage as minimal as 10 µg/mL, while *in vivo* studies detected inhibitory effects at doses as minimal as 2.5 µg/mL (Geyter *et al.*, 2007).

### Insecticidal activity

Due to the insecticidal properties of saponins, significant effects have been observed on agricultural pests- the pea aphid (*Acyrtosiphon pisum*) as well as the cotton leafworm (*Spodoptera*



**Figure 4:** Structural framework of Sapinmusaponins C-E.

*littoralis*). Experimental results showed that saponins either induced mortality or inhibited growth in these insects. While *Spodoptera* caterpillars successfully developed into seemingly normal adults when fed a diet containing 7% saponin, complete mortality of *A. pisum* was observed at a concentration as low as 0.1%. These findings suggest that saponins may serve as a promising natural alternative within Integrated Pest Management (IPM) strategies, particularly against pests that have developed resistance to conventional agricultural and horticultural chemicals (Rahman *et al.*, 2007). Furthermore, an ethanol extract of *Sapindus mukorossi* was examined for its efficacy targeting *Sitophilus oryzae* and *Pediculus humanus*. The results demonstrated significant insecticidal and repellent activity, with bioassays indicating that both toxicity and repellency were directly proportional to the extract concentration.

**Table 4: Structural framework of Sapinmusaponins C-E (Huang et al., 2007).**

Sapinmusaponins	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>
C	Glc <sub>2</sub> -Rha	-OH	-OH
D	Glc <sub>2</sub> -Rha	-OH	-OCH <sub>3</sub>
E	Glc <sub>2</sub> -Rha	-H	-OCH <sub>3</sub>

**Table 5: Structural framework of Sapinmusaponins A-B and O-P (Geyter et al., 2007).**

Sapinmusaponin	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>
A	Glc <sub>2</sub> -Rha	-H	-OH	-OH	-H
B	Glc <sub>2</sub> -Rha	-H	-OH	-OH	-OH
O	Glc <sub>2</sub> -Rha	-OH	-CH <sub>3</sub>	-H	-H
P	Glc <sub>2</sub> -Rha	-CH <sub>3</sub>	-OH	-H	-H

**Table 6: Structural framework of Sapinmusaponins K-N (Takagi et al., 1980).**

Sapinmusaponins	R <sub>1</sub>	R <sub>2</sub>
K	Ara <sub>2</sub> -Rha <sub>3</sub> -Ara <sub>3</sub> -OAc	-H
L	Ara <sub>2</sub> -Rha <sub>3</sub> -Rha <sub>4</sub> -OAc	-H
M	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>3</sub> -OAc	-H
N	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>4</sub> -OAc	-H

### Anti-Diabetic property

*Sapindus mukorossi* has demonstrated significant potential in managing diabetes, mainly due to the occurrence of saponins, flavonoids, and polyphenolic compounds. These constituents aid in regulating blood sugar by stimulating insulin production, enhancing cellular glucose absorption, and suppressing enzymes like  $\alpha$ -glucosidase and  $\alpha$ -amylase involved in carbohydrate metabolism. Experimental studies involving streptozotocin-induced diabetic rats revealed that administering fruit-derived fraction of *S. mukorossi* at dosage between 250 and 500 mg/kg body weight over 3 weeks lead to in notable reductions in Glycaemic level and improved lipid parameters. Additionally, the extract showed a shielding effect on pancreatic  $\beta$ -cells, attributed to its antioxidant activity. While the outcomes appear favourable, further human-based studies are needed to confirm its therapeutic efficacy in diabetes care (Patel et al., 2012).

### Anti-pyrexial, Anti-nociceptive and Wound recovery properties

It has been shown to have the ability to reduce pain and body temperature. *S. mukorossi* stem bark extract lowered the rectal temperature of rats injected with *Saccharomyces cerevisiae* to cause fever (Jan et al., 2016). Furthermore, the extract from *S. mukorossi* contains analgesic (pain-relieving) properties. Rat skin wounds heal more quickly after being treated with *S. mukorossi* seed oil than when left untreated (Chen et al., 2019).

**Table 7: Structural framework of Mukorozi saponin E1, G, Y1, Y2 and X (Sparg et al., 2004).**

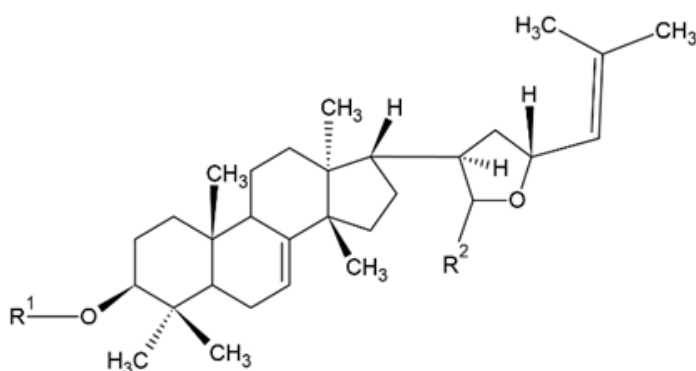
Mukorozi saponin	R <sub>1</sub>	R <sub>2</sub>
E1	Ara <sub>2</sub> -Rha	-H
G	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl	-H
Y1	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>4</sub> -Glc	-H
Y2	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>4</sub> -Glc <sub>2</sub> -Glc	-H
X	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>4</sub> -Glc -2-Glc

**Table 8: Structural framework of Sapinmusaponins F-J, Q-R (Saxena et al., 2004).**

Sapinmusaponins	R <sub>1</sub>	R <sub>2</sub>
F	Glc <sub>6</sub> -Rha	$\beta$ -OCH <sub>3</sub>
G	Glc <sub>6</sub> -Rha	$\alpha$ -OCH <sub>3</sub>
H	Glc <sub>2</sub> -Rha	$\alpha$ -OCH <sub>3</sub>
I	Glc <sub>6</sub> -Rha	$\beta$ -OCH <sub>3</sub>
J	Glc <sub>6</sub> -Rha	$\alpha$ -OCH <sub>3</sub>
Q	Glc <sub>2</sub> -Glc	$\alpha$ -OCH <sub>3</sub>
R	Glc <sub>6</sub> -Rha	$\alpha$ -OCH <sub>3</sub>

### Spermicidal activity

Saponins from *Sapindus mukorossi* have demonstrated spermicidal activity. At a low concentration (0.05%), no immediate effect was observed within one minute; however, after ten minutes, sperm showed vesicle formation and plasma membrane damage. Higher concentrations (0.1% to 5.0%) caused similar morphological alterations such as vacuolation, vesiculation, and membrane rupture in the sperm head region. These changes are likely due to saponin-induced disruption of glycoproteins in the plasma membrane of the sperm. Such properties support the potential use of *Sapindus mukorossi* saponins in the development of herbal contraceptive creams (Dhar et al., 1989).



**Figure 5:** Structural framework of Sapinmusaponins F-J, Q-R.

### Anti-Trichomonas activity

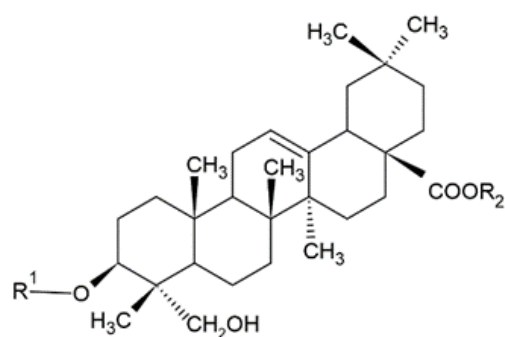
Saponins from *Sapindus mukorossi* exhibit strong anti-trichomoniasis activity at a low concentration of 0.005%, significantly lower than the minimum spermicidal dose (0.05%). These saponins inhibit *Trichomonas vaginalis* by preventing its attachment to HER HeLa host cells and reducing the parasite's proteolytic activity. This effect is associated with downregulation of cysteine proteinase gene TvCP2 and adhesin AP65, both critical for parasite adherence and invasion. Additionally, saponins disrupt the actin cytoskeleton beneath the parasite's plasma membrane, further impeding attachment. Importantly, saponin treatment does not affect the mitochondrial function or viability of host cells, indicating selective antiparasitic action with minimal cytotoxicity (Maikhuri *et al.*, 2003).

### Anti-cancer activity

Due to their diverse structural forms, saponins are known to exert anticancer effects through multiple biological pathways. There are over eleven distinct types of saponins such as lupane, hopane, taraxasterane, ursane, cycloartane, lanostane, cucurbitane, and various steroid-based structures. Members of the dammarane group, such as ginsenosides, have demonstrated the ability to inhibit tumor progression by reducing cancer cell adhesion, invasion, metastasis, and angiogenesis via suppression of vascular endothelial growth factors. Steroidal saponins like dioscin and its aglycone diosgenin also show potent anticancer potential by halting cell division and inducing programmed cell death (apoptosis). Preliminary bioassays revealed that human cancer cultured cell-including Hepa59T/VGH, NCL, HeLa, and Med-these are partially susceptible to the cell-damaging action of these compounds, with Effective Doses (ED<sub>50</sub>) ranging from 9 to 18 µg/mL. In these studies, stryquinopentamine was used as a control, and most saponins displayed activity levels at least five times lower than this standard compound (Chen *et al.*, 2010).

### Hepatoprotective activity

Extracts of Soapberry (2.5 mg/mL) and Indian rhubarb (3.0 mg/mL) have shown hepatoprotective properties in both *in vivo* and *in vitro* (primary hepatocyte cultures) studies against Carbon



**Figure 6:** Structural framework of sapinmusaponins K-N, sapindosides A-E, mukorozi saponin E1, G, Y1, Y2 and X.

Tetrachloride (CCl<sub>4</sub>)-induced liver damage. CCl<sub>4</sub> exposure typically induces liver injury, but co-treatment with these extracts significantly improved serum marker enzyme activity, indicating reduced hepatic damage. In primary monolayer hepatocyte cultures, *S. mukorossi* pericarp extract was found to mitigate cellular toxicity. The protective effect is likely due to antioxidant or membrane-stabilizing properties of the plant compounds. These findings suggest *Sapindus mukorossi* could be a promising natural agent for liver protection (Singh *et al.*, 2010).

### Anxiolytic activity

Methanolic extracts of *Sapindus mukorossi*, at doses of 200 and 400 mg/L, have shown notable anxiety-reducing effects, comparable to standard anxiolytic medications such as diazepam (2 mg/kg) and fluoxetine (10 mg/kg) (Ibrahim *et al.*, 2008).

### Molluscicidal activity

Its fruit extract exhibits strong molluscicidal activity in contrast to *Pomacea canaliculata* with LC<sub>50</sub> values decreasing over time: 85 ppm at 24 hr, 22 ppm at 48 hr, and 17 ppm at 72 hr. The outer shell (pericarp) of the fruit has shown effectiveness in deterring *Lymnaea acuminata*, a secondary host of the liver fluke *Fasciola gigantica*, which commonly infects livestock in northern India. The molluscicidal agents are found in the powdered fruit and are soluble in various organic solvents, including ethanol, ether, acetone, and chloroform. Among these, ethanol extracts show the highest toxicity, suggesting better solubility and extraction efficiency. This highlights *S. mukorossi* as a promising natural molluscicide for controlling parasite-transmitting snails in aquatic environments (Chakaraborty *et al.*, 2010).

### Tyrosinase inhibition and free radical scavenging

Research indicates that extracts from soapberry (*Sapindus mukorossi*) seeds, obtained using solvents such as methanol, ethyl acetate, or hexane, exhibit several bioactive properties, including tyrosinase inhibition, antioxidant activity, antibacterial effects, and anticancer potential. These extracts demonstrated strong and selective growth-inhibitory effects on human lung cancer and melanoma cell lines. The findings suggest that *S.*

**Table 9: Triterpenoid Saponin: Pharmacology and Structure Activity Relationship.**

Compound	Triterpenoid Skeleton Types	Pharmacological Activity	SAR Explanation
Sapimukoside A (Kuo <i>et al.</i> , 2005)	Tirucullane	Anti-inflammatory	Glycosylation at C-3 improves solubility, bioavailability and receptor interaction. Type of sugar alters potency (glucose/rhamnose ↑ activity; deoxy sugars ↑ potency but ↑ haemolysis). Removal of sugar drastically lowers activity.
Sapinmusaponin A (Sharma <i>et al.</i> , 2013)	Dammarane	Cytotoxic/Anticancer	Additional glycosylation at C-28 reduces haemolysis and cytotoxicity toward normal cells while retaining selective anticancer effects. Monodesmosidic forms (only C-3 glycoside) show stronger but less selective cytotoxicity, while bidesmosidic (C-3 + C-28) are safer and more suitable pharmacologically.
Sapinmusaponin C (Shah <i>et al.</i> , 2017)	Dammarane	Antimicrobial (antifungal and antibacterial)	The triterpenoid aglycone provides amphiphilic character enabling interaction with microbial cell membrane sterols, leading to pore formation and leakage. Sugar residues at C-3 modulate solubility and specificity, but the aglycone itself is primarily responsible for membrane-disruptive antimicrobial action.
Sapinmusaponin F (Chirva <i>et al.</i> , 1970)	Tirucullane	Wound-healing	The rhamnose substitution at C-3 enhances interaction with extracellular matrix proteins and growth factor pathways, promoting fibroblast proliferation and collagen synthesis. This sugar moiety significantly contributes to wound closure efficacy compared to analogs lacking rhamnose.
Sapinmusaponin N (Tsuzuki <i>et al.</i> , (2007)	Oleanane	Hepatoprotective	The free carboxyl at C-28, when glycosylated, reduces cytotoxicity and enhances hepatoprotective efficacy by stabilizing hepatocyte membranes and increasing antioxidant defense. Aglycone or non-glycosylated analogs at this position show weaker hepatoprotection and higher haemolytic activity.
Sapindoside E (Sharma <i>et al.</i> , 2011)	Oleanane	Immunomodulatory	The extended sugar chain at C-3 improves water solubility and facilitates immune cell receptor interaction, thereby potentiating macrophage and lymphocyte responses. Shorter sugar chains or absence of glycosylation weaken the immunostimulatory effect.
Mukurozi-saponin X (Yin <i>et al.</i> , 2011)	Oleanane	Anti-fungal	Longer sugar chains at C-3 enhance hydrophilicity and membrane-sterol binding specificity, increasing antifungal potency while slightly reducing haemolysis. Short-chain or absent glycosylation weakens antifungal efficacy.

**Table 10: Structural Framework of Sapimukoside (A-J) (Garg S et al., 1993).**

Sapimukosides	R <sub>1</sub>	R <sub>2</sub>
A	Glc <sub>2</sub> -Rha	-H
B	Glc <sub>6</sub> -Rha	-H
C	Glc <sub>2</sub> -Rha	-C <sub>2</sub> H <sub>5</sub>
D	Glc <sub>2</sub> -Rha	-CH <sub>3</sub>
E	Glc <sub>2</sub> -Rha <sub>3</sub> -Ara	-C <sub>2</sub> H <sub>5</sub>
F	Glc <sub>2</sub> -Rha <sub>3</sub> -Xyl	-C <sub>2</sub> H <sub>5</sub>
G	Glc <sub>2</sub> -Rha <sub>3</sub> -Xyl	-CH <sub>3</sub>
H	Glc <sub>2</sub> -Rha <sub>3</sub> -Ara	-C <sub>2</sub> H <sub>5</sub>
I	Glc <sub>2</sub> -Rha <sub>3</sub> -Ara	-CH <sub>3</sub>
J	Glc <sub>6</sub> -Rha	-C <sub>2</sub> H <sub>5</sub>

**Table 11: Structural framework of Sapindosides A-E (Dhar et al., 1989).**

Sapindosides	R <sub>1</sub>	R <sub>2</sub>
A	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>4</sub> -OAc	-H
B	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl <sub>4</sub> -OAc	-H
C	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl	Glc <sub>2</sub> -Glc
D	Ara <sub>2</sub> -Rha <sub>3</sub> -Xyl	Glc <sub>2</sub> -Glc
E	Ara <sub>2</sub> -Rha	Glc <sub>2</sub> -Glc

*mukorossi* extracts hold promise for Implementations in the drug development and cosmetic formulations, particularly in the development of dietary supplements, cancer treatments, antimicrobial agents, and skincare products (Singh et al., 1997).

### Anti-inflammatory activity

Studies have shown that both crude saponins and hederagenin extracted from *Sapindus mukorossi* significantly decreased granuloma formation and fluid accumulation in the hind paws of rats treated with croton oil, as well as swelling induced by carrageenan. Their influence was also examined on vascular leakage and pain behaviour triggered by acetic acid in mice. Hederagenin and other agents were effective only through oral administration, while crude saponins produced notable anti-inflammatory effects when administered both orally and via intraperitoneal injection in the carrageenan-induced edema model. Laboratory analyses revealed that hederagenin suppresses the synthesis of nitric oxide, prostaglandin E2 and key inflammation-inducing cytokines along with the LPS-stimulated upregulation of inflammatory markers for example iNOS, COX-2, and NF-κB, as well as their related mRNA levels (Tripathi et al., 2000).

### Piscicidal activity

Research was done on the effects of *Sapindactylus japonicum* on fish. He discovered that the most toxic portion of *Sapindus mukorossi* was its pericarp, and that the average survival duration

was 1.18 hr. In 12 hr, he was completely dead. He will probably destroy the pisces at quantities of 3.5 ppm to 10 ppm (LD<sub>10</sub>, LD<sub>50</sub>, LD<sub>100</sub>) within 48 hr. The pericarp of *Sapindus mukorossi* preferentially repels garfish, including azalea fossils and azaleas (Wei et al., 2021).

### Anti-platelet aggregation effect

Ethanol-based extracts of *Sapindus mukorossi* containing chirucharan-type saponins, known as Sapinmusasaponins, showed moderate activity by suppressing the early-stage antigen response linked to Epstein-Barr virus, which was stimulated by the compound TPA (12-O-tetradecanoylphorbol-13-acetate) (Santos et al., 2011).

### Fungicidal Potential

The crude extract derived from *Sapindus mukorossi* has demonstrated significant inhibitory effects on the development of *Candida albicans*, an infective yeast responsible for cutaneous candidiasis. Research conducted using extracts from the dried fruit pericarp assessed their antifungal efficacy in contrast to clinical separates of *Candida albicans* and non-*albicans* species obtained from Endovaginal swab swabs of females diagnosed with vulvovaginal candidiasis. Further investigations revealed that saponins extracted from *S. mukorossi* effectively suppressed the *in vitro* mycelial development of *Botrytis cinerea* and inhibited gray mold progression on strawberries in a concentration-dependent manner. The antifungal mechanism involved disruption of membrane integrity and potential, the formation of vacuoles resembling those seen in autophagy and interference with the balance of organelles in *B. cinerea*, as demonstrated through fluorescence staining and microscopic analysis. Additionally, the saponins induced mitochondrial damage and triggered oxidative stress within the cytoplasm, leading to the loss of cellular function. These findings indicate the potential of *S. mukorossi* saponins to serve as environmentally friendly fungicidal agents for managing gray mold in postharvest fruits (Takagi et al., 1980).

### Molecular Docking Studies of Saponins from *Sapindus mukorossi*

Triterpenoid saponins derived from soapberry including Sapimukosides (A-J), Sapinmusasaponins (A-R), Sapindosides (A-E) and Mukorozisaponins (E1, G, X, Y1, Y2)-have been widely reported for their pharmacological potential such as anti-inflammatory, antioxidant, antimicrobial and anticancer properties. To investigate their potential mechanisms at the molecular level, *in silico* molecular docking studies were performed using representative compounds from each class against therapeutically relevant protein targets (Huang et al., 2007).

Five key targets were selected based on literature-reported traditional and experimental uses of *S. mukorossi* extracts:

**Table 12: Major pharmaceutical activities of different parts of Soapberry.**

Sl. No.	Activity	Method used	Part used
1	Anti-Bacterial activity (Dwivedi <i>et al.</i> , 1990)	Ethanollic and chloroform extracts	Leaf
2	Spermicidal activity (Tiwari <i>et al.</i> , 2008)	Saponins	Fruit pericarp
3	Anti-trichomonas activity (Geyter <i>et al.</i> , 2007)	Mixing of sapindus and saponin	Fruit pericarp
4	Insecticidal activity (Geyter <i>et al.</i> , 2010)	Ethanollic extract	Seed
5	Anxiolytic activity (Man <i>et al.</i> , 2010)	Methanollic extract	Gall
6	Anti-cancer (Rashid <i>et al.</i> , 2017)	Saponin from gall extract	Gall
7	Hepatoprotective activity (Singh <i>et al.</i> , 2009)	Fruit pericarp extract	Fruit pericarp
8	Molluscicidal activity (Viridi <i>et al.</i> , 1982)	Extract	Fruit Extract
9	Piscicidal activity (Tsuzuki <i>et al.</i> , 2007)	Saponin from gall extract	Gall
10	Fungicidal activity (Takaji <i>et al.</i> , 1980)	Crude extract	Fruit pericarp
11	Anti-inflammatory (Huang <i>et al.</i> , 2007)	Crude extract / isolated saponin and hederagenin	Pericarp
12	Anti-platelet aggregation activity (Chen <i>et al.</i> , 2007)	Compound acquisition from extract	Gall
13	Tyrosine inhibition and free radical scavenging (Verma <i>et al.</i> , 2012)	Methanol-soluble fraction	Seed
14	Anti-diabetic and anti-hyperlipidimic activity (Thair <i>et al.</i> , 2016)	Hydroalcoholic extract	Fruits
15	Anti-oxidant activity (Tamura <i>et al.</i> , 2001)	Response surface methodology	Stem, bark, fruit extract

- Cyclooxygenase-2 (COX-2, PDB ID: 6COX) for inflammation,
- DNA Gyrase (PDB ID: 1KZN) for antibacterial activity,
- Lanosterol 14 $\alpha$ -demethylase (PDB ID: 5EQB) for antifungal activity,
- Keap1-Nrf2 complex (PDB ID: 5CGJ) for antioxidant response, and
- Epidermal Growth Factor Receptor (PDB ID: 1M17) for anticancer evaluation.

The docking workflow was executed with Auto Dock Vina implemented in PyRx version 0.8. Protein structures were achieved from the RCSB Protein Data Bank and organized by eliminating water molecules and heteroatoms incorporating polar hydrogens and conveying Gasteiger charges. Ligand structures were built based on published phytochemical data, energy-minimized using MMFF94 force field and changed to PDBQT format. The docking grid was centred on the active site regions of each protein based on co-crystallized ligand data.

Among the screened saponins Mukorosisaponin Y1, Sapinmusaponin D and Sapindoside C exhibited significant binding affinities oscillating from -8.6 to -10.2 kcal/mol, particularly toward COX-2 and EGFR. These molecules established crucial hydrogen bonding and hydrophobic communications with key amino acid remainders-such as

Arg120, Tyr355, Ser530 (COX-2) and Met793, Glu738 (EGFR)-consistent with known drug-binding motifs.

These results provide preliminary insight into the binding behaviour and therapeutic potential of *S. mukorossi* saponins. Further experimental validation via *in vitro* and *in vivo* studies would be valuable in translating these findings into pharmacological applications. The outcomes support the rationale for advancing these compounds as potential leads in drug discovery programs targeting inflammation, cancer, and microbial infections (Morris *et al.*, 2009).

## DISCUSSION

The present review highlights *Sapindus mukorossi* as a multipurpose medicinal plant with a long history of ethnomedicinal use and a growing body of experimental evidence supporting its pharmacological relevance. Traditional applications as an expectorant, contraceptive, anti-inflammatory and antimicrobial agent are consistent with modern phytochemical and bioactivity findings. In particular, the high concentration of triterpenoid saponins-oleanane, dammarane, tirucallane and lupane types-alongside flavonoids and fatty acids appears to underpin the wide spectrum of biological effects attributed to this species.

Across multiple studies, both crude extracts and isolated saponins have demonstrated antimicrobial, antioxidant, anticancer, hepatoprotective, insecticidal, hypoglycemic and spermicidal activities, supporting the traditional uses of the plant. The

diverse sugar substitutions in saponin structures affect solubility, bioavailability and receptor interactions, which may explain the variability in pharmacological potency reported across different fractions. While many *in vitro* and *in vivo* experiments validate individual activities, most studies have been conducted at a preclinical stage with limited mechanistic elucidation or standardization of extract composition.

Recent *in silico* docking analyses strengthen the pharmacological rationale by showing favourable binding of representative saponins to key therapeutic targets such as COX-2, DNA gyrase, lanosterol 14 $\alpha$ -demethylase, Keap1-Nrf2 complex and EGFR. These interactions correspond to the anti-inflammatory, antimicrobial, antioxidant and anticancer effects observed experimentally. However, docking results remain predictive; they require confirmation through enzyme inhibition, cell-based assays and animal models to validate biological relevance.

Another important gap is the lack of toxicological and clinical data. Despite extensive use in traditional medicine, systematic evaluation of safety, pharmacokinetics and potential interactions with other drugs is sparse. Variability in plant chemotypes, harvesting conditions and extraction methods also complicates reproducibility and dose-response relationships. To move from ethnopharmacology to evidence-based therapeutics, future research should focus on (i) comprehensive chemical profiling using standardized methods, (ii) isolation and characterization of bioactive compounds, (iii) mechanistic studies at the molecular level and (iv) well-designed clinical trials to establish efficacy and safety. Collectively, the reviewed evidence positions *S. mukorossi* as a valuable natural resource for drug discovery and development. By bridging traditional knowledge with modern phytochemistry, pharmacology and computational modelling, it is possible to identify new therapeutic leads and environmentally friendly bioactive agents. This integrative approach could accelerate the translation of *S. mukorossi* from a traditional remedy into standardized, scientifically validated health-care products.

### Future directions/research gaps

To advance from ethnopharmacology to evidence-based therapeutics, future research must focus on (i) comprehensive chemical profiling using standardized methods, (ii) isolation and characterization of specific bioactive compounds, (iii) in-depth mechanistic studies at the molecular level, and (iv) well-designed clinical trials to establish efficacy and safety in humans. There is a significant current lack of toxicological and pharmacokinetic data regarding plant chemotypes and extraction methods.

### CONCLUSION

*Sapindus mukorossi* (soapberry) emerges from this review as a multipurpose medicinal plant whose ethnobotanical uses are strongly supported by modern phytochemical and pharmacological studies. Its rich repertoire of triterpenoid

saponins, flavonoids and other secondary metabolites underpin a wide array of experimentally validated activities-including anti-inflammatory, antimicrobial, anticancer, hepatoprotective, hypoglycemic and spermicidal effects. Recent molecular docking analyses further substantiate its potential mechanisms of action and identify promising targets for drug discovery.

Despite these advances, the translation of *S. mukorossi* from traditional remedy to standardized therapeutic product is still limited by gaps in mechanistic understanding, safety assessment, pharmacokinetic profiling and clinical evaluation. Addressing these issues through rigorous, well-designed studies will be essential to confirm efficacy, ensure reproducibility and support regulatory approval. *S. mukorossi* represents a valuable natural resource with significant potential for development into novel pharmaceutical, cosmetic and agro-industrial applications, bridging traditional knowledge with contemporary scientific innovation.

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### ABBREVIATIONS

**COX-2:** Cyclooxygenase-2; **DNA:** Deoxyribonucleic acid; **EGFR:** Epidermal Growth Factor Receptor; **Keap1:** Kelch-like ECH-associated protein 1; **Nrf2:** Nuclear factor erythroid 2-related factor 2; **LPS:** Lipopolysaccharide; **iNOS:** Inducible Nitric Oxide Synthase; **NF- $\kappa$ B:** Nuclear Factor kappa B; **mRNA:** Messenger Ribonucleic Acid; **LC-MS:** Liquid Chromatography-Mass Spectrometry; **PDB:** Protein Data Bank; **ED<sub>50</sub>:** Effective Dose 50; **LC<sub>50</sub>:** Lethal Concentration 50; **LD:** Lethal Dose; **IPM:** Integrated Pest Management; **MMFF94:** Merck Molecular Force Field 94; **SAR:** Structure-Activity Relationship; **Glc:**  $\beta$ -D-Glucopyranosyl; **Rha:**  $\alpha$ -L-Rhamnopyranosyl; **Ara:**  $\alpha$ -L-Rabinopyranosyl; **Xyl:**  $\beta$ -D-Xylopyranosyl.

### CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

### AUTHOR CONTRIBUTIONS

Neeraj Maurya: Writing-original draft. Shashi Bhooshan Tiwari: Supervision, Conceptualization. Raj Pal and Ankit Kumar Verma Editing and supervision. Shiv Dev Singh, Prashant Kumar, Yogendra Pal and Pawan Kumar Gupta: Validation.

### SUMMARY

*Sapindus mukorossi*, commonly known as soapberry, is a deciduous tree extensively found in various Asian regions and has been traditionally valued in Ayurvedic, Chinese, and

indigenous medicinal practices. Different plant parts such as the pericarp, seeds, leaves, roots, and galls have been conventionally used to manage respiratory disorders, inflammation, infections, and fertility-related conditions. The present summary outlines the ethnomedicinal importance, phytochemical diversity, pharmacological potential, and molecular docking evidence associated with *S. mukorossi*. Phytochemical investigations reveal that the plant predominantly contains triterpenoid saponins of oleanane, dammarane, tirucallane, and lupane skeletons, along with flavonoids, fatty acids, and sesquiterpenoidal glycosides. Numerous *in vitro* and *in vivo* studies have reported its wide-ranging biological activities, including anti-inflammatory, antioxidant, antimicrobial, spermicidal, anticancer, hepatoprotective, hypoglycemic, and insecticidal effects. Furthermore, molecular docking studies demonstrate notable interactions between selected saponins and key biological targets such as cyclooxygenase-2, DNA gyrase, lanosterol 14 $\alpha$ -demethylase, Keap1-Nrf2 complex, and epidermal growth factor receptor, supporting their mechanistic relevance. Collectively, these findings indicate that *Sapindus mukorossi* possesses significant potential as a natural source of therapeutically active compounds, although advanced mechanistic studies, safety evaluations, and clinical investigations are required for its development into standardized medicinal products.

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