



GC -MS Characterization of Steroidal, Terpenoid and Fatty Acid Constituents in *Semicarpus anacardium* L. Bark

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ABSTRACT

Gas Chromatography–Mass Spectrometry bark of *Semecarpus anacardium* L. analysis shows presence of 30 phytochemical constituents with retention times ranging from 0.021 to 35.895 minutes. Major compounds identified included terpenoids, steroids, fatty acid esters, phenolic compounds, sulfur- and nitrogen-containing derivatives. The predominant peaks corresponded to high-molecular-weight terpenoid and steroidal compounds, contributing significantly to the total ion chromatogram area. Bioactive constituents such as patchouli alcohol, stigmasta-5,22-dien-3-ol derivatives, gorgost-5-en-3-ol, fatty acid esters, and phenolic derivatives were detected, it also possesses antioxidant, antimicrobial, anti-inflammatory, and cytotoxic activities. The presence of these diverse phytoconstituents supports the traditional medicinal use of *S. anacardium*. L. bark and suggests its potential as a source of pharmacologically important bioactive compounds. Further studies focusing on isolation and biological evaluation of the major constituents are warranted.

Keywords: *Semicarpus anacardium* L, Bark, GCMS.

INTRODUCTION

Semecarpus anacardium L. Medium size tree having family Anacardiaceae, commonly known as Bhallataka or marking nut, is an important medicinal plant. (Khare et al.2004) (Jain et al 2013) It is widely used in traditional Indian systems of medicine such as Ayurveda, Siddha, and Unani. While the nut of the plant is extensively studied, (Bhitre et al 2008) the bark has also been reported to possess significant therapeutic and pharmacological properties, including anti-inflammatory, (Ramprasth et al 2006) antimicrobial, antioxidant, anticancer, and hepatoprotective activities. (Sri Bhavmishra et al 2018). The medicinal potential of *S. anacardium* bark is attributed to the presence of diverse bioactive phytochemicals such as phenolic compounds,

fatty acids, terpenoids, aliphatic hydrocarbons, and other secondary metabolites. Scientific validation and chemical characterization of these constituents are essential to support its traditional use and to explore its potential for drug development.

Gas Chromatography–Mass Spectrometry (GC–MS) is a powerful and widely used analytical technique for the separation, identification, and quantification of volatile and semi-volatile organic compounds present in plant extracts. GC separates complex mixtures based on volatility and polarity, while MS provides structural information and molecular identification by comparing mass spectra.

MATERIAL AND METHODS

Plant Material Collection:

The bark of *Semecarpus anacardium* L. was collected from a naturally growing population in Murbad Taluka in Thane district, during the appropriate season. The plant material was identified with the help of Flora of Kolhapur district by S R Yadav and a voucher specimen was deposited in the department of Botany herbarium for future reference.

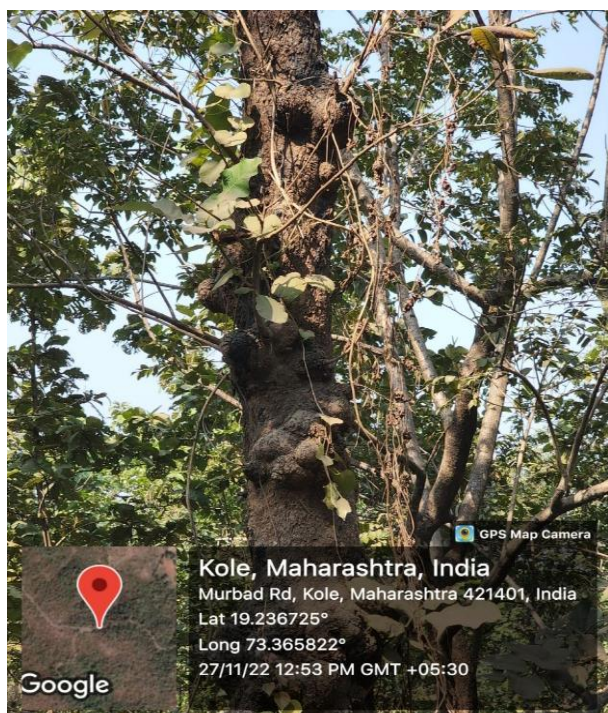


Fig 1 *Semecarpus anacardium* L. sample at 19.23 latitude and 73.36 longitude in Murbad Kole Maharashtra India. Photograph of stem and leaves (Photograph is captured by Mrs. Jyoti Waghmare Murbad Taluka in Thane district Maharashtra from same region for the use of collection study sample in this research)

Plant Morphology:

Semecarpus anacardium L. medium size tree leaves obovate-oblong grey tomentose beneath. Flowers small polygamous in terminal panicle, petals 5 - 6 stamens 5 - 6 inserted at the base of the disk, imperfect in female flowers ovary sub globose densely pilose, ground with 3 styles drupe smooth and shining black when ripe seated on a fleshy edible Orange colored thalamus. occasionally in moist deciduous forests. Plant used in ayurvedic medicine fleshy receptacles edible.

Preparation of Sample:

The collected bark was thoroughly washed with distilled water to remove adhering dust and impurities. It was then shade-dried at room temperature for several days until a constant weight was achieved. The dried bark was coarsely powdered using a mechanical grinder and stored in an airtight container until further analysis. (Baxi A J et al .2001)

Extraction of Phytochemicals:

The plant material was washed and cleaned with distilled water then kept for shade drying for two weeks till it completely dried the dried plant material was powdered with grinder. The powdered bark material was subjected to solvent extraction using methanol by Soxhlet apparatus. The extraction was carried out for 6 hours until the solvent became colorless. The extract was filtered and concentrated under reduced pressure using a rotary evaporator. The concentrated extract was stored at 4 °C for GC–MS analysis.

GC–MS Instrumentation and Analytical Conditions

GC–MS analysis was performed using a Gas Chromatograph coupled with a Mass Spectrometer equipped with an electron impact (EI) ionization system. Separation was carried out using a capillary column (e.g., HP-5MS / DB-5MS; 30 m × 0.25 mm × 0.25 µm film thickness). Peak Report TIC.

Operating conditions:

Carrier gas: Helium (99.999% purity), Flow rate: 1.0 mL/min, Injection volume: 1 µL, Injection mode: Split mode, Injector temperature: 250 °C, Oven temperature program: Initial temperature at 60 °C, increased gradually to 300 °C at a programmed rate, Ionization mode: Electron impact (EI), Ionization energy: 70 eV, Mass scan range: m/z 40–600.

Identification of Compounds:

The compounds present in the bark extract were identified by comparing their retention times, mass spectra, and fragmentation patterns with those available in standard mass spectral libraries such as NIST and Wiley. The relative percentage composition of each component was calculated on the basis of peak area normalization without using correction factors.

RESULTS AND DISCUSSION

The Total Ion Chromatogram (TIC) was recorded, and individual peaks were analyzed for retention time, peak area, and peak height. The results were expressed as relative area percentages, representing

the abundance of each phytochemical constituent present in the extract shown in table no 1.

GC-MS Profiling of *Semicarpus anacardium* Bark:

The GC-MS total ion chromatogram (TIC) of the bark extract of *Semicarpus anacardium* L. revealed a complex phytochemical profile with thirty well-resolved peaks, indicating the presence of a wide range of volatile and semi-volatile constituents. The compounds were identified based on their retention times and mass spectral data by comparison with standard library databases. The retention times of the detected compounds ranged from 0.021 to 35.895 minutes, suggesting the presence of both low-molecular-weight volatile compounds and high-boiling bioactive metabolites. The compound was expressed as peak area percentage.

Table 1: Showing retention time, peak area, peak height retention and fragmentation patterns, relative area percentages of Bark of *S. anacardium* L .

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	Name
1	0.021	0.010	0.050	28632	2.2672	28834	9.41	8-Methyl-6-nonenoic acid
2	26.155	26.140	26.200	7259	0.5748	3357	1.10	Patchouli alcohol
3	30.325	30.300	30.465	20083	1.5903	3627	1.18	2,7-dithiatricyclo[4.3.1.0(3,8)]decane,10-brom
4	31.465	31.455	31.590	20348	1.6113	3415	1.11	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethy
5	31.685	31.660	31.700	5418	0.4290	2638	0.86	Fumaric acid, 2-octyl tridec-2-yn-1-yl ester
6	31.710	31.700	31.750	11285	0.8936	3656	1.19	2,2,2-Trifluoro-N-[2-(1-hydroxy-2,2,6,6-tetra
7	31.770	31.750	31.875	59538	4.7146	7838	2.56	2-Octenoic acid, 7-hydroxy-, ethyl ester
8	31.885	31.875	31.905	10924	0.8650	7555	2.47	Card-20(22)-enolide, 3,5,14,19-tetrahydroxy-,
9	31.985	31.905	32.020	109479	8.6692	22017	7.19	4,4,6-Trimethyl-2-[p-bromophenylamino]-5,6-
10	32.035	32.020	32.140	134221	10.6284	23741	7.75	3-Tridecanone, 7-methyl-13-phenyl-
11	32.291	32.140	32.305	256820	20.3365	30664	10.01	3.beta.,22E-Stigmasta-5,22-dien-3-ol, flophem
12	32.320	32.305	32.375	62601	4.9571	24050	7.85	d,l-Xylitol, 1-O-undec-10-enoyl-
13	32.760	32.745	32.805	14098	1.1164	4547	1.48	2-ethoxy-3,5-hexadiene
14	32.815	32.805	32.890	34660	2.7446	7678	2.51	Pentasiloxane, dodecamethyl-
15	33.026	32.890	33.070	100348	7.9461	9924	3.24	2,2-Dimethyl-6-methylene-1-[3,5-dihydroxy-1
16	33.830	33.820	33.880	7534	0.5966	3661	1.20	d-Mannitol, 1-decylsulfonyl-
17	33.945	33.880	33.955	6811	0.5393	3879	1.27	Distearyl thiodipropionate
18	34.195	34.175	34.225	17559	1.3904	6799	2.22	Cyclopropane-1-carbohydrazide, 2-phenyl-N2
19	34.305	34.225	34.360	143739	11.3821	22510	7.35	7-Hexadecenal, (Z)-
20	34.380	34.360	34.395	34492	2.7313	17926	5.85	Cyclononanone, oxime
21	34.405	34.395	34.430	23083	1.8278	14783	4.83	Propanenitrile, 3-(5-diethylamino-1-methyl-3-
22	34.465	34.430	34.475	20812	1.6480	7898	2.58	2-Methylthiomethyl-4-(1-methylthioethyl)thiet
23	34.495	34.475	34.510	9954	0.7882	5967	1.95	5-Ethyl-2-formylpyridine thiosemicarbazone
24	34.595	34.510	34.610	15816	1.2524	5101	1.67	Bicyclo[5.2.0]nonan-9-one, 8,8-dichloro-
25	35.089	35.030	35.105	11911	0.9432	4073	1.33	Gorgost-5-en-3-ol, (3.beta.)-, TMS derivative
26	35.590	35.575	35.690	22639	1.7927	3750	1.22	2-Methylthiomethyl-4-(1-methylthioethyl)thiet
27	35.710	35.690	35.755	23239	1.8402	6747	2.20	1,4-Benzenediol, 2,5-bis(1,1-dimethylethyl)-
28	35.765	35.755	35.820	20094	1.5912	7624	2.49	9-Borabicyclo[3.3.1]nonane, 9-[3-(dimethylam
29	35.830	35.820	35.880	16275	1.2887	7170	2.34	3-Chloropropionic acid, undecyl ester
30	35.895	35.880	35.940	13181	1.0437	4901	1.60	Z-11-Pentadecenol

Phytochemical Constituents:

These compounds found mainly belonged to terpenoids, steroids, and long-chain lipid derivatives, which are commonly associated with medicinal properties. (Bhartiet.al.2025) Patchouli alcohol, identified at a retention time of 26.155 minutes, is a known sesquiterpene alcohol reported to exhibit antimicrobial, anti-inflammatory, and antioxidant activities. The presence of this compound enhances the therapeutic relevance of the bark extract. (Mishra et.al 2017) Steroidal compounds such as stigmasta-5,22-dien-3-ol and gorgost-5-en-3-ol derivatives were detected at higher retention times. These phytosterols are known to contribute to anti-inflammatory, anticancer, (Manoj et.al 2011) and membrane-stabilizing activities, supporting the traditional use of *S. anacardium L* in chronic inflammatory and tumor-related conditions.

Fatty Acids, Esters, and Phenolic Compounds:

The bark extract contains fatty acid derivatives such as 8-methyl-6-nonenic acid and various long-chain esters. Fatty acids and their esters are reported to possess antimicrobial and anti-inflammatory properties and may play a role in the plant's protective and therapeutic functions. Phenolic compounds, (Rao et.al1973). including substituted benzenediol derivatives. Phenolic compounds are well known for their antioxidant potential and their ability to scavenge free radicals, (Murthy et.al1983-1984).

Sulfur- and Nitrogen-Containing Compounds:

The presence of sulfur- and nitrogen-containing compounds such as thiosemicarbazone derivatives, thiodipropionate derivatives, and heterocyclic sulfur compounds is noteworthy. These compounds are often associated with antimicrobial, antifungal, and enzyme-inhibitory activities. These compounds show defense mechanisms and medicinal efficacy.

Pharmacological Significance:

The bioactive compounds with known pharmacological activities support its potential application in the development of herbal formulations and natural therapeutic agents. GC-MS analysis demonstrated that *S. anacardium L*. bark is rich in biologically active secondary metabolites. The presence of compounds with reported antioxidant, antimicrobial, anti-inflammatory, and cytotoxic properties indicates that the bark extract may serve as a valuable source of natural bioactive molecules.

Further studies involving isolation, structural characterization, and in-vitro and in-vivo biological evaluations are recommended to validate the therapeutic potential of the identified constituents.

Chromatogram (TIC) Analysis:

The compounds were separated with retention times (RT) ranging from 0.021 to 35.895 minutes, reflecting the presence of both low-boiling and high-boiling components in the extract. The identification of compounds was achieved by comparing their retention times and mass spectral fragmentation patterns with those available in standard spectral libraries. The chromatogram shows predominance of high molecular weight and less volatile compounds, such as terpenoids, steroids, fatty acid esters, and complex heterocyclic molecules. Major compounds based on area percentage: The relative abundance of compounds was calculated using peak area percentages. The most dominant peak was observed at RT 32.291 min (Peak 11), contributing 20.34% of the total chromatographic area, indicating it as the principal constituent of the sample.

Significant peaks included:

Peak 10 (RT 32.035 min) with 10.63% area, Peak 19 (RT 34.305 min) with 11.38% area, Peak 9 (RT 31.985 min) with 8.67% area, Peak 15 (RT 33.026 min) with 7.95% area, Peak 7 (RT 31.770 min) with 4.71% area, Peak 12 (RT 32.320 min) with 4.96% area, these peaks accounted for more than 65% of the total ion chromatogram, confirming that the extract is rich in a few predominant bioactive constituents.

Identification of Bioactive Compounds:

Fatty Acids and Their Esters: Early eluting compounds included 8-Methyl-6-nonenic acid (RT 0.021 min, 2.27%), indicating the presence of low molecular weight fatty acids. Additional fatty acid derivatives such as 2-Octenoic acid, 7-hydroxy-, ethyl ester and 3-chloropropionic acid, undecyl ester were detected, which are reported to possess antimicrobial and anti-inflammatory activities.

Terpenoids and Alcohols:

Patchouli alcohol (RT 26.155 min, 0.57%), a sesquiterpene alcohol known for antimicrobial and antioxidant properties, was identified in the sample. Terpenoid-based compounds contribute significantly to the medicinal properties of plant extracts.

Steroids and Triterpenoids: High retention time peaks corresponded to steroidal and triterpenoid compounds, including 3 β ,22E-Stigmasta-5,22-dien-3-ol and Gorgost-5-en-3-ol (TMS derivative). These compounds are well-known for their anti-inflammatory, anticancer, and membrane-stabilizing activities, supporting the therapeutic importance of the sample.

Sulfur- and Nitrogen-Containing Compounds: Several sulfur-containing compounds were detected, such as 2,7-dithiatriacyclo [4.3.1.0(3.8)] decane derivatives, distearyl thiodipropionate, and thiosemicarbazone derivatives. Nitrogen-containing compounds including cyclopropane-1-carbohydrazide derivatives were also identified. These compounds are frequently associated with antimicrobial, antifungal, and enzyme-inhibitory activities.

Phenolic and Polyol Compounds:

The presence of 1,4-benzenediol, 2,5-bis(1,1-dimethylethyl)-, xylitol derivatives, and mannitol derivatives suggests antioxidant potential, as phenolic compounds and polyols are effective free-radical scavengers. Aldehydes, Ketones, and Other Volatile Compounds: Compounds such as (Z)-7-hexadecenal, 3-tridecanone, 7-methyl-13-phenyl-, cyclononanone oxime, and nitrile derivatives were identified. These molecules may contribute to the biological activity and chemical defense mechanisms of the plant.

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CONCLUSION

The GC-MS analysis revealed the presence of thirty phytochemical constituents in the sample, with steroids, terpenoids, fatty acid derivatives, and sulfur-containing compounds as the major components. The predominance of bioactive compounds supports the medicinal importance of the extract and justifies its traditional therapeutic applications.

Conflict of Interest: None of the authors have any conflicts of interest to disclose.

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