ASIAN JOURNAL OF PHARMACEUTICAL AND CLINICAL RESEARCH



Research Article

# IDENTIFICATION OF BIOACTIVE COMPOUNDS BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY ANALYSIS OF *SYZYGIUM JAMBOS* (L.) COLLECTED FROM WESTERN GHATS REGION COIMBATORE, TAMIL NADU

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Received: 03 October 2016, Revised and Accepted: 15 October 2016

#### ABSTRACT

**Objective:** The aim of this study was to investigate the presence of bioactive compounds in the methanolic leaf extract of *Syzygium jambos*.

**Methods:** Collected leaves were shade dried and made into fine powder, extracted with methanol, and the methanolic extract was prepared and analyzed for the presence of bioactive compounds by gas chromatography-mass spectrometry (GC-MS). The mass spectrum of the chromatography was matched with NIST and WILEY Libraries.

**Results:** The GC-MS analysis revealed the presence of 45 active compounds in the extract. From the GC-MS investigation, 1-Deoxy-d-mannitol 3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one, 3-Pentadecylphenol, 2-biphenylene carboxylic acid, Quinoline-3-carboxylic acid, and Stigmast-5-en-3-ol are important phytoconstituents which have antipyretic and antiparasitic activities.

**Conclusion:** The present investigation revealed preliminary information on phytocompounds presented in *S. jambos* leaf extract which is very useful for the human community.

Keywords: Syzygium jambos, Gas chromatography-mass spectrometry analysis, 1-Deoxy-d-mannitol, Phytoconstituents, Methanolic leaf extract.

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#### INTRODUCTION

Herbal plants are cherished gift of nature for mankind and these plants harbor various phytoconstituents which are used by people around the world have healed the sick with plant-derived medicines and handed over to the next generation. Medicinal plants are capable of synthesizing variety of organic compounds with low molecular weight (MW) which is called as secondary metabolites, which are usually with unique and complex structures [1], and it is used as traditional medicine to maintain healthiness, as well as to inhibit, identify, and recover physical and mental illnesses for human and animal [2]. These medicinal products directly acted as medicine or as a source for modern drug development for various fungal and bacterial infections, an antimalarial drug, and anticancer drugs [3-5]. In recent decades, it increases the pharmacological evaluation of phytoconstituents and their medicinal values [6,7]. Many modern methods were used for identification and quantification of bioactive compounds in plant materials. Rather than, gas chromatography-mass spectrometry (GC-MS) has become confidently developed as a key scientific platform for low molecular (secondary) metabolite profiling in both plant and animal species [8,9].

*Syzygium jambos* (L.) (Myrtaceae) is a small tree, popularly known as 'Rose apple which is cultivated throughout India for the edible fruit (black plum) and is testified to contain gallic acid, vitamin C, cyanidin, tannins, anthocyanins, and other components [10,11]. For diabetes mellitus, the leaf extract is used as a remedy in many countries [12,13]. Homeopathic medicine is prepared from the seeds and used as a drug in clinical conditions such as acne, pimples, heartburn nausea, headache, abdominal colic, diarrhea, and fever [14,15]. In the novelty of this study, the previous researchers have studied the preliminary phytochemical analysis and bioactivity of this plant against clinical pathogens, but in our present study, it is designed to explore the bioactive compounds by GC-MS presented in the methanolic leaf extract of *S. jambos*.

#### **METHODS**

### Collection and authentication of plant leave

*S. jambos* leaves were collected from Semmedu (Fig. 1) (Western Ghats's region), Coimbatore, Tamil Nadu, South India. Identification and authentication was done at Botanical Survey of India (BSI) (South Zone), Coimbatore, India. The voucher specimen was deposited in the Laboratory, Department of Microbiology, Dr. N.G.P. Arts and Science College, Coimbatore.

### Preparation of leaf extract

Collected leaves were washed with water, chopped, and shade dried. The dried leaves were made fine power and used for extraction. Before extraction, the leaf powder (10 g) was defatted with hexane. The defatted leaf powder was extracted with methanol by cold maceration method for 48 hrs. The mixture was filtered and concentrated by rotary vacuum evaporator. The extract was stored in the refrigerator for further use.

#### GC-MS analysis for bioactive compounds

GC-MS analysis was performed at PSG College of Arts and Science, Coimbatore India. 5 ml of methanolic leaf extract was dried and few micrograms was dissolved in 1 ml methanol and the extract was analyzed with GC-MS. Separation process was carried out with CE GC 8000 top MSMD 8000 Fyson instrument with Db 35 mr column (10 m×0.5 mm, 0.25 mm film thickness). For separation, heating programs were executed with the help of helium carrier gas from 100 to 250°C for 3 minutes at the flow rate of 1ml/min in the split mode (1:50). An aliquot (2  $\mu$ l) of methanol extract was injected into the column with the injector heater at 250°C.

#### Identification of components

The mass spectra of compounds in the sample were attained by electron ionization (E1) at eV, and the detector operated in scan mode from 20

to 600 atomic mass units. Molecular structure, molecular mass, and fragmentations were used for identifications. The phytoconstituents were identified with the help of standard mass spectral database of WILEY and NIST Libraries [16,17].

# RESULTS

In the present study, the collected plant was identified and authenticated as *S. jambos* (BSI/SRC/5/23/2012/Tech.1270) in BSI, South zone, Coimbatore, Tamil Nadu, India.

# GC-MS analysis

The methanolic leaf extract of *S. jambos* was analyzed for the presence of phytocompounds by GC-MS as shown in Fig. 2.

Totally, 45 effective compounds were identified from the chromatogram. The bioactive compounds were predicted by their retention time (RT),

peak area percentage (%), MW, molecular formula, and their biological activities with the help of PubChem Compound (NCBI), Wiley and NIST Libraries (Table 1).

The first active compound 4-Quinolinol,4-ethenyl-1-ethyldecahydro-2-methyl-(2.alpha,4.alpha,4a.alpha,8a.beta.) was identified in less RT (5.472) (0.10 %), and the last compound Stigmast-5-en-3-ol was identified in much longest RT (46.573) and high percentage peak area (3.97) was observed. Among these 45 compounds, too many phytocompounds having different biological activities, rather than the compounds categorized in different forms based on their biological activities such as antipyretic, antiparasitic (antimalarial), antibacterial, antifungal, and antiviral compounds, are shown in Tables 2 and 3. 4-Methylbenzyl chloride was observed in the 16.117 RT which showed anticancer activity and used as a drug for genital disorders. No biological activity was reported for the compounds of RT1-3, 7, 8, 10, 15, 16, 17, 19, 20, 24, 27, 28, 31-34, 41 (Table 1).



Fig. 1: Map showing the place where leaf samples were collected



Fig. 2: Gas chromatography-mass spectrometry spectrum of methanolic leaf extract of Syzygium jambos

Peak	RT	Compound name	Molecular formula	Molecular weight (g/mol)	Peak area (%)	Biological activity
1	5.472	4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl-(2.	$C_{14}H_{25}NO$	223.3544	0.10	No activity reported
2 3	5.912 7.539	Glucitol, 6-0-nonyl Octadecanoic acid, 9,10-epoxy-18-(trimethylsiloxy)-, methyl	$\begin{array}{c} {C_{{}_{15}}{H_{{}_{32}}{O_{6}}}}\\ {C_{{}_{22}}{H_{{}_{44}}{O_{4}}}{Si}} \end{array}$	308.41098 282.46136	0.01 0.04	No activity reported No activity reported
4	9.272	ester, cis- 1-Deoxy-d-mannitol	$C_{6}H_{14}O_{5}$	166.17236	0.02	Antibacterial,
5	11.000	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin	$C_{11}H_{10}N_4O_3S$	278.2871	-0.01	Antipyretic Antipyretic,
6	11.384	-4-yipyrimidin-4-one. 2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)	$C_{15}H_{12}Br_4O_2$	543.87058	0.36	Antiinflamatory Anticancer
7 8	13.493 14.585	4Cyclopropylmethylbenzonitrile Caryophyllen alcohol ((3Z)-4,8,11,11-tetramethylbicyclo[7.2.0]	$\substack{C_{11}H_{11}N\\C_{15}H_{26}O}$	157.21174 222.36634	0.44 0.23	No activity reported No activity reported
9	16.117	4-Methylbenzyl chloride, 1-(Chloromethyl)-4-methylbenzene	C <sub>8</sub> H <sub>9</sub> Cl	140.61006	0.03	Anticancer, mucolytics, drug for
10	16.858	Methyl 18-fluorooctadecanoate, octadecanoic acid,	C <sub>19</sub> H <sub>37</sub> FO <sub>2</sub>	316.49428	0.01	genital disorder No activity reported
11	17.852	E-15-Heptadecenal, (E)-heptadec-15-enal	$C_{17}H_{32}O$	252.43538	0.23	Fatty acid amide
12	18.565	2,6,10-trimethyl, 14-ethylene-14-pentadecne	$C_{20}H_{38}$	278	0.93	Antiproliferative
13	19.289	3,7,11,15-Tetramethyl-2-hexadecen-1-ol (2-Hexadecen-1-ol, 3,7,11,15-tetramethyl)	$C_{20}H_{40}O$	296.5310	0.36	Precursor of synthetic forms of vitamin E and
14	20.091	Hexadecanoic acid, methyl ester (palmitic acid)	$C_{17}H_{34}O_2$	270.4507	1.20	vitamin K1 Used to produce soaps, cosmetics, and release agents
15 16 17 18	20.891 23.923 24.074 24.350	PENTADECANOIC ACID, pentadecylic acid Methyl (9Z,12Z)-9,12-heptadecadienoate Linolenic acid, pinolenic acid, 5,9,12-octadecatrienoic acid 3,7,11,15-Tetramethyl-2-hexadecen-1-ol. (2-Hexadecen-1-ol, 3,7,11,15-tetramethyl)	$\begin{array}{c} C_{15}H_{30}O_2\\ C_{18}H_{32}O_2\\ C_{18}H_{30}O_2\\ C_{20}H_{40}O\end{array}$	242.3975 280.445 278.4296 296.5310	1.89 0.71 1.12 1.51	No activity reported No activity reported No activity reported Precursor of synthetic forms of vitamin E and vitamin K1
19	24.624	Tetradecanoic acid, 12-methyl-, methyl ester. (Methyl 12-methyltetradecanoate)	$C_{16}H_{32}O_{2}$	256.4241	0.36	No activity reported
20 21	24.841 24.991	Ethyl (9É,12E)-9,12-octadecadienoate Butyl (9E,12E,15E)-9,12,15-octadecatrienoate	$\begin{array}{c} C_{20}H_{36}O_{2}\\ C_{22}H_{38}O_{2} \end{array}$	308.499 334.536	0.45 1.11	No activity reported Antiinflammatory, hypocholesterolemic, cancer preventive,
22	26.308	(E,3R)-2-BENZYLIDENE-3-HYDRO	$C_{11}H_{12}O_{3}$	192	0.00	Antineoplastic, drugs for dermatological
23	29.296	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	$C_4H_2BrN_3O_4$	235.98	0.01	problem Bradykinin B <sub>1</sub> receptor antagonists to relieve adverse symptoms in
24 25	31.432 31.745	1-O-hexadecylglycerol - bis-trimethylsi 3-Pentadecylphenol (3-n-Pentadecylphenol)	$\begin{array}{c} C_{_{19}}H_{_{40}}O_{_{3}}\\ C_{_{21}}H_{_{36}}O\end{array}$	316.52 304.50994	0.09 4.75	mammals No activity reported Antipyretic, antibacterial, anti-inflammatory
26	33.409	TETRACOSANE,(N-Tetracosane)	$C_{24}H_{5}0$	338.6538	0.24	etc. Drugs for dermatological, genital disorders, antibacterial and
27	34.679	(E, E)-1,4,4-Trimethyl-8-methylene-1,5-cycloundecadiene; (betaHumulene)	$\mathrm{C_{15}H_{24}}$	204.35106	29.76	urinary problem No activity reported

Table 1: Phytocompounds present in the methanolic leaf extract of Syzygium jambos

(Contd...)

### Table 1: (Continued)

Peak	RT	Compound name	Molecular formula	Molecular weight (g/mol)	Peak area (%)	Biological activity
28	34.849	Methyl (Z)-5,11,14,17-eicosatetraenoate (RACNRUFXUGWSBR-IOSOIELISA-N)	$C_{21}H_{34}O_2$	318.49346	36.59	No activity reported
29	35.096	3-Pentadecylphenol (Phenol, 3-pentadecyl)	$C_{21}H_{36}O$	304.50994	2.97	Drug for dermatological disorders, antibacterial activity.
30	35.217	methyl (4R,9R,10R,15R)-4- (cyanomethyl)-4,9,10-trimethyl-3- [2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino) propan-2-yl]-15-prop-1-en-2-yl-2,3,5,6,7,8,11,12,14,15,16,17 -dodecahydro-1H-cyclopenta[a] phenanthrene-13-carboxylate	$C_{34}H_{49}N_3O_3S$	579.83616	0.57	Ultra-violet absorbing properties, cerebral vasodilation activity
31	35.367	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol; 2-{2-[2-(4-NONYLPHENOXY) ETHOXY] ETHOXY} ETHANOL	$C_{21}H_{36}O_4$	352.50814	1.23	No activity reported
32 33	35.426 35.521	Phenylacetic acid, 2-(1-adamantyl) ethyl ester 2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol; 2-{2-[2-(4-NONYLPHENOXY] ETHOXY] ETHOXY] ETHANOL	$\begin{array}{c} C_{_{20}}H_{_{26}}O_{_2}\\ C_{_{21}}H_{_{36}}O_{_4} \end{array}$	298.41924 352.50814	0.76 0.61	No activity reported No activity reported
34	35.667	Ethyl 7-amino[1,2,4]triazolo[1,5-a] pyrimidine-6-carboxylate( 7-amino- ethyl ester)	$C_8 H_9 N_5 O_2$	207.18936	1.04	No activity reported
35	36.134	1H-Indole-2-carboxylic acid (Indole-2-carboxylic acid)	$C_9H_7NO_2$	161.15738	0.55	Antitussive agent, antiasthmatic
36	36.914	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl	$C_{30}H_{5}0$	410.7180	2.44	Drug for dermatological disorders, used to
37	37.318	2,5-Di-tert-amylhydroquinone (79-74-3; Santouar A)	$C_{16}H_{26}O_{2}$	250.37644	0.26	treat wound, ulcer Drug for dermatological
38	37.600	2-BIPHENYLENECARBOXYLIC ACID	$C_{17}H_{14}O_4$	282	0.45	disorders, anticancer Antimalarial, drug for nervous
39	37.869	(Z)-7-Hexadecenal, 7-Hexadecenal, (Z)	$C_{16}H_{30}O$	238.4088	0.59	Antiviral activity,
40	38.661	S-Ethyl ethanethioate, S-Ethyl thioacetate	$C_5H_{10}OS$	118.197	0.35	Drug for skeletal disorder, nervous
41	38.858	Phenanthro (1,2-b) furan-10,11-dione, 6,7,8,9-tetrahydro-7-hydroxy-6-(hydroxymethyl)-1-methyl-;	$C_{18}H_{16}O_5$	312.31664	0.37	No activity reported
42	39.371	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	$C_{14}H_{22}O_{2}$	222	0.50	Drug for dermatological disorders, acting as
43	40.475	Quinoline-3-carboxylic acid (3-Quinolinecarboxylic acid)	$C_{10}H_7NO_2$	173.16808	0.21	analgesics Antiparasitic, antimalarial, antibacterial, antibiotic, antiseptic
44	42.012	alphaTocopherolbetaD-mannoside (2,5,7,8-Tetramethyl-2-	$C_{35}H_{60}O_{7}$	592.8467	0.58	etc. Antineoplastic activity, quaternary
45	46.573	hexofuranoside) Stigmast-5-en-3-ol, Azuprostat; Nimbosterol; .alphaPhytosterol	C <sub>29</sub> H <sub>50</sub> O	414.7067	3.97	compounds Antipyretic, antipruritic

From these 45 active compounds, six phytocompounds exhibited antipyretic and antiparasitic (antimalarial) (Table 2) activity such as 1-Deoxy-d-mannitol (C6H1405), 3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one (C11H10N403S), 3-Pentadecylphenol (C21H360), 2-biphenylene carboxylic acid (C17H1404), Quinoline-3-carboxylicacid (C10H7N02), and Stigmast-5-en-3-ol (C29H500). Moreover, TETRACOSANE(C24H50), (E,3R)-2-BENZYLIDENE-3-HYDROXYBUTANOIC ACID (C11H1203),3-Pentadecylphenol (),2,6,10,14,18,22-Tetracosahexaene (C30H50), 1,4-Benzenediol, 2,5-bis(1,1-dimethylethyl), and (Z)-7-Hexadecenal(C16H30O) are exhibited antifungal, antibacterial, and antiviral activity.

# DISCUSSION

Nowadays, the study of the organic compounds for biological activity from natural resources has increased. The combination of GC-MS is a great technique for separation and identification of volatile and semi-

S. No.	Compound name	Structure of the compound	Biological activity
1	1-Deoxy-d-mannitol	HO OH OH	Antipyretic activity
2	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one		Antipyretic activity
3	3-Pentadecylphenol (3-n-Pentadecylphenol)		Antipyretic activity
4	2-BIPHENYLENECARBOXYLIC ACID	L'AL	Antiparasitic and antimalarial activity
5	Quinoline-3-carboxylic acid( 3-Quinolinecarboxylic acid)		Antiparasitic and antimalarial activity
6	Stigmast-5-en-3-ol, Azuprostat; Nimbosterol;.alphaPhytosterol		Antipyretic activity

# Table 2: Antipyretic and antiparasitic compounds present in *S. jambos* leaf extract

S. jambos: Syzygium jambos

Table 3: Antibacterial	, antifungal and antiviral	compounds present i	n <i>S. jambos</i> leaf extract
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S. No.	Compound name	Structure of the compound	Biological activity
1	TETRACOSANE, (N-Tetracosane)	~~~~~~	Drugs for dermatological problem, antibacterial activity
2	(E,3R)-2-BENZYLIDENE-3-HYDROXYBUTANOIC ACID		Drugs for dermatological problem
3	3-Pentadecylphenol (Phenol, 3-pentadecyl)	HO CONTRACTOR OF	Drugs for dermatological problem, antibacterial activity
4	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl	hopeday	Drugs for dermatological problem, antibacterial activity
5	(Z)-7-Hexadecenal, 7-Hexadecenal, (Z)		Antiviral activity, organic fertilizer
6	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	HO	Drug for dermatological disorders, acting as analgesics
		ОН	

S. jambos: Syzygium jambos

volatile bioactive compounds [18]. In general, the reliability of medicinal plant for its usage is evaluated by correlating the phytochemical compounds with their biological activities [19].

In the present exploration, totally 45 bioactive chemical constituents were identified in methanolic leaf extract of *S. jambos* having biological properties. From the GC-MS investigation, too many numbers of

bioactive compounds were present in the leaf extract which is mentioned in Table 1. 1-Deoxy-d-mannitol, 3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one, 3-Pentadecylphenol, 2-biphenylene carboxylic acid, Quinoline-3-carboxylic acid and Stigmast-5-en-3-ol are important phytoconstituents which have antipyretic and antiparasitic activities. Hexadecanoic acid, Octadecanoic, and Octadecadienoic compounds are observed in our study; these compounds are previously identified in different plant extracts reported. Hexadecanoic acid had been reported in alcohol extract of the leaves of Kigelia pinnata [20] and M. officinalis [21,22]. We identified 17 compounds with n-Hexadecanoic acid and Octadecanoic acid as the major compounds in the leaves of Cleistanthus collinus. GC-MS analysis of ethyl acetate extract of Goniothalamus umbrosus revealed the presence of n-Hexadecanoic acid [23]. n-hexadecanoic acid. Hexadecanoic acid. Phytol. 9. 12-Octadecadienoic acid, 9, 12, 15-Octadecatrienoic. There is a growing awareness of the importance of the phytochemical components and their biological activities [24,25].

#### CONCLUSION

*S. jambos* is a tree used as medicine by our ancient people; however, there are no reports on the thorough phytochemical analysis of the plant. GC-MS analysis reported the important biological components presented in our selected plant. Secondary metabolites will be rich in plants which are widely used in traditional medicine to treat and cure various ailments as well as in the modern medicine. The secondary metabolites such as alkaloids, phenols, tannins, and flavonoids are acted against different biological problems. The present investigation has given preliminary information of phytocompounds present in *S. jambos* leaf extract which is useful for the human community. Further investigations are needed *in silico* for these bioactive compounds which may add new knowledge to the information of *S. jambos* which is useful for pharmacological evaluation.

### ACKNOWLEDGMENTS

The authors would like to thank the Central Instrument Facility, PSG College of Arts and Science, Coimbatore, for providing required facilities to carry out this research work.

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