

Comprehensive GC-MS/MS Profiling Of Bioactive Compounds in *Syzygium Stocksii* (Duthie) Gamble (Myrtaceae)

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ABSTRACT:

The genus *Syzygium* comprises 1200–1800 species that belong to the family of Myrtaceae. Moreover, plants that are belonged to this genus are being used in the traditional system of medicine in various countries, including India, from the ancient times. The aim of this research is to describe the scientific works and to provide organized information of the compounds and functional groups found in *Syzygium stocksii* through the GC-MS/MS and FTIR techniques. Bioactive compounds found in leaves and stem of *Syzygium stocksii* have various applications in pharmaceutical industries and this finding will be beneficial to treat various illness as they show different biological activities. The information related to genus *Syzygium* was done through searching variant scientific electronic databases, including scientific databases, including PubMed, Google Scholar, Science Direct, Web of Science, Wiley Online Library, Springer, Research Gate link, published books, and conference proceedings. However, many members of the species of the genus *Syzygium* need further comprehensive studies regarding phytochemical constituents and mechanism based pharmacological activities.

I. INTRODUCTION:

The plants are being widely used for their natural resources isolated from various parts of a plant and have been used in the treatment of human diseases. According to 'World Health Organization' 80 % of the people living in rural area depend on medicinal herb as primary health care system. Due to the presence of various alkaloids, Flavonoids, Steroids, Polyphenols (Dhru et al. 2016, Loc and Kiet, 2011). *Syzygium* is an entirely old-world genus. In past, many *Syzygium* species were originally described in *Eugenia* L. or *Jambosa* Adans. Taxonomic confusion in *Eugenia* and *Syzygium* resulted from the considerable overlap of macro- and micromorphological characters. Currently, it is clear that these genera

are significantly different. Recent molecular evidence supports a scenario in which these two genera are in fact independent lineages (Widodo, 2011). The genus *Syzygium* comprises 1200–1800 species that belong to the family of Myrtaceae. It has a subtropical to tropical distribution, from Africa extending east to the Hawaiian Islands and from India and China southwards to southern Australia and New Zealand. The centres of diversity are the Southern Asian, Southeast Asian, Malaysian, Australian and New Caledonian regions with decreasing species richness elsewhere (Craven 2001, Parnell et al. 2006).

Accordingly, numerous of research works have been conducted on plants from the genus *Syzygium* to elucidate its chemistry and pharmacology. Occurrence of polyphenols, flavonoids, tannins, and sterols from *Syzygium* species, Meanwhile, plant extracts and compounds also claimed a broad spectrum of activities from antibacterial to anti-inflammatory activities through analgesic, antiviral, anti-dermatophyte, anticancer and hepato-protective properties (Sobeh et al. 2018).

II. MATERIAL AND METHODS:

2.1 COLLECTION OF SPECIMENS:

Barsu, Rajapur tehsil of Ratnagiri District Maharashtra, India, was selected for collection of plant species for experiment. The different plant materials are collected during May month. Leaves and Stems were collected. The collected material was washed properly and allowed to shade dry for 15-20 days. Then the material was crushed into fine powder and was kept in air tight container.

2.2 PREPARATION OF EXTRACT:

1gm fine powder of Stem and Leaves each was taken and mixed in 10ml of 70% Methanol to obtain the methanolic extract. The extract was sonicated at 20°C for 15 min. and centrifuged at 10,000 rpm for 10 min. Supernatant was subjected to GC-MS/MS analysis.

2.3 SAMPLE ANALYSIS:

2.3.1 GC-MS/MS ANALYSIS:

The extract was sonicated at 20°C for 15 minutes and centrifuged at 10,000 rpm for 10 min. The supernatant was subjected to GC-MS/MS analysis. GC-MS/MS analysis was performed on a Shimadzu TQ 8050 plus HS 20 from Japan, with helium as the carrier gas. The following conditions were maintained for the analysis: column oven temperature at 40°C, injection temperature at 270°C, injection mode as split, flow control mode with linear velocity, pressure at 49.5 kPa, total flow at 74.0 mL/min, and column flow at 1.00 mL/min.

III. RESULTS:

Compounds which are detected in methanolic extracts of both leaves and stem, are tabulated in Tables 1 and 2 with their Retention times and Area of percentage. The detected compound shows various biological activities as enlisted and compare as follows: It is found that the methanolic extracts of stem contains various compounds viz. Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dim, Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-m, alpha.-Pinene, D-Limonene, Nonane, 4,5-dimethyl-, 1-Butoxy-1-isobutoxybutane, Caryophyllene, (1R,3aS,8aS)-7-Isopropyl-1,4-dimethyl- 1,2,3, Humulene, 1H-Cycloprop[e]azulene, 1a,2,3,5,6,7,7a,7b-o, n-Butyl ether, Propanoic acid, 2-methyl-, 2-methylpropyl ester, tau.-Cadinol, Neophytadiene, Tetracosamethyl- cyclododecasiloxane, Sulfurous acid, cyclohexylmethyl pentadecyle, 1,1':3',1"-Terphenyl, 5'- phenyl-, Sulfurous acid, cyclohexylmethyl octadecyl ester, Borinic acid, diethyl-, (2-ethyl-1,3,2-dioxabor and Cholesta-4,6-dien-3-ol, (3.beta.). On the other hand it was found that the methanolic extracts of leaves contains various compounds viz. Acetic acid, butyl ester, Propanoic acid, 2-methyl-, 2- methylpropyl ester, alpha.-Pinene, Camphene, D-Limonene, Nonane, 4,5- dimethyl-, Dimethyl [bis(2-methylpropoxy)]silan e, 1,1-Diisobutoxy-isobutane, Bornyl acetate, alpha.-Guaiene, 1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-o, Bicyclo[5.2.0]nonane, 2-methylene-4,8,8- trim, Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8, Neointermedeol, Neophytadiene, 3,7,11,15-Tetramethyl-2- hexadecen-1-ol, Hexadecanoic acid, methyl ester, 6-Octadecenoic acid, methyl ester, (Z)-, Methyl stearate and Tetrapentacontane. These compounds show various activities viz. Antibacterial, Antimicrobial, apoptotic, antimetastatic, and antibiotic, Antioxidant,

antidiabetic, anticancer, anti-inflammatory, cardioprotective, gastroprotective, hepatoprotective, immune modulatory, anti-fibrotic, anti- genotoxic, anti-hemolytic, Analgesic, antipyretic and Cytotoxic activity. Bioactive compounds found in leaves and stem of *Syzygium stocksii* have various applications in pharmaceutical industries and this finding will be beneficial to treat various illness as they show different biological activities.

IV. CONCLUSION:

The GC-MS spectroscopic analysis of methanolic extracts of *Syzygiumstocksii* leaves and stem revealed the presence of various functional groups. In total, 20 compounds were detected from 35 functional groups in the methanolic extracts. The presence of functional groups such as acetylenic (alkyne), aromatic ring (aryl), olefinic (alkene), aliphatic organohalogen, saturated aliphatic (alkane/alkyl), and amine and amino compounds was confirmed through the identification of specific peaks in the FTIR spectra. These findings indicate the chemical complexity and potential bioactivity of the methanolic extracts of *Syzygiumstocksii*.

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Captions:

Table 1. GC-MS/MS of Syzygiumstocksii Stem.

Sr.No.	Name	R.T	Area%	Formula	MW	Properties	Reference
1	Naphthalene,1,2,4a,5,8,8a-hexahydro-4,7-dim	23.037	0.22	C ₁₅ H ₂₄	204	Antibacterial	TayyebGhaffari,etal.2019
2	Naphthalene,1,2,3,4,4a,5,6,8a-octahydro-7-m	23.276	0.51	C ₁₅ H ₂₄	204	Antibacterial	TayyebGhaffari,et al.2019
3	alpha.-Pinene	7.038	1.05	C ₁₀ H ₁₆	136	Antimicrobial,apoptotic,antimetastatic, and antibioticproperties	Manoj KPandey,etal.2022
4	D-Limonene	9.860	0.29	C ₁₀ H ₁₆	136	Antioxidant,antidiabetic,anticancer, anti-inflammatory,cardioprotective,gastroprotective,hepatoprotective,immunomodulatory, antifibrotic, anti-genotoxic	PandiAnandakumar,etal.2020
5	Nonane,4,5-dimethyl-	10.560	-0.20	C ₁₁ H ₂₄	156	Norecord	-
6	1-Butoxy-1-isobutoxy-butane	13.769	0.20	C ₁₂ H ₂₆ O ₂	202	Antioxidant,antibacterial,anti-hemolytic,anti-inflammatory,antidiabetic,and anticancerousactivity	MuhammadNaveed,etal.2023

7	Caryophyllene	20.825	0.96	C ₁₅ H ₂₄	204	Anticancer and analgesic activities	Yulia Vyacheslavovna Gyrdymova, et al. 2021
8	(1R,3aS,8aS)-7-Isopropyl-1,4-dimethyl-1,2,3,	21.397	1.40	C ₁₅ H ₂₄	204	Norecord	-
9	Humulene	21.789	0.32	C ₁₅ H ₂₄	204	Antibacterial activity	Nasser A. Awadh, et al., 2017
10	1H-Cycloprop[e]azulene, 1a,2,3,5,6,7,7a,7b-o	22.730	0.60	C ₁₅ H ₂₄	204	Antimicrobial activity	Juntao Chen, et al. 2018
11	n-Butylether	5.680	19.18	C ₈ H ₁₈ O	130	Norecord	-
12	Propanoic acid, 2-methyl-, 2-methylpropylester	6.549	0.53	C ₈ H ₁₆ O ₂	144	Norecord	-
13	tau.-Cadinol	26.478	1.75	C ₁₅ H ₂₆ O	222	Anti-inflammatory activity	Ana M. González, et al. 2012
14	Neophytadiene	30.984	0.75	C ₂₀ H ₃₈	278	Analgesic, antipyretic, anti-inflammatory, antimicrobial, antioxidant compound	Mallappa Kumara Swamy, et al. 2017
15	Tetracosamethylcyclododecasiloxane	40.200	8.56	C ₂₄ H ₇₂ O ₁₂ S ₁₂	888	Cytotoxic and antimicrobial properties.	Mohammed Al Bratty, et al. 2020
16	Sulfurous acid, cyclohexylmethylpentadecyle	42.276	4.33	C ₂₂ H ₄₄ O ₃ S	388	Norecord	-
17	1,1':3',1''-Terphenyl, 5'-phenyl-	44.068	14.5	C ₂₄ H ₁₈	306	Norecord	-
18	Sulfurous acid, cyclohexylmethyloctadecylester	46.740	21.19	C ₂₅ H ₅₀ O ₃ S	430	Antimicrobial and cytotoxic activity	Purity Kinya Kaaria, 2018

19	Borinic acid, diethyl-, (2-ethyl-1,3,2-dioxabor	48.449	6.98	C ₉ H ₂₀ B ₂ O ₃	198	Norecord	-
20	Cholesta-4,6-dien-3-ol, (3-beta.)-	48.654	16.59	C ₂₇ H ₄₄ O	384	Norecord	-

Table 2. GC-MS/MS of SyzygiumstocksiiLeaves.

SrNo	Name (leaf)	R.Time	Area%	Formula	Mol.wt	Properties	Reference
1	Acetic acid, butylester	3.975	0.64	C ₆ H ₁₂ O ₂	116	Antifungal and antitumor	Izzah Farhah Zambari, et al. 2022
2	n-Butylether	5.506	35.21	C ₈ H ₁₈ O	130	Norecord	-
3	Propanoic acid, 2-methyl-, 2-methylpropylester	6.401	1.12	C ₈ H ₁₆ O ₂	144	Norecord	-
4	alpha.-Pinene	6.900	7.55	C ₁₀ H ₁₆	136	Antimicrobial, apoptotic, antimetastatic, and antibiotic properties	Manoj K Pandey, et al. 2022
5	Camphene	7.382	1.02	C ₁₀ H ₁₆	136	Antibacterial, antifungal, anticancer, antioxidant, antiparasitic, antidiabetic, anti-inflammatory, and hypolipidemic activities	Naoufal ELHachlafi, et al. 2021

6	D-Limonene	9.799	2.12	C ₁₀ H ₁₆	136	Antioxidant, antidiabetic, anticancer, anti-inflammatory, cardioprotective, gastroprotective, hepatoprotective, immunomodulatory, antifibrotic, anti-genotoxic	PandiAnandakumar,etal.2020
7	Nonane, 4,5-dimethyl-	10.508	0.46	C ₁₁ H ₂₄	156	Norecord	-
8	Dimethyl[bis(2-methylpropoxy)]silane	12.003	4.14	C ₁₀ H ₂₄ O ₂ Si	204	Norecord	-
9	1,1-Diisobutoxyisobutane	13.755	0.96	C ₁₂ H ₂₆ O ₂	202	Norecord	-
10	Bornylacetate	17.365	0.70	C ₁₂ H ₂₀ O ₂	196	Norecord	-
11	Caryophyllene	20.993	1.32	C ₁₅ H ₂₄	204	Anticancer and analgesic activities	YuliaVyacheslavovnaGyrdymova,etal.2021
12	alpha. -Guaiene	21.372	2.91	C ₁₅ H ₂₄	204	Antibacterial activity.	-
13	1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-o	22.384	1.44	C ₁₅ H ₂₄	204	Norecord	-
14	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trim	22.785	3.03	C ₁₅ H ₂₄	204	Norecord	-

15	Naphthalene,1,2,3,4,4a,5,6,8a-octahydro-4a,8	22.951	1.48	C ₁₅ H ₂₄	204	Norecord	-
16	Neointermedeol	26.939	1.44	C ₁₅ H ₂₆ O	222	Antibacterial activity	WangoYaxin,etal.2020
17	Neophytadiene	30.994	10.47	C ₂₀ H ₃₈	278	Analgesic, antipyretic, anti-inflammatory, antimicrobial, and antioxidant compound	MallappaKumaraSwamy,etal.2017
18	3,7,11,15 Tetramethyl-2-hexadecen-1-ol	31.630	2.64	C ₂₀ H ₄₀ O	296	Antioxidant, antimicrobial	ThiyagarajanBharathi, et al.2023
19	Hexadecanoic acid,methylester	33.314	2.36	C ₁₇ H ₃₄ O ₂	270	Larvicidal, pesticide,Antifungal.	Abdullah, R.2019 Ali,etal.2022
20	6-Octadecenoic acid,methylester,(Z)-	37.126	2.34	C ₁₉ H ₃₆ O ₂	296	Antioxidant, antimicrobial.	Adeniyi SAdegoke,etal.2019
21	Methylstearate	37.684	1.87	C ₁₉ H ₃₈ O ₂	298	Antioxidant, antifungal.	Javaid,etal.2021
22	Tetrapentacontane	42.530	10.06	C ₅₄ H ₁₁₀	758	Antidiabetic and Anticancer effects.	Abuzer, et al.2021

Captions:

Figure 1. GC-MS/MS Chromatogram of Syzygiumstocksii Stem

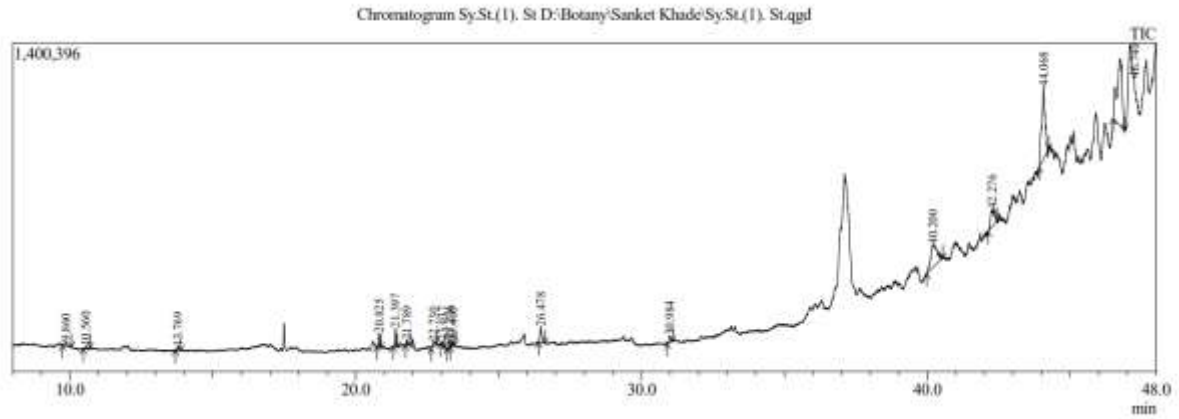


Figure 1.GC-MS/MS Chromatogram of Syzygiumstocksii Leaves

