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# Gas Chromatography and Mass Spectroscopic Analysis of Bioactive Compounds from *Scoparia dulcis* Whole Plant Extract

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**Abstract:** Worldwide, human beings have traditionally employed many folkloric herbal resources as complementary and alternative remedies, and these remedies have played a pivotal role in modern medicines for many decades, as scientists have used them to develop drugs. The use of plants and plant products for medicinal purposes has increased in recent times. The plants are considered to be safe for use and potentially with fewer side effects. These plants are also freely available to the users. But, many of these medicinal plants possess poisonous phytochemicals which can even cause death if taken in higher concentrations. It is very important to gain a good amount of knowledge before their use. In this study, the whole plant of *Scoparia dulcis* were extracted using hydro-alcoholic and screened to identify active phytoconstituents using gas chromatography mass spectrometry. A total of thirty compounds appeared in GC-MS chromatogram, fourteen major bioactive compounds were identified in the present study. The major components of the hydro-alcoholic extract were found to be 2,3-dihydro-benzofuran, 3-pyridinecarboxylic acid, Nonanoic acid, 10,11-dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl acetate, hexadecanoic acid, methyl ester, n-hexadecanoic acid, oleic acid, 9,12-octadecadienoic acid, methyl ester, 9,12,15-octadecatrienoic acid, methyl ester, phytol, octadecanoic acid, methyl ester, 9-octadecenoic acid, 9,12,15-octadecatrien-1-o and octadecanoic acid. Hence, the presence of these phytochemicals could be responsible for the therapeutic effects of the plant.

**Keywords:** *Scoparia dulcis*, GC-MS analysis, Phytochemicals, Bioactive compounds

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## Introduction

Most people have entrusted plants with having qualities of an important source of medicine for decades. The practice of using herbal remedies to cure and heal sick individuals has persisted

through families for decades. Traditional medicine is an amalgam of expertise. It is carried out in accordance with varied cultural theories, beliefs, and traditional practices that are

employed to uphold health, identify, prevent, and treat diseases. Natural products, especially plants derived chemicals are considered as promising source for the development of new agents with safe therapeutic window (Atanasov *et al.*, 2015). Medicinal plants are rich in secondary metabolites with many biological activities including antioxidant, anti-inflammatory, anticancer, antiviral, antifungal, and antibacterial agents (Gololo *et al.*, 2021). Phytochemicals that are regarded as bioactive compounds in plants have been confirmed to be safe effective, relatively cheap, and recently predicted as a suitable substitute to antibiotics (Ahmed *et al.*, 2019). About 80% of the world's inhabitants (Nxumalo *et al.*, 2020) and more than 90% of those listed in developing countries adopted herbal medicine for preliminary health care. Recently, medicinal plants have played an important role in pharmacological research and drug apperception (Bourhia *et al.*, 2020).

Many phytochemical compounds have been utilized by thousands of physicians in their practices and are consumed under medical management by tens of millions of people (Yuan *et al.*, 2016). Crude plant extracts and medicines manufactured on the values of natural compounds even by pharmaceuticals companies may lead to large-scale exposure of humans to natural products (Ghosh *et al.*, 2016). The major reason for continued use of herbal remedies is their usefulness, easy availability, low price, and moderately less or no toxic property (Alexandra *et al.*, 2018). It can act on the body as powerful as pharmaceutical drugs, and it can start healing itself. As various phytochemicals with pharmacological activity have been isolated from several traditional Indian medicinal plants, it is pertinent to investigate the therapeutic effects of the traditional Indian medicinal plants (Kshetrimayum *et al.*, 2017). GC-MS is the best sensitive technique used for separation and identification of the many structurally complex components that are present in plant extracts.

Gas chromatography-mass spectrometry (GC-

MS) is the accurate technique employed for the detection of functional groups and identification of various bioactive therapeutic compounds that are present in medicinal plants (Fan *et al.*, 2018; Satapute *et al.*, 2019). In recent years GC-MS studies have been increasingly applied for the analysis of medicinal plants as this technique has proved to be a valuable method for the analysis of non-polar components and volatile essential oil, fatty acids, lipids and alkaloids (Sosa *et al.*, 2016). Hence, the present study was aimed to find the bioactive compounds present in the hydro-alcoholic extract of whole plant of *Scoparia dulcis* by GC-MS analysis. On the basis of qualitative and quantitative analysis of different extractions of whole plant of *Scoparia dulcis*, the hydro-alcoholic extract showed better results and used for GC-MS analysis.

## Materials and Methods

### *Collection of plant materials:*

The whole plant of *Scoparia dulcis* were collected from Thiruppanandal, Thanjavur (District), Tamil Nadu, India from a single herb. The whole plant of *Scoparia dulcis* was identified and authenticated by Dr. K. Sankarganesh. Department of Botany. D.G. Government Arts College for Women, Mayiladuthurai. Tamil Nadu. India.

### *Preparation of extract:*

The collected *Scoparia dulcis* plants were washed several times with distilled water to remove the traces of impurities from the plant. The plants were dried at room temperature and coarsely powdered. The powder was extracted with hydro-alcohol (70%) using Soxhlet extraction. A semi solid extract was obtained after complete elimination of solvent under reduced pressure. The *Scoparia dulcis* extracts were stored in refrigerator until used for GCMS analysis.

### *GC-MS analysis:*

GC MS analysis was carried out on Shimadzu 2010 plus comprising a AOC-20i auto sampler and gas chromatograph interfaced to a mass spectrometer instrument employing the following

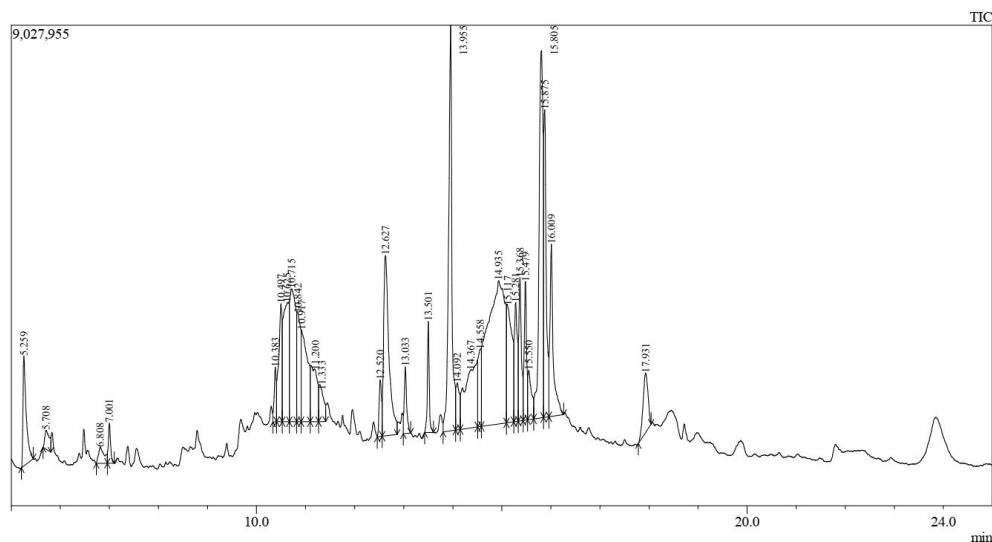


Fig. 1: Chromatogram of *Scoparia dulcis* whole plant.

conditions: column RTX 5Ms (Column diameter is 0.32 mm, column length is 30 m, column thickness 0.50  $\mu\text{m}$ ), operating in electron impact mode at 70eV, Helium gas (99.999%) was used as carrier gas at a constant flow of 1.73 ml/min and an injection volume of 0.5  $\mu\text{l}$  was employed (split ratio of 10:1), injector temperature 270  $^{\circ}\text{C}$ , ion-source temperature 200 $^{\circ}\text{C}$ . The oven temperature was programmed from 40 $^{\circ}\text{C}$  (isothermal for 2 min), with an increase of 8 $^{\circ}\text{C}/\text{min}$ , to 150 $^{\circ}\text{C}$ , then 8 $^{\circ}\text{C}/\text{min}$  to 250 $^{\circ}\text{C}$ , ending with a 20 min isothermal at 280 $^{\circ}\text{C}$ . Mass spectra were taken at 70eV; a scan interval of 0.5 sec and fragments from 40 to 450 Da. Total GC running time is 51.25 min. The relative percentage amount of each component was calculated by comparing its average peak area to the total areas. Software adopted to handle mass spectra and chromatograms was a Turbo Mass Ver 5.2.0 (Srinivasan *et al.*, 2013).

#### Identification of components:

Interpretation on GCMS was conducted using the database of National Institute Standard and Technology (NIST) and WILEY8 having more than 62,000 patterns. The spectrum of the unknown component was compared with the spectrum of the known components stored in the NIST library. The name, molecular weight and structure of the

components of the test materials were ascertained (Dukes, 2013).

### Results and Discussion

In general, the effectiveness of medicinal plants is assessed by correlating the phytochemical compounds to the biological activities of the plants (Belkacem *et al.*, 2013). Different bioactive compounds of the hydro-alcoholic extracts of whole plant of *Scoparia dulcis* were analyzed by using GC-MS. The bioactive phyto-compounds were recognized and characterized based on their retention and elution order in an analytical column. The mass spectra are matched with the inbuilt database of the NIST and WILEY8 library to identify the compound present. The chromatograms of the extract is shown in Figure 1 and in Tables 1 and 2. GC-MS chromatogram of *Scoparia dulcis* whole plant extract showed peaks which indicated the presence of 30 different bioactive compounds. The results revealed that the percentage of major bioactive compounds viz., 2,3-dihydro-benzofuran, 3-pyridinecarboxylic acid, Nonanoic acid, 10,11-dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl acetate, hexadecanoic acid, methyl ester, n-hexadecanoic acid, oleic acid, 9,12-octadecadienoic acid, methyl ester, 9,12,15-octadecatrienoic acid, methyl ester, phytol, octadecanoic acid, methyl ester, 9-octadecenoic

Table 1: Identification of active compounds in *Scoparia dulcis* whole plant using GCMS

Peak	R. Time	Area %	Height %	Molecular Formula	Molecular Weight	Name of the compounds
1	5.259	2.31	3.13	C <sub>8</sub> H <sub>8</sub> O	120	2,3-dihydro-benzofuran
2	5.708	0.58	0.53	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	123	3-pyridinecarboxylic acid
3	6.808	0.60	0.46	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	164	Beta.-D-Ribopyranoside, methyl
4	7.001	0.56	1.14	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	170	2,6-dimethyl-1,7-octadiene-3,6-diol
5	10.383	0.74	1.56	C <sub>17</sub> H <sub>28</sub> O <sub>4</sub>	296	Nerolidol-epoxyacetate
6	10.497	2.61	3.36	C <sub>15</sub> H <sub>26</sub> O <sub>2</sub>	238	9-(3,3-Dimethyloxiran-2-yl)-2,7-dimethylnona-2,6-dien-1-ol
7	10.625	4.39	3.39	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>	194	Methyl .beta.-d-galactopyranoside
8	10.715	5.04	3.79	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	158	Nonanoic acid
9	10.842	2.52	3.09	C <sub>11</sub> H <sub>14</sub> O <sub>4</sub>	210	Tricyclo[4.2.1.0(3,7)]nonane-9-carboxylic acid
10	10.917	3.57	2.61	C <sub>7</sub> H <sub>15</sub> NO <sub>8</sub>	241	1-deoxy-1-nitroheptitol
11	11.200	2.32	1.46	C <sub>12</sub> H <sub>20</sub> O	180	Cyclohexene, 1,5,5-trimethyl-6-acetylmethyl-
12	11.333	1.07	0.88	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116	1-(1-Hydroxyethyl),1-(hydroxymethyl)cyclopropane
13	12.520	0.90	1.61	C <sub>13</sub> H <sub>18</sub> O <sub>3</sub>	222	2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-4-(3-oxo-1-butenyl)-
14	12.627	6.20	5.13	C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub>	165	6-Methoxy-2-benzoxazolinone
15	13.033	1.00	1.90	C <sub>17</sub> H <sub>30</sub> O <sub>4</sub>	298	10,11-dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl acetate
16	13.501	1.31	3.16	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270	Hexadecanoic acid, methyl ester
17	13.955	8.71	11.55	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256	n-Hexadecanoic acid
18	14.092	1.02	1.34	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	210	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-
19	14.367	4.97	1.65	C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub>	205	N-(2-oxo-tetrahydro-furan-3-yl)-benzamide
20	14.558	1.53	2.21	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	172	4-Octanone, 5-hydroxy-2,7-dimethyl-
21	14.935	16.01	4.08	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	180	Inositol
22	15.117	4.05	3.33	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282	Oleic Acid
23	15.281	2.37	3.39	C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>	294	9,12-Octadecadienoic acid, methyl ester
24	15.368	2.36	4.09	C <sub>19</sub> H <sub>32</sub> O <sub>2</sub>	292	9,12,15-Octadecatrienoic acid, methyl ester
25	15.479	2.10	3.94	C <sub>20</sub> H <sub>40</sub> O	296	Phytol
26	15.550	1.12	1.41	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	298	Octadecanoic acid, methyl ester
27	15.805	9.68	10.46	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282	9-octadecenoic acid
28	15.875	4.84	8.76	C <sub>18</sub> H <sub>32</sub> O	264	9,12,15-Octadecatrien-1-o
29	16.009	3.62	4.90	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	298	Octadecanoic acid
30	17.931	1.91	1.69	C <sub>18</sub> H <sub>30</sub> N <sub>2</sub> OS	322	Tridecanoic acid, thiophen-2-ylmethylenehydrozide

acid, 9,12,15-octadecatrien-1-o and octadecanoic acid were found as the major compounds in the hydro alcoholic extract of leaf of *Scoparia dulcis* (Table 2).

Table 2 represents the biological activity of compounds identified in *Scoparia dulcis* whole plant using GCMS. 2,3-dihydro-benzofuran act as Diabetic retinopathy and arthritis. 3-pyridine-carboxylic acid showed the antimicrobial, anti-inflammatory activities. Nonanoic acid, Anti-

bacterial activity, flavors and cosmetics. 10,11-dihydroxy- 3, 7, 11- trimethyl- 2, 6-dodeca-dienyl acetate possess antimicrobial and antioxidant activities. Hexadecanoic acid methyl ester exhibited antioxidant, pesticide hypocholesterolemic, anti-androgenic, hemolytic, alpha reductase inhibitor, antibacterial and anti-fungal properties. n-Hexadecanoic acid shows anti-oxidant, hypocholesterolemic, nematocidal, pesticidal, hemolytic, antiandrogenic, hemolytic

Table 2: Biological activity of compounds identified in *Scoparia dulcis* whole plant using GCMS

R. Time	Name of the compounds	Biological activity**
5.259	2,3-dihydro-benzofuran	Diabetic retinopathy and arthritis
5.708	3-pyridinecarboxylic acid	Antimicrobial, anti-inflammatory
10.715	Nonanoic acid	Antibacterial activity, flavors and cosmetics
13.033	10,11-dihydroxy-3,7,11-trimethyl-2,6-dodecadienyl acetate	Antimicrobial, antioxidant
13.501	Hexadecanoic acid, methyl ester	Antioxidant, pesticide hypocholesterolemic, anti-androgenic, hemolytic, alpha reductase inhibitor, antibacterial and antifungal
13.955	n-Hexadecanoic acid	Antioxidant, hypocholesterolemic, nematocidal, pesticidal, hemolytic, antiandrogenic, hemolytic, 5-alpha reductase inhibitor
15.117	Oleic Acid	Anti-inflammatory, anti-androgenic, cancer preventive, hypocholesterolemic, 5-alpha reductase inhibitor
15.281	9,12-Octadecadienoic acid, methyl ester	Antiinflammatory, nematocide, insectifuge, hypocholesterolemic, cancer preventive, hepatoprotective, antihistaminic, antiacne, antiarthritic, antieczemic, anticoronary
15.368	9,12,15-Octadecatrienoic acid, methyl ester	Anti-inflammatory, insectifuge hypocholesterolemic, Anticancer, nematocide, hepatoprotective, insectifuge, antihistaminic, antieczemic, antiacne, 5-alpha reductase inhibitor, antiandrogenic, antiarthritic and anticoronary
15.479	Phytol	Antimicrobial, anticancer, diuretic, anti-inflammatory activity.
15.550	Octadecanoic acid, methyl ester	Anti-inflammatory, antiandrogenic, cancer preventive, dermatitigenic activity
15.805	9-octadecenoic acid	Anticancer, antimicrobial anemiagenic, insectifuge, antiandrogenic, dermatitigenic activity
15.875	9,12,15-Octadecatrien-1-o	Antioxidant, anticancer, antiradical
16.009	Octadecanoic acid	Lower LDL Cholesterol level

\*\*Source: Dr. Duke's phytochemical and ethnobotanical databases [Online database].

and 5-alpha reductase inhibitor. Oleic acid may play a significant role in the anti-inflammatory, anti-androgenic, cancer preventive, hypocholesterolemic and 5-alpha reductase inhibitors. 9,12-Octadecadienoic acid, methyl ester revealed the antiinflammatory, nematocide, insectifuge, hypocholesterolemic, cancer preventive, hepatoprotective, antihistaminic, antiacne, antiarthritic, antieczemic and anticoronary. 9,12,15-Octadecatrienoic acid, methyl ester have the anti-inflammatory, insectifuge hypocholesterolemic, anticancer, nematocide, hepatoprotective, insectifuge, antihistaminic, antieczemic, antiacne, 5-alpha reductase inhibitor, antiandrogenic, antiarthritic and anticoronary. Phytol may play an important role in the antimicrobial, anticancer,

diuretic and anti-inflammatory activity. Octadecanoic acid, methyl ester have shown anti-inflammatory, antiandrogenic, cancer preventive, dermatitigenic activity. 9-octadecenoic acid may act as anticancer, antimicrobial anemiagenic, insectifuge, antiandrogenic, dermatitigenic activity. 9,12,15-Octadecatrien-1-o showed the antioxidant, anticancer, antiradical activity. Octadecanoic acid may Lower LDL Cholesterol level. Using Dr. Duke's phytochemical and ethnobotanical database (online), the biological activity of the identified phytocomponents was ascertained (Duke's, 2016; Kavitha and Nadu, 2021).

Major bioactive components found in the examined extract was revealed by the



investigation. They were known to have pharmacological properties that might affect the plant's potential for therapeutic use. The therapeutic use of the plant is supported by the chemicals in *Scoparia dulcis* extract that have been shown to have these biological actions. The discovery of these substances in the plant serves as a starting point for further biological and pharmacological research by providing evidence of the plant's potential health benefits. (Paz *et al.*, 1995; Rishikesh *et al.*, 2012). The phyto-compounds are well known to have curative activity against several human problems such as diuretics, skin diseases (Kirtikar and Basu, 1980), hypercholesterolemia (Sharma and Pant, 1992) and hyperglycemic disorders (Sharmila *et al.*, 2007; Rai *et al.*, 2008) and could suggest the folk use of the medicinal plants. The spectrum profile of GC-MS confirmed the presence of main components with their retention time. The heights of the peak show the relative concentrations of the components present in the extracts. In comparison of the mass spectra of the constituent with the NIST library, the phytoconstituents were characterized and identified.

GC-MS analysis showed 30 compounds from *Scoparia dulcis* which is one of the first steps towards understanding the nature of active principles in medicinal plants and to decide whether the plant species has any individual compound or group of compounds. Overall, the presence of various bioactive compounds in the *Scoparia dulcis* whole plant extract suggests its potential medicinal applications.

## Conclusion

The GC-MS analysis helps to identify the source of many chemical constituents from the peak pattern of chromatograms. Based on the results obtained in the present investigation, thirty compounds were identified from *Scoparia dulcis* and the biological activities of the identified phytocomponents used for anti-microbial, anti-inflammatory, anti-diabetic, antihypercholesterolemic, and anti-cancer activities. The

importance of the study is due to the biological activity of some of these compounds present that might support the pharmacological activity of the plants. The present study is considered to be the preliminary study that reveals the presence of components in *Scoparia dulcis*. Further studies on the biological activities of compounds need to be carried out.

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