Phytochemistry of plants
PHYTOCHEMISTRY OF PLANTS

Large number of medicinal plants are used in Ayurveda and Unani systems of medicine to cure various diseases. The secondary metabolites in the plant are responsible for curing diseases in human beings and animals. Plants are rich source of secondary metabolites which are biologically active. These secondary metabolites with variety of structural arrangements and properties sources of are important medicines (Fatima et al. 2006). The nature of these secondary metabolites is different in different plants, and hence medicinal uses of plants differ from plant to plant. The pharmaceutical companies isolate these medicinally active phytocomstituents and use in the preparation of drugs to cure disease. Thus phytocomstituents are the sources of drugs and are used drug preparations. In developing countries about 80% population really depends traditional medicines for primary healthcare. There is a need to screen medicinal plants for bioactive compounds as a basis for further pharmacological studies (Saha et al. 2008). In recent years, gas chromatography mass spectroscopy (GC-MS) has been applied to identify the structure of different phytocomstituents with great success. (Prasain et al. 2004 and Rijke et al. 2006). Present chapter deals with the detection of phytocomstituents from medicinal plant parts and their studies on their chemical structure using gas chromatography mass spectroscopy (GC-MS) technique.
1. *Helicteres isora* L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Helicteres isora* L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 8.

### Table No.8

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-hydroxy-5-methylbenzaldehyde</td>
<td><img src="image1.png" alt="Structure" /></td>
<td>12.7</td>
<td>C₈H₈O₂</td>
<td>136.05</td>
</tr>
<tr>
<td>2-ethoxyphenethylamine</td>
<td><img src="image2.png" alt="Structure" /></td>
<td>12.7</td>
<td>C₁₀H₁₅O₄</td>
<td>165.12</td>
</tr>
<tr>
<td>Benzenepropanoic acid, 4-dihydroxy, methyl ester</td>
<td><img src="image3.png" alt="Structure" /></td>
<td>16.3</td>
<td>C₁₀H₁₂O₄</td>
<td>196.23</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr.Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 2-hydroxy-5-methylbenzaldehyde, 2-Ethoxyphenethylamine, 4-dihydroxy methyl ester Benzenepropanoic acid. The spectrum profile of GC-MS confirmed the presence of seven major components with the retention time 8.6, 10.4, 12.7, 16.3, 19.8, 21.5, 26.7 respectively (Figure 1A). The individual fragmentation patterns of the components were illustrated in Figure 1B-D. The mass spectrum of the compound with retention time 12.7 (Hit 1) gave 6 major peaks (m/z) at 51, 77, 90, 107, 118, 136.
(Figure 1B). The mass spectrum of the compound with retention time 12.7 (Hit 2) gave 7 major peaks (m/z) at 51, 65, 77, 91, 108, 136, 135 (Figure 1C). The mass spectrum of the compound with retention time 16.3 (Hit 2) gave 6 major peaks (m/z) at 51, 77, 91, 107, 137, 178 (Figure 1D).

In the present study we characterized the chemical profile of *Helicteres isora* L. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Helicteres isora* L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Helicteres isora* L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
*Helicteres isora* L.

![Graph](image-url)
Chapter VII

Phytochemistry of plants

Acq. Data Name: E87VSDr
External Sample Id: R
Average(MS[1] Time:10.4..10.4)
x10^3 Area (26420)

Acq. Data Name: E87VSDr
External Sample Id: R
Average(MS[1] Time:12.7..12.7)
x10^3 Area (31069)

Acq. Data Name: E87VSDr
External Sample Id: R
Average(MS[1] Time:6.0..6.0)
x10^3 Area (50821)

Ionization Mode: 1:EI+

m/z

91.07
121.99
120.08
150.10
135.07
99.96
135.09
137.10
Chapter-VII

Phytochemistry of plants
Chapter VII: Phytochemistry of plants

**Fig 1B**

Hit 1: 2-Hydroxy-5-methylbenzaldehyde
C8H8O2; MF: 148; RMF: 757; Prob 7.47%; CAS: 813-84-3; Lib: mainlib; ID: 99251.

---

**Fig 1C**

Hit 2: 2-Ethoxyphenethylamine
C10H15NO; MF: 183; RMF: 702; Prob 4.30%; CAS: 39590-27-7; Lib: mainlib; ID: 1233.
Chapter VII

Fig 1D

Hit 1: Benzenepropanoic acid, \(\alpha,\beta\)-dihydroxy-, methyl ester  
C10H12O4, MF: 178; RMF: 872; Prob 66.0%; CAS: 51095-47-7; Lib: replib; ID: 14401.

Hit 2: Benzenepropanoic acid, \(\alpha,\beta\)-dihydroxy-, methyl ester  
C10H12O4, MF: 776; RMF: 843; Prob 68.0%; CAS: 51095-47-7; Lib: replib; ID: 14803.
2. *Tribulus terrestris* L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Tribulus terrestris* L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 9.

**Table No.9**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3-dihydro-3,5dihydro-3,5-dihydroxy-6-methyl</td>
<td></td>
<td>7.2</td>
<td>C_{4}H_{8}O_{4}</td>
<td>144.13</td>
</tr>
<tr>
<td>Ethanone, 1-(2-hydroxy-5-methylphenyl)</td>
<td></td>
<td>10.4</td>
<td>C_{9}H_{10}O_{2}</td>
<td>150.17</td>
</tr>
<tr>
<td>2-Methoxy-4-vinylphenol</td>
<td></td>
<td>10.4</td>
<td>C_{9}H_{16}O_{2}</td>
<td>148.09</td>
</tr>
<tr>
<td>3,5-dimethoxyacetophenone</td>
<td></td>
<td>17.0</td>
<td>C_{10}H_{12}O_{3}</td>
<td>180.20</td>
</tr>
<tr>
<td>2,4-dimethoxyacetophenone</td>
<td></td>
<td>17.0</td>
<td>C_{10}H_{12}O_{3}</td>
<td>180.20</td>
</tr>
<tr>
<td>Hexadecanoic acid, methyl ester</td>
<td></td>
<td>19.4</td>
<td>C_{17}H_{34}O_{2}</td>
<td>270.26</td>
</tr>
<tr>
<td>9,12-octadecadienoic acid, methyl ester</td>
<td></td>
<td>21.5</td>
<td>C_{19}H_{34}O_{2}</td>
<td>294.30</td>
</tr>
<tr>
<td>9,12-octadecadienoic acid, octadecadienoic acid</td>
<td></td>
<td>21.5</td>
<td>C_{18}H_{32}O_{2}</td>
<td>280.33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22.5</td>
<td>C_{18}H_{30}O_{2}</td>
<td>284.55</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 2,3-dihydro-3,5-dihydroxy-6-methyl, Ethanone, 1-(2-hydroxy-5-methylphenyl), 2-methoxy-4-vinylphenol, 3,5-dimethoxyacetophenone, 2,4-dimethoxyacetophenone, hexadecanoic acid, methyl ester, 9,12-Octadecadienoic acid (z,z)-methyl ester, octadecanoic acid. The spectrum profile of GC-MS confirmed the presence of eight major components with the retention time 7.2, 10.4, 17.0, 18.0, 19.9, 22.1, 22.2, 22.5 respectively (Figure 2A). The individual fragmentation patterns of the components were illustrated in Figure 2B-I. The mass spectrum of the compound with retention time 7.2 (Hit 1) gave 11 major peaks (m/z) at 53, 55, 58, 73, 87, 101,115, 119, 126, 134,144 (Figure 2B). The mass spectrum of the compound with retention time 10.4 (Hit 1) gave 14 major peaks (m/z) at 51, 55, 63, 67, 75, 77, 79, 85, 91, 107, 121, 131, 135, 150 (Figure 2C). The mass spectrum of the compound with retention time 10.4 (Hit 2) gave 14 major peaks (m/z) at 51, 55, 63, 69, 75, 77, 79, 81, 86, 89, 107, 118, 135, 150 (Figure 2D). The mass spectrum of the compound with retention time 17.0 (Hit 1) gave 14 major peaks (m/z) at 51,55, 63, 69, 74, 77,85, 92,107, 122, 137, 151, 165, 180 (Figure 2E). The mass spectrum of the compound with retention time 19.4 (Hit 1) gave 17 major peaks (m/z) at 55, 69,74, 87, 97, 115, 129, 143, 157, 171, 185, 199, 213, 227, 239, 270 (Figure 2F). The mass spectrum of the compound with retention time 21.5 (Hit 1) gave 19 major peaks (m/z) at 55, 59, 67, 81, 95, 109, 123, 136, 150, 164, 178, 191, 205, 220, 234, 245, 263, 279, 294 (Figure 2G). The mass spectrum of the compound with retention time 22.1 (Hit 1) gave 17
major peaks (m/z) at 55, 60, 67, 81, 95, 110, 124, 137, 150, 168, 182, 196, 210, 220, 237, 264, 280 Figure 2H). The mass spectrum of the compound with retention time 22.5 (Hit 1) gave 19 major peaks (m/z) at 60, 69, 73, 83, 97, 115, 129, 143, 157, 171, 185, 199, 213, 227, 241, 255, 267, 284. (Figure 2I).
In the present study we characterized the chemical profile of *Tribulus terrestris* L. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Tribulus terrestris* L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Tribulus terrestris* L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Tribulus terrestris L.

Fig 2 A
Fig 2 B

Hit 1: 4H-Pyrano-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
C8H8O4; MF: 925; RMF: 925; Prob 95.7%; CAS: 28556-83-2; Lib: replib; ID: 1857.

Hit 2: 4H-Pyrano-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
C8H8O4; MF: 872; RMF: 878; Prob 95.7%; CAS: 28556-83-2; Lib: mainlib; ID: 6348.
**Search Report Page 1 of 1**

Unknown: MDT[(CTR[1.0000...1.0000,0,Center,15,2,0,Area];BCK[DF],SMT[SA,5]] E8TVSD.7RE8TVSDs.7tw
Compound in Library Factor = -155

Hit 1: Ethanone, 1-(2-hydroxy-5-methylphenyl); C9H10O2; MF: 855; RMP: 901; Prob 28.4%; CAS: 1450-72-2; Lib: mainlib; ID: 97712.

**Fig 2 C**

Hit 2: 2-Methoxy-4-vinylphenol; C9H10O2; MF: 851; RMP: 894; Prob 24.0%; CAS: 7786-61-0; Lib: mainlib; ID: 97710.

**Fig 2 D**
**Search Report Page 1 of 1**

Unknown: MDTCTR|1,000,0.1,000,80,Center,15.2,0,Area:BC:K[D]:SMT[S:SA,5]|E87VSD.7FNE87VSDs.7tw
Compound in Library Factor = 402

**Hit 1:** 3,5-Dimethoxyacetophenone
C10H12O3; MF: 781; RMF: 808; Prob 49.1%; CAS: 39151-19-4; Lib: replib; ID: 21878.

**Hit 2:** 2,4-Dimethoxyacetophenone
C10H12O3; MF: 745; RMF: 765; Prob 12.1%; CAS: 829-20-9; Lib: replib; ID: 21662.

Fig 2 E
**Search Report Page 1 of 1**

Unknown: MDT[CTR][1,0000,1,0000,80,Center,15,2,0,Area];BCK[DF];SMT[SA,5] E87VSD.7mE87VSDs.7w

Compound in Library Factor = 200

Hit 1: Hexadecanoic acid, methyl ester
C17H34O2; MF: 904; RMF: 904; Prob 77.8%; CAS: 112-39-0; Lib: replib; ID: 9052.

Fig 2 F

Hit 2: Hexadecanoic acid, methyl ester
C17H34O2; MF: 895; RMF: 895; Prob 77.8%; CAS: 112-39-0; Lib: mainlib; ID: 38248.
**Search Report Page 1 of 1**

Unknown: MDT[CTR][1.0000. 1.0000.80, Center, 15.2.0, Area]: BCK[DF], SMT:SA, 5] E87VSD.78fE87V/SDs.7rw 21.5 min

Compound in Library Factor = -103

**Hit 1**: 9,12-Octadecadienoic acid (Z,Z)-methyl ester
C19H34O2; MF: 298; RMF: 936; Prob 31.9%; CAS: 112-63-0; Lib: mainlib; ID: 28886.

**Fig 2 G**

**Hit 2**: 9,12-Octadecadienoic acid (Z,Z)-methyl ester
C19H34O2; MF: 298; RMF: 923; Prob 31.9%; CAS: 112-63-0; Lib: repplib; ID: 7214.
** Search Report Page 1 of 1 **

Unknown: MDT[CTR][1,000;0.1,000,0.8,Center,15,2,0,Area],[BCK[DF],[SMT][SA,S]] E87VSD.78E87VSDs.7nw 92.1 min

Compound in Library Factor = 298

Fig 2 H

Hit 1: 9,12-Octadecadienoic acid (Z,Z)-
C18H32O2; MF: 914; RMF: 914; Prob: 59.8%; CAS: 80-33-3; Lib: mainlib; ID: 28864.

Hit 2: 9,12-Octadecadienoic acid (Z,Z)-
C18H32O2; MF: 900; RMF: 900; Prob: 59.8%; CAS: 60-33-3; Lib: replib; ID: 7212.
3. *Oxalis corniculata* L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the Methanolic extract of *Oxalis corniculata* L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 10.

**Table No.10**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-hexadecanoic acid</td>
<td></td>
<td>19.8</td>
<td>C_{16}H_{32}O_{2}</td>
<td>256.24</td>
</tr>
<tr>
<td>Proline, 5-oxo, methylester</td>
<td></td>
<td>11.4</td>
<td>C_{6}H_{10}O_{3}N</td>
<td>143.21</td>
</tr>
<tr>
<td>9,12,15-octadecadienoic acid</td>
<td></td>
<td>22.1</td>
<td>C_{18}H_{30}O_{2}</td>
<td>278.55</td>
</tr>
<tr>
<td>Butyl-9,12,15-octadecadienoic acid</td>
<td></td>
<td>22.1</td>
<td>C_{22}H_{36}O_{2}</td>
<td>334.28</td>
</tr>
<tr>
<td>9,12,15-octadecadienoic acid, methyl ester</td>
<td></td>
<td>21.6</td>
<td>C_{19}H_{32}O_{2}</td>
<td>292.88</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of n-hexadecanoic acid, 9,12,15-Octadecadienoic acid, proline, 5-oxo,methyl ester, Butyl-9,12,15-octadecatrienoate, Butyl-9,12,15-octadecatrienoate,
Methyl ester. The spectrum profile of GC-MS confirmed the presence of five major components with the retention time 8.8, 11.4, 19.4, 21.5, 21.6 respectively (Figure 3A). The individual fragmentation patterns of the components were illustrated in Figure 3B-F. The mass spectrum of the compound with retention time 19.8 (Hit 1) gave 11 major peaks (m/z) at 60, 73, 83, 97, 115, 129, 157, 185, 213, 227, 256 (Figure 3B). The mass spectrum of the compound with retention time 11.4 (Hit 1) gave 8 major peaks (m/z) at 56, 59, 66, 84, 88, 98, 115, 143 (Figure 3C). The mass spectrum of the compound with retention time 22.1 (Hit 1) gave 11 major peaks (m/z) at 55, 67, 79, 93, 108, 121, 149, 173, 222, 249, 278. (Figure 3D). The mass spectrum of the compound with retention time 22.1 (Hit 2) gave 14 major peaks (m/z) at 55, 67, 79, 95, 108, 121, 149, 163, 191, 217, 243, 261, 305, 334.(Figure 3E). The mass spectrum of the compound with retention time 22.6 (Hit 1) gave 12 major peaks (m/z) at 55, 67, 79, 95, 108, 121, 149, 163, 191, 236, 261, 292 (Figure 3F).

In the present study we characterized the chemical profile of *Oxalis corniculata* L. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its
kind to analyze the chemical constituents of *Oxalis corniculata* L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Oxalis corniculata* L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Oxalis corniculata L.

Fig 3 A
** Search Report Page 1 of 1 **

Unknown: MDT|CTR[30.0000..30.0000,10,Center,80,0,0,Area];SMT[SA,3]|E87VSD.7R|E87VSD.7w|21.6m

Compound in Library Factor = -324

Hit 1: 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-
C19H32O2; MF: 792; RMF: 824; Prob 24.5%; CAS: 301-00-8; Lib: mainlib; ID: 41712.

** Fig 3 F **

Hit 2: 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-
C19H32O2; MF: 791; RMF: 817; Prob 24.5%; CAS: 301-00-8; Lib: replib; ID: 9679.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Cullen corylifolium* (L.) Medik. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 11.

**Table No.11**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>2H-Flu[2,3-H]-1-benzopyran-2-one</td>
<td><img src="image1" alt="Structure" /></td>
<td>17.6</td>
<td>C_{11}H_{6}O_3</td>
<td>186.03</td>
</tr>
<tr>
<td>2H-Flu[2,3-H]-1-benzopyran-2-one</td>
<td><img src="image2" alt="Structure" /></td>
<td>17.6</td>
<td>C_{11}H_{6}O_3</td>
<td>186.03</td>
</tr>
<tr>
<td>Phenol, 4-(3,7-dimethyl-3-ethylocta-1,6-dienyl)</td>
<td><img src="image3" alt="Structure" /></td>
<td>21.9</td>
<td>C_{18}H_{24}O</td>
<td>256.38</td>
</tr>
<tr>
<td>Phenanthrene, 7-ethenyl-dodecahydro-4,7-dimethyl-1-methylene</td>
<td><img src="image4" alt="Structure" /></td>
<td>21.9</td>
<td>C_{16}H_{24}</td>
<td>256.22</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytological and Ethnobotanical Databases. The results revealed that the presence of 2H-Furo [2,3-H]-1-benzopyran-2-one, 2H-Furo [3,2-g] [1] benzopyran-7-one, phenol, 4-(3,7-dimethyl-3-ethylocta-1,6-dienyl), Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-4a, 7-dimethyl-1-methylene-[4As-(4aa,4a]. The spectrum profile of GC-MS confirmed the presence of three major components with the retention time 17.6, 18.3, 22.0 respectively (Figure 4A). The individual fragmentation patterns of the components were illustrated in Figure 4B-E. The mass spectrum of
the compound with retention time 17.6 (Hit 1) gave 9 major peaks (m/z) at 51, 63, 75, 79, 93, 102, 130, 158, 186 (Figure 4B). The mass spectrum of the compound with retention time 17.6 (Hit 2) gave 6 major peaks (m/z) at 51, 76, 102, 130, 158, 186 (Figure 4C). The mass spectrum of the compound with retention time 21.9 (Hit 1) gave 17 major peaks (m/z) at 55, 68, 77, 83, 91, 107, 120, 131, 145, 159, 173, 185, 199, 213, 227, 241, 256 (Figure 4D). The mass spectrum of the compound with retention time 21.9 (Hit 2) gave 16 major peaks (m/z) at 55, 67, 79, 91, 105, 119, 131, 145, 157, 171, 186, 199, 213, 227, 241, 256 (Figure 4E).

In the present study we characterized the chemical profile of *Cullen corylifolium* (L.) Medik. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Cullen corylifolium* (L.) Medik. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Cullen corylifolium* (L.) Medik.
for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.

*Cullen corylifolium* (L.) Medik.
** Search Report Page 1 of 1 **

Unknown: MDTCTR(30.0000, 30.0000, 10, Center, 80.000, Area): SMT[S, 3] E87VSD 7fE87VSD p7tw 21-9

Compound in Library Factor = 133

Hit 1: Phenol, 4-(3,7-dimethyl-3-ethyloclocta-1,6-diencyl)-
C18H24O; MF: 845; RMF: 845; Prob 93.2%; Lib: mainlib; ID: 128377.

Fig 4 D

Hit 2: Phenanthrene, 7-ethynyl-1,2,3,4,4a,5,6,7,8,10,10a-dodecahydro-4a,7-dimethyl-1-methylene-,[4aS-(4aR,4a
C19H28; MF: 716; RMF: 716; Prob 3.93%; CAS: 26549-04-2; Lib: mainlib; ID: 50302.

Fig 4 E
5. *Ludwigia perennis* L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Ludwigia perennis* L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 12.

**Table No.12**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-Methoxypyrrolidin-2-one</td>
<td><img src="image1" alt="Structure" /></td>
<td>7.8</td>
<td>C₅H₄O₂N</td>
<td>115.62</td>
</tr>
<tr>
<td>2-Pyrrolidinone</td>
<td><img src="image2" alt="Structure" /></td>
<td>7.8</td>
<td>C₅H₄O₂N</td>
<td>115.68</td>
</tr>
<tr>
<td>Proline, 5-oxo, methylester</td>
<td><img src="image3" alt="Structure" /></td>
<td>11.4</td>
<td>C₆H₈O₃N</td>
<td>143.21</td>
</tr>
<tr>
<td>Proline, 5-oxo, methylester</td>
<td><img src="image4" alt="Structure" /></td>
<td>11.4</td>
<td>C₆H₈O₃N</td>
<td>143.21</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 5-methoxypyrrolidin-2-one, 2-pyrrolidinone,5-(hydroxymethyl), DL-proline, 5oxo, methyl ester, L-proline,5-oxo,methyl ester. The spectrum profile of GC-MS confirmed the presence of six major components with the retention time 7.8, 11.4, 19.4, 19.8, 19.9, 21.5 respectively (Figure 5A). The individual fragmentation patterns of the components were
illustrated in Figure 5B-D. The mass spectrum of the compound with retention time 7.8 (Hit 1) gave 6 major peaks (m/z) at 56, 60, 71, 84, 100, 115 (Figure 5B). The mass spectrum of the compound with retention time 7.8 (Hit 2) gave 5 major peaks (m/z) at 56, 84, 91, 98, 115 (Figure 5C). The mass spectrum of the compound with retention time 11.4 (Hit 2) gave 5 major peaks (m/z) at 56, 84, 98, 115, 143 (Figure 5D).

In the present study we characterized the chemical profile of *Ludwigia perennis* L. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Ludwigia perennis* L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Ludwigia perennis* L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Ludwigia perennis L.
Chapter VII

Phytochemistry of plants

** Search Report Page 1 of 1 **

Unknown: MDT\[CTR\[30.0000, 30.0000, \text{Center}, 80, 0, 0, \text{Area}\]; SMT\[SA, 3\]] E87VSD.7RE87VSDv.7w 11.4

Compound in Library Factor = 103

Hit 1: DL-Proline, 5-oxo-, methyl ester
C8H9NO3; MF: 198; RMF: 911; Prob 43.7%; CAS: 54571-66-3; Lib: mainlib; ID: 45666.

Fig 5 D

Hit 2: L-Proline, 5-oxo-, methyl ester
C8H9NO3; MF: 198; RMF: 908; Prob 43.4%; CAS: 4931-66-2; Lib: mainlib; ID: 45655.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Echinops echinatus* Roxb. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 13.

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>2H-Flun[2,3-H]-1-benzopyran-2-one</td>
<td><img src="image1" alt="Structure" /></td>
<td>12.7</td>
<td>C₄H₁₂O₆</td>
<td>180.16</td>
</tr>
<tr>
<td>D-glucopyranoside, D-glucopyranosyl-D fructofuranosyl</td>
<td><img src="image2" alt="Structure" /></td>
<td>12.7</td>
<td>C₁₆H₂₈O₁₆</td>
<td>504.17</td>
</tr>
<tr>
<td>4(1E)-3-hydroxy-1-propenyl-2-methoxyphenol</td>
<td><img src="image3" alt="Structure" /></td>
<td>17.0</td>
<td>C₁₀H₁₂O₃</td>
<td>180.12</td>
</tr>
<tr>
<td>4(1E)-3-hydroxy-1-propenyl-2-methoxyphenol</td>
<td><img src="image4" alt="Structure" /></td>
<td>17.0</td>
<td>C₁₀H₁₂O₃</td>
<td>180.12</td>
</tr>
<tr>
<td>Thianthrene</td>
<td><img src="image5" alt="Structure" /></td>
<td>19.4</td>
<td>C₁₂H₈S₂</td>
<td>256.22</td>
</tr>
<tr>
<td>Anobin</td>
<td><img src="image6" alt="Structure" /></td>
<td>23.0</td>
<td>C₁₅H₂₅O₃</td>
<td>280.13</td>
</tr>
<tr>
<td>Terthiophene</td>
<td><img src="image7" alt="Structure" /></td>
<td>23.0</td>
<td>C₁₂H₈S₅</td>
<td>248</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of d-Mannose, D-Glucopyranoside, O-α-D-glucopyranosyl-(fwdarw.3)-β-D-fructofuranosyl, 3-hydroxy-1-propenyl)-2-methoxyphenol, phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy, Thianthrene, Anobin, 3,4-dihydroxy-1,5,7 guai-10(15),11(13)-diene-6, 12-olide, 2,2’, 5’, 2”-Terthiophene. The spectrum profile of GC-MS confirmed the presence of ten major components with the retention time 5.8, 7.2, 8.8, 13.8, 19.4, 19.8, 22.1, 23.0, 23.6, 33.8 respectively (Figure 6A). The individual fragmentation patterns of the components were illustrated in Figure 6B-H. The mass spectrum of the compound with retention time 12.7 (Hit 1) gave 6 major peaks (m/z) at 60, 73, 85, 103, 149, 179 (Figure 6B). The mass spectrum of the compound with retention time 12.7 (Hit 2) gave 7 major peaks (m/z) at 60, 73, 85, 97, 126, 145, 191 (Figure 6C). The mass spectrum of the compound with retention time 17.0 (Hit 1) gave 7 major peaks (m/z) at 51, 77, 91, 124, 137, 147, 180 (Figure 6D). The mass spectrum of the compound with retention time 17.0 (Hit 2) gave 8 major peaks (m/z) at 51, 77, 91, 109, 124, 137, 151, 180 (Figure 6E). The mass spectrum of the compound with retention time 19.4 (Hit 1) gave 6 major peaks (m/z) at 69, 108, 139, 171, 184, 216 (Figure 6F). The mass spectrum of the compound with retention time 23.0 (Hit 1) gave 13 major peaks (m/z) at 53, 79, 91, 105, 122, 131, 161, 179, 190, 203, 221, 246, 264 (Figure 6G). The mass spectrum of the compound with retention time 23.8 (Hit 1) gave 6 major peaks (m/z) at 69, 96, 127, 171, 190, 203 (Figure 6H).

In the present study we characterized the chemical profile of *Echinops echinatus* Roxb. using GC-MS. The gas chromatogram shows
the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Echinops echinatus* Roxb. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Echinops echinatus* Roxb. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Echinops echinatus** Roxb.

![Diagram](image-url)

**Fig 6 A**

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Phytochemistry of plants

[Image of charts and graphs related to phytochemistry]
Chapter-VII

Phytochemistry of plants
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** Search Report Page 1 of 1 **

Unknown: MDI[CCTR:30.0000..30.0000,10.,Center,80.0,0.Area]:SMT[SA,3] E87VSD:78|E87VSDq:7w 12

Compound in Library Factor = -1276

Hit 1: d-Mannose

Fig 6 B

Hit 2: α-D-Glucopyranoside, O-α-D-glucopyranosyl-(1→2;α)-β-D-fructofuranosyl

Fig 6 C
** Figure 6 D **

Hit 1: 4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol
C_{10}H_{12}O_{3}; MF: 186; RMF: 915; Prob 78.0%; Lib: mainlib; ID: 100190.

** Figure 6 E **

Hit 2: Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-
C_{10}H_{12}O_{3}; MF: 178; RMF: 826; Prob 13.6%; CAS: 458-35-5; Lib: mainlib; ID: 100191.
Fig 6 F
**Search Report Page 1 of 1**

Unknown: MDT[CTR]30.0000, 30.0000, 10, Center, 60.0, 0.0, Area; SMT[SA, 3]]

Compound in Library Factor = 478

Hit 1: 2,2',5',2"-Terthiophene
C12H8S3; MF: 968; RMF: 901; Prob 71.8%; CAS: 1081-34-1; Lib: replib; ID: 26292.

**Fig 6 H**

Hit 2: 2,2',9',2"-Terthiophene
C12H8S3; MF: 912; RMF: 868; Prob 71.8%; CAS: 1081-34-1; Lib: mainlib; ID: 164830.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Eclipta prostrata* (L.) L. Mant. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 14.

**Table no.14**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.7,11,15-tetramethyl-2-hexadecen-1-ol</td>
<td><img src="image1.png" alt="Structure" /></td>
<td>18.3</td>
<td>C_{24}H_{40}O</td>
<td>296.31</td>
</tr>
<tr>
<td>3-Eicosyne</td>
<td><img src="image2.png" alt="Structure" /></td>
<td>18.3</td>
<td>C_{26}H_{34}</td>
<td>278.30</td>
</tr>
<tr>
<td>9,12-octadecadienoic acid</td>
<td><img src="image3.png" alt="Structure" /></td>
<td>22.1</td>
<td>C_{18}H_{32}O_{2}</td>
<td>280.24</td>
</tr>
<tr>
<td>9,12,15-octadecatrienoic acid</td>
<td><img src="image4.png" alt="Structure" /></td>
<td>22.1</td>
<td>C_{18}H_{30}O_{2}</td>
<td>278.22</td>
</tr>
<tr>
<td>Stigmasterol</td>
<td><img src="image5.png" alt="Structure" /></td>
<td>29.5</td>
<td>C_{25}H_{40}O</td>
<td>412.37</td>
</tr>
<tr>
<td>Tricyclo [3,3.1.0.3,7] deca-5,9-dien-2,6-diol</td>
<td><img src="image6.png" alt="Structure" /></td>
<td>33.1</td>
<td>C_{15}H_{25}O_{2}N_{2}</td>
<td>226.17</td>
</tr>
<tr>
<td>5,8,11,14-eicosatetraynoic acid</td>
<td><img src="image7.png" alt="Structure" /></td>
<td>33.1</td>
<td>C_{20}H_{24}O_{2}</td>
<td>296.18</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 3,7,11,15-Tetramethyl-2-hexadecen-1ol, 3-Eicosyne, Tricyclo [3.3.1.1 (3, 7)] decane-2,6-diol, Stigmasterol, 9,12-Octadecadienoic acid, 9, 12, 15-Octadecatrienoic acid, 2,6-bis (aminomethyl), 5,8,11,14-Eicosatetraynoic acid, The spectrum profile of GC-MS confirmed the presence of five major components with the retention time 7.2, 18.3, 19.8, 22.0, 33.1 respectively (Figure 7A). The individual fragmentation patterns of the components were illustrated in Figure 1B-H. The mass spectrum of the compound with retention time 18.3 (Hit 1) gave 9 major peaks (m/z) at 55, 71, 81, 95, 109, 123, 137, 179, 278 (Figure 7B). The mass spectrum of the compound with retention time 18.3 (Hit 2) gave 10 major peaks (m/z) at 55, 67, 82, 95, 109, 123, 137, 166, 249, 278 (Figure 7C). The mass spectrum of the compound with retention time 22.1 (Hit 1) gave 10 major peaks (m/z) at 67, 81, 95, 109, 123, 151, 182, 222, 256, 280 (Figure 7D). The mass spectrum of the compound with retention time 22.1 (Hit 2) gave 11 major peaks (m/z) at 55, 67, 79, 93, 108, 121, 149, 173, 222, 249, 278 (Figure 7E). The mass spectrum of the compound with retention time 29.5 (Hit 1) gave 18 major peaks (m/z) at 55, 69, 83, 95, 133, 159, 173, 213, 229, 255, 271, 283, 300, 314, 351, 369, 394, 412 (Figure 7F). The mass spectrum of the compound with retention time 33.1 (Hit 1) gave 6 major peaks (m/z) at 57, 95, 117, 167, 196, 224 (Figure 7G). The mass spectrum of the compound with retention time 33.1 (Hit 2) gave 14 major peaks (m/z) at 55, 67, 77, 91, 115, 128, 152, 165, 179, 193, 207, 239, 267, 295 (Figure 7H).
In the present study we characterized the chemical profile of _Eclipta prostrata_ (L.) L. Mant. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of _Eclipta prostrata_ (L.) L. Mant. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of _Eclipta prostrata_ (L.) L. Mant. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Eclipta prostrata** (L.) L. Mant.

Fig 7A
** Search Report Page 1 of 1 **

Unknown: MDT[CTR[30.0000_30.0000.10.Center.80.0.0.Area:SMT[S,3]] E87VSD.7tE87VSDo.7w18.3m

Compound in Library Factor = .197

** Fig 7B **

Hit 1: 3,7,11,15-Tetramethyl-2-hexadecen-1-ol
C20H40O; MF: 840; RMF: 926; Prob 35.6%; CAS: 102608-53-7; Lib: mainlib; ID: 43206.

** Fig 7C **

Hit 2: 3-Eicosyne
C20H38; MF: 784; RMF: 824; Prob 6.78%; CAS: 61886-66-6; Lib: mainlib; ID: 29111.
Fig 7 D

Hit 1: 9,12-Octadecadienoic acid (Z,Z)-C18H32O2, MF: 788, RMF: 812; Prob 8.84%, CAS: 60-33-3; Lib: replib; ID: 7185.

Fig 7 E

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**Fig 7G**

Unknown: MDT[CTR][30.0000,30.0000,10,Center,80.0,0.Area]; SMT[SA,3]E87VSD.78; E87VSDo.7tw

Compound in Library Factor = 1298

Hit 1: Tricyclo(3.3.1.1^3.7)^decane-2,6-diol, 2,6-bis(aminomethyl)-C_{12}H_{22}N_{2}O_{2}; MF: 595; RMF: 702; Prob 25.3%; CAS: 39751-02-5; Lib: mainlib; ID: 143551.

**Fig 7H**

Hit 2: 5,8,11,14-Eicosatetraynoic acid; C_{20}H_{24}O_{2}; MF: 588; RMF: 634; Prob 22.4%; CAS: 1191-85-1; Lib: mainlib; ID: 122564.
8. *Glossocardia bosvallea* (L.f.) DC.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Glossocardia bosvallea* (L.f.) DC. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 15.

**Table No.15**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>9,12-Octadecadienoic acid</td>
<td><img src="image1" alt="Structure" /></td>
<td>22.1</td>
<td>C_{12}H_{22}O_{2}</td>
<td>280.24</td>
</tr>
<tr>
<td>Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)</td>
<td><img src="image2" alt="Structure" /></td>
<td>13.4</td>
<td>C_{15}H_{24}</td>
<td>204.19</td>
</tr>
<tr>
<td>1,2,3,5-Cyclohexanetetrol</td>
<td><img src="image3" alt="Structure" /></td>
<td>15.3</td>
<td>C_{6}H_{12}O_{4}</td>
<td>148.16</td>
</tr>
<tr>
<td>Quinic acid</td>
<td><img src="image4" alt="Structure" /></td>
<td>15.3</td>
<td>C_{7}H_{12}O_{6}</td>
<td>190.08</td>
</tr>
<tr>
<td>6-hydroxy-9-oxa-bicyclo[3.3.1]nonan-3-one</td>
<td><img src="image5" alt="Structure" /></td>
<td>15.4</td>
<td>C_{8}H_{12}O_{3}</td>
<td>156.44</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 9,12-Octadecadienoic acid, Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl), 1,2,3,5-Cyclohexanetetrol, Quinic acid, 6-hydroxy-9-oxa-biclo [3,3,1] nonan-3-one. The spectrum profile of GC-MS confirmed the presence of six major components with the retention time 11.8, 13.4, 15.3, 15.4, 19.8, 22.1 respectively (Figure 8A). The individual fragmentation patterns of the components were illustrated in Figure 8B-G. The mass spectrum of the compound with retention time 22.1 (Hit 1) gave 15 major peaks (m/z) at 55, 67, 81, 95, 110, 124, 137, 150, 168, 182, 196, 210, 223, 237, 264, 280 (Figure 8B). The mass spectrum of the compound with retention time 13.4 (Hit 1) gave 18 major peaks (m/z) at 51, 53, 55, 65, 67, 77, 79, 81, 89, 91, 105, 121, 133,147, 161, 175, 189, 204 (Figure 8C). The mass spectrum of the compound with retention time 15.3 (Hit 1) gave 16 major peaks (m/z) at 53, 55, 57, 60, 71, 73, 86, 89, 97, 102, 112, 130, 148 (Figure 8D). The mass spectrum of the compound with retention time 15.3 (Hit 2) gave 13 major peaks (m/z) at 53, , 57, 60, 69, 71, 73, 89, 100, 111, 118, 129, 138, 147, 156 (Figure 8E). The mass spectrum of the compound with retention time 15.4 (Hit 1) gave 14 major peaks (m/z) at 53, 55, 60, 69, 71, 84, 95, 97, 99, 113, 123, 128, 138, 156 (Figure 8F). The mass spectrum of the compound with retention time 15.4 (Hit 2) gave 11 major peaks (m/z) at 53, 55, 57, 60, 71, 73, 86, 89, 97, 102, 112, 130, 148 (Figure 8G).

In the present study we characterized the chemical profile of *Glossocardia bosvallea* (L.f.) DC. using GC-MS. The gas
chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Glossocardia bosvallea* (L.f.) DC. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Glossocardia bosvallea* (L.f.) DC. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Glossocardia bosvallea (L.f.) DC.**

![Chart Image]

**Fig 8 A**
**Search Report Page 1 of 1**

Unknown: MDT[CTR]1.0000.0.0000.80.Center.15.2.0.Area].BCK[DF].SMT[SA.5]] E87VSD.7F8E87VSDm.7tw2.1

Compound in Library Factor = 109

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**Fig 8 B**

Hit 1: 9,12-Octadecadienoic acid (Z,Z)-C18H32O2; MF: 856; RMF: 877; Prob 48.2%; CAS: 60-33-3; Lib: mainlib; ID: 28864.

Hit 2: 9,12-Octadecadienoic acid (Z,Z)-C18H32O2; MF: 854; RMF: 873; Prob 48.2%; CAS: 60-33-3; Lib: repilib; ID: 7212.
**Search Report Page 1 of 1**

Unknown: MDTCTR1.00000.00000.80, Center, 15,2.0, Area]; BCK[DF]: SMT[SA, S], ES7VSD.78E7VSDm.7tw

Compound in Library Factor = -107

**Fig 8 C**

Hi 1: Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethyl)-, [4aR-(4aa,7a,8aβ)]-

Hi 2: Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethyl)-, [4aR-(4aa,7a,8aβ)]-
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Unknown: MDT [CTR] 1.0000.1.0000.80.Center.15.2.0.Area].BCK[DF].SMT[SA.5] E87VSD.7fE87VSDm.7rw 15.3

Compound in Library Factor = -1.187

**Fig 8 D**

Hit 1: 1,2,3,5-Cyclohexanetetrol, (1o,2B,3o,5B)-C8H12O4; MF: 625; RMF: 723; Prob 15.4%; CAS: 53585-08-3; Lib: mainlib; ID: 27135.

**Fig 8 E**

Hit 2: (1R,3R,4R,5R)-(-) Quinic acid
C7H12O6; MF: 624; RMF: 630; Prob 14.8%; CAS: 77-95-2; Lib: mainlib; ID: 27098.
9. *Tridax procumbence* (L.) L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Tridax procumbence* (L.) L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 16.

**Table No.16**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-Butanol, 3-methyl-formate</td>
<td><img src="image1" alt="structure" /></td>
<td>6.2</td>
<td>C₆H₁₂O₂</td>
<td>116.08</td>
</tr>
<tr>
<td>1-Butanol, 3-methyl-acetate</td>
<td><img src="image2" alt="structure" /></td>
<td>6.2</td>
<td>C₇H₁₄O₂</td>
<td>130.10</td>
</tr>
<tr>
<td>4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl</td>
<td><img src="image3" alt="structure" /></td>
<td>7.2</td>
<td>C₄H₆O₄</td>
<td>144.04</td>
</tr>
<tr>
<td>1-(3,6,6-Trimethyl-1,6,7,7a-tetrahydro-cyclopenta[c]pyran-1-yl)-ethanone</td>
<td><img src="image4" alt="structure" /></td>
<td>11.9</td>
<td>C₁₃H₁₄O₂</td>
<td>206.13</td>
</tr>
<tr>
<td>phenol, 2,6-Di-tert-butyl</td>
<td><img src="image5" alt="structure" /></td>
<td>11.9</td>
<td>C₁₄H₁₉O</td>
<td>206.17</td>
</tr>
<tr>
<td>3-Ethyl-5-(2-ethyl-butyl)-octadecane</td>
<td><img src="image6" alt="structure" /></td>
<td>29.2</td>
<td>C₂₅H₅₄</td>
<td>366.42</td>
</tr>
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</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 1-Butanol, 3-methyl-formate, 1-Butanol, 3-methyl-acetate, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, 1-(3,6,6-Trimethyl 1,6,7,7a-tetrahydro-cyclopenta[c]pyran-1-yl)-ethanone, phenol-2,6-Di-tert-butyl, 3-Ethyl-5-(2-ethyl-butyl)-octadecane. The spectrum profile of GC-MS confirmed the presence of five major components with the retention time 6.2, 7.2, 11.9, 31.1 and 31.4, respectively (Figure 9A). The individual fragmentation patterns of the components were illustrated in Figure 1B-G. The mass spectrum of the compound with retention time 6.2 (Hit 1) gave 4 major peaks (m/z) at 55, 70, 87 and 113 (Figure 9B). The mass spectrum of the compound with retention time 6.2 (Hit 2) gave 6 major peaks (m/z) at 55, 70, 87, 97 and 115, 130 (Figure 9C). The mass spectrum of the compound with retention time 7.2 gave 6 major peaks (m/z) at 55, 72, 85, 101, 115 and 144 (Figure 9D). The mass spectrum of the compound with retention time 11.9 (Hit 1) gave 9 major peaks (m/z) at 55, 77, 91, 121, 131, 149, 163, 191 and 206 (Figure 9E). The mass spectrum of the compound with retention time 11.9 (Hit 2) gave 8 major peaks (m/z) at 57, 74, 91, 115, 131, 163, 191 and 206 (Figure 9F). The mass spectrum of the compound with retention time 29.2 gave 9 major peaks (m/z) at 57, 71, 85, 97, 113, 141, 183, 281 and 364 (Figure 9G).

In the present study we characterized the chemical profile of *Tridax procumbence* (L.) L. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass
spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Tridax procumbence* (L.) L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Tridax procumbence* (L.) L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Tridax procumbence (L.) L.**

![Graph](image_url)

**Table 1**

<table>
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<tr>
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<th>Type</th>
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<th>Area [Intens * se]</th>
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<th>Description</th>
<th>Start Point</th>
<th>Height</th>
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<th>End Point</th>
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** Search Report Page 1 of 1 **

Unknown: MDT[CTR\(30.0000.30.0000.10\),Center,80.0.0,Area:SMT[SAA,3]] E87VSD.7flE87VSDh.7tw 6.2m

Compound in Library Factor = .941

**Fig 9 B**

Hit 1: 1-Butanol, 3-methyl-, formate
C8H12O2; MF: 681; RMF: 729; Prob 34.7%; CAS: 110-45-2; Lib: mainlib; ID: 18425.

**Fig 9 C**

Hit 2: 1-Butanol, 3-methyl-, acetate
C7H14O2; MF: 669; RMF: 728; Prob 23.1%; CAS: 123-92-2; Lib: replib; ID: 2362.
Chapter-VII  Phytochemistry of plants
** Search Report Page 1 of 1 **

Unknown: MDTCTR[30.0000..30.0000,10.Center,80.0,0.Area]:SMTISA.3] E87VSD.7fEB7VSDh.7rw 11.9men

Compound in Library Factor = .225

Hit 1 : 1-(3,6,6-Trimethyl-1,6,7,7a-tetrahydropyrene)cyclopenta[c]pyran-1-yl)ethanone
C13H18O2; MF: 201; RMF: 263; Prob 57.9%; Lib: mainlib; ID: 146436.

Fig 9 E

Hit 2 : Phenol, 2,6-bis[1,1-dimethyllethy]...
C14H22O; MF: 172; RMF: 211; Prob 77.4%; CAS: 128-39-2; Lib: replib; ID: 23708.

Fig 9 F
Fig 9 G
10. *Mimusops elengi* L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Mimusops elengi* L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 17.

**Table No. 17**

<table>
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<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
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<td>$C_{18}H_{23}ClO_3N_2S$</td>
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<td>Alanine, N-propargyloxycarbonyl, isohexyl ester</td>
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<td>$C_{13}H_{21}O_4N$</td>
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<td>4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl</td>
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<td>7.2</td>
<td>$C_6H_6O_3$</td>
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<td>2-furancarboxaldehyde, 5-(hydroxymethyl)</td>
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<td>n-hexadecanoic acid</td>
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<td>19.6</td>
<td>$C_{16}H_{32}O_2$</td>
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<td>6-octadecenoic acid</td>
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<td>$C_{18}H_{34}O_2$</td>
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<tr>
<td>cis-13-octadecenoic acid</td>
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<td>C(<em>{18})H(</em>{34})O(_2)</td>
<td>282.26</td>
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<tr>
<td>octadecanoic acid</td>
<td><img src="octadecanoic.jpg" alt="Structure" /></td>
<td>22.5</td>
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<td>31.7</td>
<td>C(<em>{19})H(</em>{30})O(_3)</td>
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<tr>
<td>Tungsten, dicarbonyl, tetranethyl ethanediamine</td>
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<td>31.7</td>
<td>C(<em>{19})H(</em>{40})N(_2)W</td>
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</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of Clindamycin, D-Alanine, N-propargyloxycarbonyl, isohexyl ester, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, Hexadecanoic acid, methyl ester, 2 Furancarboxaldehyde, 5-(hydroxymethyl),n-
Hexadecanoic acid, 6-Octadecenoic acid, cis-13-Octadecenoic acid, Octadecanoic acid, Tungsten, dicarbonyl, tetramethyl ethanediamine 1,4,5,8-Dimethanonaphthalene-2,3diol The spectrum profile of GC-MS confirmed the presence of eight major components with the retention time 5.9, 7.2, 8.9, 19.4, 19.6, 22.2, 22.5, 31.7. respectively (Figure 10A). The individual fragmentation patterns of the components were illustrated in Figure 10B-L. The mass spectrum of the compound with retention time 5.9 (Hit 1) gave 5 major peaks (m/z) at 55, 70, 82, 96 and 126 (Figure 10B). The mass spectrum of the compound with retention time 5.9 (Hit 2) gave 4 major peaks (m/z) at 55, 67, 82, 126 (Figure 10C). The mass spectrum of the compound with retention time 7.2 gave 6 major peaks (m/z) at 55, 72, 85, 101, 115 and 144 (Figure 10D). The mass spectrum of the compound with retention time 8.9 (Hit 1) gave 7 major peaks (m/z) at 53, 69, 81, 95, 97, 109, 123, 126 (Figure 10E). The mass spectrum of the compound with retention time 19.4 (Hit 1) gave 14 major peaks (m/z) at 55, 74, 87, 97, 115, 129, 143, 171, 185, 199, 213, 227, 239, 270 (Figure 10F). The mass spectrum of the compound with retention time 19.6 (Hit 1) gave 17 major peaks (m/z) at 57, 60, 73, 83, 97, 115, 129, 143, 157, 171, 185, 199, 213, 256 (Figure 10G). The mass spectrum of the compound with retention time 22.2 (Hit 1) gave 12 major peaks (m/z) at 55, 69, 83, 97, 111, 125, 151, 180, 222, 246, 264, 282 (Figure 10H). The mass spectrum of the compound with retention time 22.2 (Hit 2) gave 10 major peaks (m/z) at 55, 69, 83, 97, 111, 125, 151, 180, 222, 264 (Figure 10I). The mass spectrum of the compound with retention time 22.5 (Hit 1) gave 14 major peaks (m/z) at 60, 73, 83, 97, 115, 129, 143, 171, 185, 199, 227, 241, 255, 284 (Figure 10J). The
mass spectrum of the compound with retention time 31.7 (Hit 1) gave 11 major peaks (m/z) at 67, 79, 107, 116, 144, 167, 237, 301, 387, 405, 447 (Figure 10K). The mass spectrum of the compound with retention time 31.7 (Hit 2) gave 10 major peaks (m/z) at 58, 72, 81, 115, 286, 326, 354, 375, 403, 448 (Figure 10L).

In the present study we characterized the chemical profile of *Mimusops elengi* L. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Mimusops elengi* L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Mimusops elengi* L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Mimusops elengi L.**

**Fig 10 A**
Chapter-VII
Phytochemistry of plants

** Search Report Page 1 of 1 **

Unknown: MDT\[CTR\{30.0000...30.0000,10,Center,80.0,0,Area\}SMT[SA,3]\] E87VSD.7F8E87VSD.7F7w

Compound in Library Factor = -509

Hit 1: Clindamycin
C18H33CIN2OSS; MF: 793; RMF: 805; Prob 18.7%; CAS: 18323-44-9; Lib: replib; ID: 17369.

Fig 10 B

Hit 2: D-Alanine, N-propargyloxy carbonyl, isohexyl ester
C13H21NO4; MF: 789; RMF: 824; Prob 15.8%; Lib: mainlib; ID: 89068.

Fig 10 C
**Search Report Page 1 of 1**

Unknown: MDT[CTR]30.0000. 30.0000,10,Center,80,0,0,Area];SMT[SA,3] E87VSD.7rfE87VSDl.7rw
Compound in Library Factor = 257

Hit 1: 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
C6H8O4; MF: 877; RMF: 923; Prob 93.2%; CAS: 28564-83-2; Lib: mainlib; ID: 6348.

**Fig 10 D**

Hit 2: 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
C6H8O4; MF: 874; RMF: 920; Prob 93.2%; CAS: 28564-83-2; Lib: replib; ID: 1856.

L-5
** Search Report Page 1 of 1 **

Unknown: MDTCTR30.0000...30.0000,10,Center,80.0.0,Area]SMT[SA,3] E87VSD.7RE87VSDL7rw
Compound in Library Factor = 475

Hit 1: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
C8H6O3; MF: 927; RMF: 929; Prob 95.9%; CAS: 67-47-0; Lib: mainlib; ID: 60271.

Hit 2: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
C8H6O3; MF: 909; RMF: 920; Prob 95.9%; CAS: 67-47-0; Lib: replib; ID: 12795.

Fig 10 E
Unknown: MDT[CTR(30,0000,30,0000,10,Center,0,0,Area)].SMT[SA,3]  E87V5D.7RE87V5D.7rw
Compound in Library Factor = 177

Hit 1: Hexadecanoic acid, methyl ester
C17H34O2; MF: 891; RMF: 897; Prob 58.8%; CAS: 112-39-0; Lib: mainlib; ID: 36248.

** Fig 10 F **

Hit 2: Hexadecanoic acid, methyl ester
C17H34O2; MF: 881; RMF: 892; Prob 56.8%; CAS: 112-39-0; Lib: replib; ID: 9052.
** Fig 10 G **

Hit 1: n-Hexadecanoic acid
C16H32O2; MF: 886; RMF: 887; Prob 80.4%; CAS: 57-10-3; Lib: replib; ID: 2558.

Hit 2: n-Hexadecanoic acid
C16H32O2; MF: 867; RMF: 874; Prob 80.4%; CAS: 57-10-3; Lib: replib; ID: 6723.
**Search Report Page 1 of 1**

Unknown: MDTCTR[30.0000,30.0000,10,Center,80.0,0,Area], SMT[S,A,3], E87VSD, 7RE87VSD, 7w
Compound in Library Factor = -217

Fig 10 H

Hit 1: 6-Octadecenoic acid, (Z)-
C18H34O2; MF: 876; RMF: 892; Prob 10.9%; CAS: 593-39-5; Lib: mainlib; ID: 17306.

Fig 10 I

Hit 2: cis-13-Octadecenoic acid
C18H34O2; MF: 875; RMF: 897; Prob 10.5%; CAS: 13125-39-1; Lib: mainlib; ID: 18239.
Chapter VII

Phytochemistry of plants

** Search Report Page 1 of 1 **

Unknown: MDT[CTR30.0000..30.0000,10,Center,80.0,0.Area]:SMT[SA,3] E87VSD,7fE87VSDL.7w
Compound in Library Factor = -857

Hit 1: 1,4,5,8-Dimethanonaphthalene-2,3-diol, 5,6,7,8,9,9-hexachloro-1,2,3,4,4a,5,8,8a-octahydro-, diacetate, (1α,2α C16H14Cl6O4; MF: 554; RMF: 555; Prob 33.4%; CAS: 34408-22-5; Lib: mainlib; ID: 13642.

Fig 10 K

Hit 2: Tungsten, dicarbonyl-(1,4-pinocarvone)-N,N,N',N'-tetraethylethanediamine C16H30N2O3W; MF: 533; RMF: 552; Prob 6.73%; Lib: mainlib; ID: 25968.

Fig 10 L
11. *Rauvolfia tetraphyla* L.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of root of *Rauvolfia tetraphyla* L. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 18.

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
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<tr>
<td>Phthalic acid dibutyl ester</td>
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<td>19.9</td>
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<td>5,5'-Dimethoxy-3,7,3',7'-tetramethyl-[2,2']binaphthalenyl-1,4,1',4'-tetrone</td>
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<td>C&lt;sub&gt;26&lt;/sub&gt;H&lt;sub&gt;22&lt;/sub&gt;O&lt;sub&gt;6&lt;/sub&gt;</td>
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<td>Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandrost-8-en-17-yl)</td>
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<td>C&lt;sub&gt;27&lt;/sub&gt;H&lt;sub&gt;42&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;</td>
<td>430.62</td>
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The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 3,4,5-Trimethoxy-benzoic acid methyl ester and Phthalic acid 1-butyl...
ester 2-decyl ester, Phthalic acid dibutyl ester, 5,5'-Dimethoxy-3,7,3',7'-tetramethyl-[2,2']binaphthalenyl-1,4,1',4'-tetraone, Propanoic acid, 2-(3-acetoxy-4-4,14-trimethylandrost-8-en17-yl). The spectrum profile of GC-MS confirmed the presence of six major components with the retention time 16.8, 19.7, 19.8, 19.9, 20.6, and 31.4, respectively (Figure 11A). The individual fragmentation patterns of the components were illustrated in Figure 11B-F. The mass spectrum of the compound with retention time 16.8 gave 8 major peaks (m/z) at 66, 81, 125, 155, 183, 195, 211 and 226 (Figure 11B). The mass spectrum of the compound with retention time 19.8 gave 7 major peaks (m/z) at 55, 76, 104, 149, 167, 223 and 307 (Figure 11C). The mass spectrum of the compound with retention time 19.9 gave 6 major peaks (m/z) at 76, 104, 149, 160, 223 and 278 (Figure 11D). The mass spectrum of the compound with retention time 31.3 gave 11 major peaks (m/z) at 57, 71, 90, 97, 149, 165, 191, 215, 255, 415 and 430 (Figure 11E). The mass spectrum of the compound with retention time 31.3 gave 17 major peaks (m/z) at 55, 69, 83, 121, 159, 173, 187, 213, 233, 247, 281, 309, 337, 355, 370, 415 and 430 (Figure 11F).

In the present study we characterized the chemical profile of *Rauvolfia tetraphyla* L. Using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at
different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Rauvolfia tetraphyla* L. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Rauvolfia tetraphyla* L. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Rauvolfia tetraphyla L.

Fig. 11 A
** Search Report Page 1 of 1 **

Unknown: MDTCTR[30.0000. 30.0000.10, Center, 80.0, 0.0, Area]: SMT[S,A,3] E87VSID. 7rE57VSID. 7w

Compound in Library Factor = 224

Fig 11 B

HIT 1: Benzoic acid, 3,4,5-trimethoxy-, methyl ester

HIT 2: Benzoic acid, 3,4,5-trimethoxy-, methyl ester
Chapter-VII

Phytochemistry of plants

** Search Report Page 1 of 1 **

Unknown: MDI[CTR[30.0000..30.0000,10,Center.80,0,Area]:SMT[SA,3]] E87VSD.7IIE87VSDa.7tw
Compound in Library Factor = .568

Hit 1: 1,2-Benzene dicarboxylic acid, butyl deoxy ester
C22H34O4; MF: 311; RMF: 908; Prob 7.88%; CAS: 89-19-0; Lib: repbib; ID: 20042.

Fig 11 C

Hit 2: Dibutyl phthalate
C16H22O4; MF: 308; RMF: 914; Prob 7.05%; CAS: 84-74-2; Lib: mainlib; ID: 110431.

Fig 11 D
Chapter-VII

Phytochemistry of plants

** Search Report Page 1 of 1 **

Unknown: MDT[CTR]30.0000.30.0000.10.Center,80.0.0.Area]; SMT[SA,3] E87VSD.7RE87VSDa.7nw

Compound in Library Factor = -1101

** Fig 11 E **

Hit 1: 5.5'-Dimethoxy-3,3',7,7'-tetramethyl-2,2'-binaphthalene-1,1',4,4'-tetrone
C26H22O6; MF: 594; RMF: 679; Prob 34.1%; CAS: 85485-13-8; Lib: mainlib; ID: 188850.

** Fig 11 F **

Hit 2: Propanoic acid, 2-[(3-acelecoxy-4,4,14-trimethylandrost-8-en-17-yl)-
C27H42O4; MF: 593; RMF: 597; Prob 32.7%; Lib: mainlib; ID: 185178.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Hemidesmus indicus* (L.) R. Br. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 19.

**Table No.19**

<table>
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<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
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</tr>
</thead>
<tbody>
<tr>
<td>2-Hydroxy-4-methoxy-benzaldehyde</td>
<td><img src="image1" alt="Structure" /></td>
<td>10.7</td>
<td>C₆H₆O₃</td>
<td>152.05</td>
</tr>
<tr>
<td>Tetradecane</td>
<td><img src="image2" alt="Structure" /></td>
<td>11.8</td>
<td>C₁₄H₃₀</td>
<td>198.23</td>
</tr>
<tr>
<td>Methyl-(3,4-Dimethoxy-phenyl)-hydroxy-acetate</td>
<td><img src="image3" alt="Structure" /></td>
<td>14.3</td>
<td>C₁₁H₁₄O₃</td>
<td>226.08</td>
</tr>
<tr>
<td>Benzaldehyde, 3,4-dimethoxy, methylnonoacetal</td>
<td><img src="image4" alt="Structure" /></td>
<td>14.3</td>
<td>C₁₀H₁₄O₄</td>
<td>198.09</td>
</tr>
<tr>
<td>Dibutyl phthalate</td>
<td><img src="image5" alt="Structure" /></td>
<td>19.9</td>
<td>C₁₀H₂₂O₄</td>
<td>278.15</td>
</tr>
<tr>
<td>Heptacosane</td>
<td><img src="image6" alt="Structure" /></td>
<td>31.1</td>
<td>C₂₇H₅₆</td>
<td>380</td>
</tr>
<tr>
<td>Nonacosane</td>
<td><img src="image7" alt="Structure" /></td>
<td>31.1</td>
<td>C₂₅H₄₀</td>
<td>408</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of
Benzaldehyde, 2-hydroxy-4-methoxy, Tetradecane, Methyl (3,4-dimethoxyphenyl)-hydroxy acetate, Benzaldehyde, 3,4-dimethoxy, methylmonoacetel, Dibutyl phthalate, Heptacosane, Nonacosane. The spectrum profile of GC-MS confirmed the presence of five major components with the retention time 10.7, 11.8, 14.3, 19.9 and 31.1, respectively (Figure 12A). The individual fragmentation patterns of the components were illustrated in Figure 12B-H. The mass spectrum of the compound with retention time 10.7 gave 10 major peaks (m/z) at 53, 65, 69, 74, 81, 95, 108, 123, 134, and 151 (Figure 12B). The mass spectrum of the compound with retention time 11.8 gave 7 major peaks (m/z) at 57, 71, 85, 99, 127, 155 and 198 (Figure 12C). The mass spectrum of the compound with retention time 14.3 (Hit 1) gave 7 major peaks (m/z) at 81, 109, 137, 152, 167, 195 and 226 (Figure 12D). The mass spectrum of the compound with retention time 14.3 (Hit 2) gave 7 major peaks (m/z) at 79, 109, 137, 152, 167, 182 and 198 (Figure 12E). The mass spectrum of the compound with retention time 19.9 gave 11 major peaks (m/z) at 50, 57, 65, 76, 93, 104, 121, 132, 149, 205 and 223 (Figure 12F). The mass spectrum of the compound with retention time 31.1 (Hit 1) gave 10 major peaks (m/z) at 57, 71, 85, 99, 113, 141, 169, 197, 225 and 380 (Figure 12G). The mass spectrum of the compound with retention time 31.1 (Hit 2) gave 11 major peaks (m/z) at 57, 71, 85, 99, 113, 141, 169, 197, 225, 253 and 408 (Figure 12H).

In the present study we characterized the chemical profile of *Hemidesmus indicus* (L.) R.Br using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative...
concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Hemidesmus indicus* (L.) R.Br using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Hemidesmus indicus* (L.) R.Br for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Hemidesmus indicus** (L.) R.Br.

![Graph](image-url)

**Fig 12 A**
Chapter-VII

Phytochemistry of plants
Unknown: MDHOTR1.0000.1.0000.0, Center: 15.2.0, Area: 5.64.0, SMT[SA, 5] E87 VSD.7 RES7 VSD 7 w
Compound in Library Factor = 141

Fig 12 B

Hit 1: Benzaldehyde, 2-hydroxy-4-methoxy-
C8H5O3: MF: 1541; RMP: 1541; Prob 79.0%; CAS: 673-23-3; Lib: reposlib; ID: 20289.

Hit 2: Benzaldehyde, 2-hydroxy-4-methoxy-
C8H5O3: MF: 941; RMP: 941; Prob 78.0%; CAS: 673-22-3; Lib: mainlib; ID: 112728.
** Search Report Page 1 of 1 **

Unknown: MDT [CTR] 1.0000. 1.0000.80. Center, 15.2.0. Area: BCK[DF]: SMT[SA,5] E87VSD. 7NE87VSDc.7rw
Compound in Library Factor = -117

Fig 12 C

Hit 1: Tetradecane
C14H30; MF: 863; RMF: 914; Prob 40.7%; CAS: 629-59-4; Lib: mainlib; ID: 21935.

Hit 2: Tetradecane
C14H30; MF: 848; RMF: 900; Prob 40.7%; CAS: 629-59-4; Lib: replib; ID: 5512.
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Fig 12 D

Hit 1: Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate
C11H14O5; MF: 282; RMF: 289; Prob 48.3%; Lib: mainlib; ID: 124358.

Fig 12 E

Hit 2: Benzaldehyde, 3,4-dimethoxy-, methylmonoaacetel
C10H14O4; MF: 282; RMF: 832; Prob 42.7%; Lib: mainlib; ID: 124357.
Unknown: MDTCTR1.0000, 1.0000, 80, Center, 15, 2, 0, Area]; BCK[DF]; SMT[SA, 5]; E87VSD, 7RE87VSDc, 7nw
Compound in Library Factor = -124

Hi 1: Dibutyl phthalate
C16H22O4, MF: 920; RMF: 920; Prob 13.4%; CAS: 84-74-2; Lib: replib; ID: 20027.

Fig 12 F

Hi 2: Dibutyl phthalate
C16H22O4, MF: 914; RMF: 914; Prob 13.4%; CAS: 84-74-2; Lib: mainlib; ID: 110431.
** Search Report Page 1 of 1 **

Unknown: MDTCTR[1.0000; 1.0000; 80; Center, 15, 2, 0, Area].BCK[DF]; SMT[S, A, 5]; E87VSD.7RE8VSDc.7yw
Compound in Library Factor = 0.25

Hit 1: Heptacosane
C27H56; MF: 391; RMF: 280; Prob 48.4%; CAS: 593-49-7; Lib: replib; ID: 5508.

Fig 12 G

Hit 2: Nonacosane
C29H58; MF: 742; RMF: 793; Prob 8.93%; CAS: 630-03-5; Lib: replib; ID: 5478.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Nanorrhinum ramosissimum* (Wall.) Batsche. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 20.

### Table No.20

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclohexen-1-one, 4-Hydroxy-3,5,5-trimethyl-4-(3-methyl-1,3-butadienyl)</td>
<td><img src="image1.png" alt="Structure" /></td>
<td>13.3</td>
<td>C₁₄H₂₀O₂</td>
<td>220.15</td>
</tr>
<tr>
<td>2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)</td>
<td><img src="image2.png" alt="Structure" /></td>
<td>13.3</td>
<td>C₁₀H₁₂O₂</td>
<td>164.08</td>
</tr>
<tr>
<td>1,2,3,4-tetrahydroisoquinolin-6-ol, 1-[3-hydroxybenzyl]</td>
<td><img src="image3.png" alt="Structure" /></td>
<td>14.3</td>
<td>C₁₆H₂₇NO₂</td>
<td>255.13</td>
</tr>
<tr>
<td>Benzenemethanamine,2,5,7-octatrienyl-N-propyl</td>
<td><img src="image4.png" alt="Structure" /></td>
<td>14.3</td>
<td>C₁₈H₃₅N</td>
<td>255.20</td>
</tr>
<tr>
<td>Oleic acid</td>
<td><img src="image5.png" alt="Structure" /></td>
<td>22.2</td>
<td>C₁₈H₃₄O₂</td>
<td>282.26</td>
</tr>
<tr>
<td>6-Octadecenoic acid</td>
<td><img src="image6.png" alt="Structure" /></td>
<td>22.2</td>
<td>C₁₄H₂₄O₂</td>
<td>282.26</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 2-Cyclohexen-1-one, 4-hydroxy-3, 5, 5-trimethyl-4-(3-methyl-1,3-butadienyl, Oleic acid, 6-Octadecenoic acid. 2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl), 1, 2, 3, 4-tetradyroisoquinolin-6-ol, 1-[3-hydrobenzyl], Benzenemethanamine, 2,5,7-octatrienyl-N-propyl, 6-Octadecenoic acid. The spectrum profile of GC-MS confirmed the presence of six major components with the retention time 13.3, 14.3, 18.3, 19.8, 22.1, and 22.2, respectively (Figure 13A). The individual fragmentation patterns of the components were illustrated in Figure 13B-G. The mass spectrum of the compound with retention time 13.3 (Hit 1) gave 8 major peaks (m/z) at 55, 77, 93, 136, 149, 164, 177 and 220 (Figure 13B). The mass spectrum of the compound with retention time 13.3 (Hit 2) gave 7 major peaks (m/z) at 53, 77, 93, 108, 121, 149 and 164 (Figure 13C). The mass spectrum of the compound with retention time 14.3 (Hit 1) gave 7 major peaks (m/z) at 51, 77, 91, 133, 148, 236 and 255 (Figure 13D). The mass spectrum of the compound with retention time 14.3 (Hit 2) gave 10 major peaks (m/z) at 79, 91, 106, 148, 155, 165, 178, 196, 226 and 255 (Figure 13E). The mass spectrum of the compound with retention time 22.2 (Hit 1) gave 11 major peaks (m/z) at 55, 69, 83, 97, 111, 125, 151, 180, 222, 264 and 282 (Figure 13F). The mass spectrum of the compound with retention time 22.2 (Hit 2) gave 11 major peaks (m/z) at 55, 69, 83, 97, 111, 123, 180, 222, 246, 264 and 282 (Figure 13G).

In the present study we characterized the chemical profile of Nanorrhinum ramosissimum (Wall.) Betsche. using GC-MS. The gas
chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Nanorrhinum ramosissimum* (Wall.) Batsche. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Nanorrhinum ramosissimum* (Wall.) Batsche. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Kickxia ramosissima (Wall.) Janchen.

**Fig 13 A**
** Search Report Page 1 of 1 **

Unknown: MDT(CTR[30.0000..30.0000,10,Center,80.0.0.Area]:SMT[SA,3]) E87VSD.7fE87VSD.d.7w 15.3
Compound in Library Factor = -898

Hit 1 : 2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-4-(3-methyl-1,3-butadienyl)-, [S-(E)]; C14H12O2; MF: 215; RMF: 219; Prob 11.6%; CAS: 131883-26-6; Lib: mainlib; ID: 122202.

Fig 13 B

Hit 2 : 2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)-; C10H12O2; MF: 199; RMF: 223; Prob 6.70%; CAS: 410-91-8; Lib: mainlib; ID: 122067.

Fig 13 C
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Unknown: MDT[CTR][30.0000.. 30.0000.10.Center,80.0.0.Area].SMT[S,4.3].E87VSD.78/E87VSD.d.7tw 22.2

Compound in Library Factor = -359

Hit 1: Oleic Acid
C18H34O2; MF: 835; RMF: 839; Prob 15.1%; CAS: 112-80-1; Lib: replib; ID: 4483.

Fig 13 F

Hit 2: 6-Octadecenoic acid
C18H34O2; MF: 817; RMF: 855; Prob 7.81%; Lib: mainlib; ID: 19139.

Fig 13 G

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Verbascum chinese* (L.) Santapau. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 21.

**Table No.21**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>D-Alanine, N-proparglyloxycarbonyl, isoheptyl ester</td>
<td><img src="image1" alt="Structure" /></td>
<td>5.8</td>
<td>C_{17}H_{29}O_{4}N</td>
<td>256.44</td>
</tr>
<tr>
<td>D-Alanine, N-proparglyloxycarbonyl, decyl ester</td>
<td><img src="image2" alt="Structure" /></td>
<td>5.8</td>
<td>C_{17}H_{31}O_{4}N</td>
<td>311.10</td>
</tr>
<tr>
<td>2-furancarboxaldehyde, 5-hydroxymethyl</td>
<td><img src="image3" alt="Structure" /></td>
<td>8.8</td>
<td>C_{6}H_{10}O_{3}</td>
<td>126.33</td>
</tr>
<tr>
<td>n-hexadecanoic acid</td>
<td><img src="image4" alt="Structure" /></td>
<td>19.8</td>
<td>C_{16}H_{32}O_{2}</td>
<td>256.44</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of D-Alanine, N-propargyloxycarbonyl, isoheptyl ester, D-Alanine, N-propargyloxycarbonyl, decyl ester, 2-Furancarboxaldehyde, 5-hydroxymethyl, n-Hexadecanoic acid. The spectrum profile of GC-MS confirmed the presence of nine major components with the retention time 5.9, 7.2, 8.8, 11.6, 12.4, 17.4, 19.8, 19.9 and 22.2 respectively (Figure 1A). The individual fragmentation patterns of the components were illustrated in Figure 14B-E. The mass spectrum of the compound with retention time 5.8 (Hit 1) gave 3 major peaks (m/z) at 55, 82, 126 (Figure 14B). The mass spectrum of the compound with retention time 5.8 (Hit 2) gave 4 major peaks (m/z) at 55, 70, 82, 126 (Figure 14C). The mass spectrum of the compound with retention time 8.8 gave 6 major peaks (m/z) at 53, 69, 81, 97, 109, 126 (Figure 14D). The mass spectrum of the compound with retention time 19.8 (Hit 1) gave 13 major peaks (m/z) at 57, 60, 73, 83, 97, 115, 129, 157, 171, 185, 213, 227 and 256 (Figure 14E).

In the present study we characterized the chemical profile of Verbascum chinese (L.) Santapau. using GC-MS The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound.
which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Verbascum chinese* (L.) Santapau. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Verbascum chinese* (L.) Santapau. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
**Verbascum chinese** (L.) Santapau.

![Graph](image)

Fig 14 A
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Unknown: MDT[CTR[30.0000..30.0000,10,Center,80,0,0,Area];SMT[SA,3]] E87VSD,7fhE87VSD.7tw

Compound in Library Factor = -778

---

**Fig 14 B**

Hit 1: D-Alanine, N-propargyloxycarbonyl-, isohexyl ester
C13H21NO4; MF: 758; RMF: 828; Prob 17.6%; Lib: mainlib; ID: 89068.

---

**Fig 14 C**

Hit 2: D-Alanine, N-propargyloxycarbonyl-, decyl ester
C17H29NO4; MF: 751; RMF: 799; Prob 13.5%; Lib: mainlib; ID: 89422.

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J-14
**Search Report Page 1 of 1**

Unknown: MDT[CTR]0.0000, 30.0000, 10, Center, 80, 0, 0, Area; SMT[SA, 3]; E87VSD; 7%E87VSD; 7%w 8K

Compound in Library Factor = 168

Hit 1: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
C6H6O3; MF: 841; RMF: 845; Prob 90.8%; CAS: 67-47-0; Lib: replib; ID: 12795.

**Fig 14 D**

Hit 2: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
C6H6O3; MF: 824; RMF: 880; Prob 90.8%; CAS: 67-47-0; Lib: mainlib; ID: 60271.
Unknown: MDT[CTR[30.0000..30.0000,10,Center,80,0,0,Area];SMT[SA,3]] E87VSD.r(E87VSD),7rw 19.8 m

Compound in Library Factor = -156

Hit 1: n-Hexadecanoic acid
C16H32O2; MF: 256; RMF: 856; Prob 72.1%; CAS: 57-10-3; Lib: repub; ID: 2556.

Fig 14 E

Hit 2: n-Hexadecanoic acid
C16H32O2; MF: 846; RMF: 856; Prob 72.1%; CAS: 57-10-3; Lib: repub; ID: 6723.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Dolichandrone falcata* (Wall. ex DC.) Seem. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 22.

**Table No.22**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-phenyl</td>
<td><img src="image1" alt="Structure" /></td>
<td>28.7</td>
<td>C_{15}H_{12}O_{4}</td>
<td>256.07</td>
</tr>
<tr>
<td>Pectolinaringenin</td>
<td><img src="image2" alt="Structure" /></td>
<td>32.8</td>
<td>C_{17}H_{14}O_{6}</td>
<td>314.08</td>
</tr>
<tr>
<td>4H-1-Benzopyran-4-one, 5-hydroxy-(4-hydroxyphenyl)-6,7-dimethoxy</td>
<td><img src="image3" alt="Structure" /></td>
<td>32.8</td>
<td>C_{17}H_{14}O_{6}</td>
<td>314.08</td>
</tr>
<tr>
<td>Chrysin</td>
<td><img src="image4" alt="Structure" /></td>
<td>33.1</td>
<td>C_{15}H_{10}O_{4}</td>
<td>254.06</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 4H-
1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-phenyl, Chrysin. 4H-1-Benzopyran-4-one, 5-hydroxy-2-(4-hydroxyphenyl)-6,7-dimethoxy, Pectolinaringenin. The spectrum profile of GC-MS confirmed the presence of five major components with the retention time 16.4, 19.8, 28.7, and 33.1, 32.9, respectively (Figure 15A). The individual fragmentation patterns of the components were illustrated in Figure 15B-E. The mass spectrum of the compound with retention time 28.7 gave 11 major peaks (m/z) at 51, 63, 69, 104, 124, 131, 152, 179, 213, 238 and 256 (Figure 15B). The mass spectrum of the compound with retention time 32.8 gave 5 major peaks (m/z) at 133, 167, 217, 299 and 314 (Figure 15C). The mass spectrum of the compound with retention time 32.8 gave 15 major peaks (m/z) at 53, 69, 77, 91, 119, 135, 153, 167, 181, 195, 239, 271, 285, 299 and 314 (Figure 15D). The mass spectrum of the compound with retention time 33.1 gave 15 major peaks (m/z) at 51, 69, 77, 96, 113, 124, 141, 152, 165, 181, 197, 213, 226, 239 and 254 (Figure 15E).

In the present study we characterized the chemical profile of *Dolichandrone falcata* (Wall. ex DC.) Seem. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is
the first of its kind to analyze the chemical constituents of *Dolichandrone falcata* (Wall. ex DC.) Seem using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Dolichandrone falcata* (Wall. ex DC.) Seem. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Dolichandrone falcata (Wall.ex DC.) Seem.

Fig 15 A
Chapter-VII

Phytochemistry of plants
** Search Report Page 1 of 1 **

Unknown: MDT([CTR][30,0000,30,0000,10,Center,80,0,0,Area];5MT[S=3]] E87VSD.7hE87VSDb.7hw 287m

Compound in Library Factor = 851

Hit 1: 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-phenyl, (S)-
C15H12O4; MP: 917; RMP: 921; Prob 96.5%; CAS: 480-39-7; Lib: mainlib; ID: 167176.

Fig 15 B

Hit 2: 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-phenyl, (S)-
C15H12O4; MP: 769; RMP: 838; Prob 96.5%; CAS: 480-39-7; Lib: replib; ID: 26528.
16. *Hygrophilla auriculata* (Schumach.) Heine

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Hygrophila auriculata* (Schumach.) Heine. These compounds were identified through mass spectrometry attached with GC. The results of the present study were evaluated in Table 23.

### Table No.23

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-furancarboxaldehyde, 5(hydroxymethyl)</td>
<td>[Structure image]</td>
<td>8.8</td>
<td>C₆H₆O₃</td>
<td>126.03</td>
</tr>
<tr>
<td>5-(Hydroxymethyl)-2-(dimethoxymethyl)furan</td>
<td>[Structure image]</td>
<td>10.1</td>
<td>C₈H₁₀O₄</td>
<td>172.18</td>
</tr>
<tr>
<td>Methyl, 2,6-difluorobenzene</td>
<td>[Structure image]</td>
<td>10.1</td>
<td>C₈H₆O₂F₂</td>
<td>172.14</td>
</tr>
<tr>
<td>Elaidic acid, isopropyl ester</td>
<td>[Structure image]</td>
<td>22.1</td>
<td>C₂₁H₄₀O₂</td>
<td>324.54</td>
</tr>
<tr>
<td>Oleic acid</td>
<td>[Structure image]</td>
<td>22.1</td>
<td>C₁₈H₃₄O₂</td>
<td>282.44</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 2-furancarboxaldehyde, 5-(hydroxymethyl), oleic acid, elaidic acid, isopropylester, 5-(hydroxymethyl)-2 (dimethoxymethyl) furan, methyl 2,6-difluorobenzoate. The spectrum profile of GC-MS confirmed the presence of four major components with the retention time 8.8, 10.1, 29.4, 31.5 respectively (Figure 16A). The individual fragmentation patterns of the components were illustrated in Figure 16 B-F. The mass spectrum of the compound with retention time 8.8 (Hit 1) gave 6 major peaks (m/z) at 53, 69, 81, 97, 109, 126 (Figure 16B). The mass spectrum of the compound with retention time 10.1 (Hit 1) gave 9 major peaks (m/z) at 53, 69, 75, 81, 95, 109, 124, 141(Figure 16C). The mass spectrum of the compound with retention time 10.1 (Hit 2) gave 14 major peaks (m/z) at 50, 63, 68, 74, 81, 87, 93, 101, 113, 127, 141, 153, 172 (Figure 16D). The mass spectrum of the compound with retention time 22.1 (Hit 1) gave 11 major peaks (m/z) at 55, 69, 83, 97, 111, 125, 151, 180, 222, 264, 282 (Figure 16E). The mass spectrum of the compound with retention time 22.1 (Hit 1) gave 16 major peaks (m/z) at 55, 69, 83, 97, 111, 125, 139, 165, 193, 222, 245, 264, 282, 324 (Figure 16F).

In the present study we characterized the chemical profile of *Hygrophila auriculata* (Schumach.) Heine using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large
compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Hygrophilla auriculata* (Schumach) Heine. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Hygrophila auriculata* (Schumach) Heine. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Hygrophila auriculata (Schumach.) Heine

Fig 16 A
Chapter VII

Phytochemistry of plants

Figure 16 B
**Search Report Page 1 of 1**

Unknown: MDT|CTR(30.0000,30.0000,10,Center,80,0,0,Area);SMT(SA,3) E87VSD.78IE87VSDu.7rw 10.1

Compound in Library Factor = -207

Hit 1: 5-(Hydroxymethyl)-2-(dimethoxymethyl)furan  
C8H12O4; MF: 764; RMF: 793; Prob 51.8%; CAS: 90200-14-9; Lib: mainlib; ID: 103719.

Fig 16 C

Hit 2: Methyl 2,6-difluorobenzoate  
C8H6F2O2; MF: 666; RMF: 772; Prob 4.12%; CAS: 13671-00-6; Lib: repilb; ID: 19171.

Fig 16 D
**Search Report Page 1 of 1**

Unknown: MD[CTR]30.0000-30.0000,10,Cent0,0.0,Area]:SMT[SA,3] E87VSD.7RE87VSDu.7tw 2.0, 1
Compound in Library Factor = 1679

**Fig 16 E**

Hit 1: Oleic Acid
C18H34O2; MF: 644; RMF: 757; Prob 4.58%; CAS: 112-80-1; Lib: replib; ID: 4483.

**Fig 16 F**

Hit 2: Elaidic acid, isopropyl ester
C21H40O2; MF: 642; RMF: 766; Prob 4.23%; CAS: 22147-34-8; Lib: mainlib; ID: 17860.
17. *Phyla nodiflora* (L.) Greene.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Phyla nodiflora* (L.) Greene. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 24.

**Table No.24**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-furancarboxaldehyde, 5-hydroxymethyl</td>
<td><img src="image1" alt="Structure" /></td>
<td>8.8</td>
<td>C_6H_6O_3</td>
<td>126.55</td>
</tr>
<tr>
<td>2,7-dioxatricyclo [4,3,1] 3,8] decan-4-one</td>
<td><img src="image2" alt="Structure" /></td>
<td>11.8</td>
<td>C_9H_10O_3</td>
<td>154.08</td>
</tr>
<tr>
<td>Cyclobutal [1,2,3,4] dicyclooctene, hexadecahydro</td>
<td><img src="image3" alt="Structure" /></td>
<td>11.8</td>
<td>C_16H_28</td>
<td>220.22</td>
</tr>
<tr>
<td>1,6-dihydro-5-(2-hydroxyethyl) 4-methyl-6-oxopyrimidine</td>
<td><img src="image4" alt="Structure" /></td>
<td>16.6</td>
<td>C_7H_10O_2N_2</td>
<td>154.07</td>
</tr>
<tr>
<td>Octopamine</td>
<td><img src="image5" alt="Structure" /></td>
<td>16.6</td>
<td>C_8H_11O_2N</td>
<td>153.08</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 2-Furancarboxaldehyde, 5-(hydroxymethyl) 2,7-dioxatricyclo[4.3.1.0(3,8)]
decan-4-one, Cyclobuta-[1,2,3,4]-dicycloctene, hexadecahydro, 1,6-dihydro-5-(2-hydroxyethyl)-4-methyl-6-oxopyrimidine, octopamine. The spectrum profile of GC-MS confirmed the presence of eight major components with the retention time 3.8, 7.2, 8.8, 11.9, 13.1, 16.6, 19.8, 22.2 respectively (Figure 17A). The individual fragmentation patterns of the components were illustrated in Figure 1B-F. The mass spectrum of the compound with retention time 8.8 (Hit 1) gave 8 major peaks (m/z) at 53, 69, 81, 95, 97, 109, 123, 126 (Figure 17B). The mass spectrum of the compound with retention time 11.8 (Hit 1) gave 7 major peaks (m/z) at 55, 68, 82, 98, 110, 136, 154 (Figure 17C). The mass spectrum of the compound with retention time 11.8 (Hit 2) gave 7 major peaks (m/z) at 54, 67, 82, 95, 110, 192, 220 (Figure 17D). The mass spectrum of the compound with retention time 16.6 (Hit 1) gave 8 major peaks (m/z) at 55, 68, 79, 96, 106, 124, 136, 154 (Figure 17E). The mass spectrum of the compound with retention time 22.1 (Hit 2) gave 10 major peaks (m/z) at 51, 60, 67, 77, 91, 95, 107, 123, 136, 154 (Figure 17F).

In the present study we characterized the chemical profile of *Phyla nodiflora* (L.) Greene using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its
kind to analyze the chemical constituents of *Phyla nodiflora* (L.) Greene using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Phyla nodiflora* (L.) Greene for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Phyla nodiflora L.

Fig 17 A
Chapter-VII
Phytochemistry of plants

N-3
Chapter-VII Phytochemistry of plants
Unknown: MDT[CTR30.0000,30.0000,10.Center,80.0,0.Area]/SMT[SA,3] E87VSD.7RE87VSDn.7rw
Compound in Library Factor = 588

Hit 1: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
C8H6O3; MF: 930; RMF: 931; Prob 96.8%; CAS: 67-47-0; Lib: mainlib; ID: 60271.

**Fig 17 B**

Hit 2: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
C8H6O3; MF: 926; RMF: 934; Prob 96.8%; CAS: 67-47-0; Lib: replib; ID: 12795.
Chapter-VII Phytochemistry of plants
Chapter VII

Phytochemistry of plants

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Unknown: MDTCTR30.0000..30.0000,10,Center,80.0,0.0,Area],SMT[SA,3] E8TVS6.77E8TVS6n.7nw 16-6

Compound in Library Factor = -941

Hit 1: 1,5-Dihydro-5-(2-hydroxyethyl)-4-methyl-6-oxopyrimidine
C7H10N2O2; MF: 168; RMF: 704; Prob 42.3%; CAS: 89643-37-3; Lib: mainlib; ID: 67809.

Fig 17 E

Hit 2: Octopamine
C8H11NO2; MF: 162; RMF: 756; Prob 15.5%; CAS: 104-14-3; Lib: replib; ID: 16882.

Fig 17 F

N-7
18. *Lavandula bipinnata* (Roth.) Kuntze.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Lavandula bipinnata* (Roth.) Kuntze. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 25.

**Table No.25**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenol, 3-(1,1-dimethylethyl)-4-methoxy</td>
<td><img src="image1" alt="Structure" /></td>
<td>11.0</td>
<td>C₁₁H₁₆O₂</td>
<td>180.12</td>
</tr>
<tr>
<td>3-tert-Butyl-4-hydroxyanisole</td>
<td><img src="image2" alt="Structure" /></td>
<td>11.0</td>
<td>C₁₁H₁₆O₂</td>
<td>180.12</td>
</tr>
<tr>
<td>2H-1-Benzopyran-2-one</td>
<td><img src="image3" alt="Structure" /></td>
<td>12.6</td>
<td>C₈H₆O₂</td>
<td>146.04</td>
</tr>
<tr>
<td>2H-1-Benzopyran-2-one, 7-methoxy</td>
<td><img src="image4" alt="Structure" /></td>
<td>12.6</td>
<td>C₁₀H₈O₃</td>
<td>176.05</td>
</tr>
<tr>
<td>Hexadecanoic acid</td>
<td><img src="image5" alt="Structure" /></td>
<td>19.8</td>
<td>C₁₆H₃₁O₂</td>
<td>256.24</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of
Phenol, 3-(1,1-dimethyl-ethyl)-4-methoxy, 3-tert-Butyl-4-hydroxyanisole, 2H-1-Benzopyran-2-one, Hexadecanoic acid. 2H-1-Benzopyran-2-one, 7-methoxy. The spectrum profile of GC-MS confirmed the presence of Seven major components with the retention time 4.0, 6.5, 11.0, 12.6, 12.7, 16.9 and 19.8, respectively (Figure 18A). The individual fragmentation patterns of the components were illustrated in Figure 18B-F. The mass spectrum of the compound with retention time 11.0 (Hit 1) gave 13 major peaks (m/z) at 51, 55, 65, 69, 77, 81, 91, 107, 121, 137, 150, 165 and 180 (Figure 18B). The mass spectrum of the compound with retention time 11.0 (Hit 2) gave 14 major peaks (m/z) at 51, 55, 65, 69, 77, 82, 91, 107, 115, 124, 131, 137, 150, 165 and 180 (Figure 18C). The mass spectrum of the compound with retention time 12.6 gave 5 major peaks (m/z) at 51, 63, 90, 118 and 146 (Figure 18D). The mass spectrum of the compound with retention time 16.9 gave 11 major peaks (m/z) at 51, 63, 69, 77, 79, 89, 105, 120, 133, 148 and 176 (Figure 18E). The mass spectrum of the compound with retention time 19.8 gave 14 major peaks (m/z) at 57, 60, 73, 83, 97, 115, 129, 157, 171, 185, 213, 227, 239 and 256 (Figure 18F).

In the present study we characterized the chemical profile of *Lavandula bipinnata* (Roth.) Kuntze. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of
peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Lavandula bipinnata* (Roth.) Kuntze. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Lavandula bipinnata* (Roth.) Kuntze for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Lavandula bipinnata (Roth.) Kuntze.
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Unknown: MDT[CTR[1.0000, 1.0000, 80, Center, 15, 2.0, 0, Area], BCK[DF], SMT[SA, 5], E87VSD, 7RE87VSD, E7tw II M

Compound in Library Factor = -315

**Fig 18 B**

**Fig 18 C**

Hit 1: Phenol, 3-(1,1-dimethylethyl)-4-methoxy-
C11H16O2, MF: 182; RMF: 181; Prob 62.6%; CAS: 88-32-4; Lib: mainlin; ID: 123132.

Hit 2: 3-tert-Butyl-4-hydroxyanisole
C11H16O2, MF: 197; RMF: 197; Prob 26.0%; CAS: 121-00-6; Lib: replib; ID: 21629.
Fig 18 D

Hit 1: 2H-1-Benzopyran-2-one
CAS: 91; MF: 93; RMF: 93; Prob 87.0%; CAS: 91-64-5; Lib: rep; ID: 15854.

Hit 2: 2H-1-Benzopyran-2-one
CAS: 91; MF: 93; RMF: 93; Prob 87.0%; CAS: 91-64-5; Lib: rep; ID: 15853.
Chapter-VII

Phytochemistry of plants

** Search Report Page 1 of 1 **

Unknown: MDT[CTR[1.0000...1.0000,80,Center,15.2.0,Area];BCK[DF];SMT][SA,5]] E87VSD.7ml87VSD,7w66,7w99,9men

Compound in Library Factor = 454

Hit 1: 2H-1-Benzopyran-2-one, 7-methoxy- C10H8O3; MF: 936; RMF: 936; Prob 92.3%; CAS: 531-59-9; Lib: replib; ID: 18131.

** Fig 18 E **

Hit 2: 2H-1-Benzopyran-2-one, 7-methoxy- C10H8O3; MF: 934; RMF: 934; Prob 92.3%; CAS: 531-59-9; Lib: mainlib; ID: 130845.
** Search Report Page 1 of 1 **

Unknown: MDT[CTR[1.0000..1.0000,80,Center,15.2.0,Area],BCK[DF],SMT[S.A,5]] E87VSD, 7fE87VSD, 7w

Compound in Library Factor = 216

** Fig 18 F **

Hit 1: n-Hexadecanoic acid
C16H32O2, MF: 915; RMF: 915; Prob 87.0%; CAS: 57-10-3; Lib: replib; ID: 2558.

Hit 2: n-Hexadecanoic acid
C16H32O2, MF: 884; RMF: 884; Prob 87.0%; CAS: 57-10-3; Lib: replib; ID: 6723.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Leucas cephalotes* (Roth.) Spreng. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 26.

**Table No.26**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>9,12,15-Octadecatrienoic acid</td>
<td><img src="image1" alt="Structure" /></td>
<td>22.2</td>
<td>C₁₈H₂₀O₂</td>
<td>278.10</td>
</tr>
<tr>
<td>9,12-Octadecadienoic acid</td>
<td><img src="image2" alt="Structure" /></td>
<td>22.2</td>
<td>C₁₈H₂₂O₂</td>
<td>280.63</td>
</tr>
<tr>
<td>8,11,14-Eicosatrienoic acid</td>
<td><img src="image3" alt="Structure" /></td>
<td>22.6</td>
<td>C₂₀H₄₂O₂</td>
<td>306.26</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 9, 12, 15-Octadecatrienoic acid, 9,12-Octadecadienoic acid, 8, 11, 14-Eicosatrienoic acid. The spectrum profile of GC-MS confirmed the presence of seven major components with the retention time 12.3, 14.9, 17.0, 19.8, 22.1, 22.2 and 22.6, respectively (Figure 19A). The individual fragmentation patterns of the components were illustrated in Figure 19B-D. The mass spectrum of the compound with retention time 22.2 (Hit 1) gave 9 major peaks (m/z) at 55, 67, 79, 93, 108, 121, 149,
191 and 278 (Figure 19B). The mass spectrum of the compound with retention time 22.2 (Hit 2) gave 7 major peaks (m/z) at 55, 67, 81, 95, 109, 123 and 280 (Figure 19C). The mass spectrum of the compound with retention time 22.6 (Hit 1) gave 8 major peaks (m/z) at 55, 67, 79, 93, 108, 121,149,173, 222, 249, 278 (Figure 19D). The mass spectrum of the compound with retention time 22.6 (Hit 2) gave 8 major peaks (m/z) at 55, 67, 79, 93, 107, 150, 208 and 306 (Figure 19E).

In the present study we characterized the chemical profile of \textit{Leucas cephalotes} (Roth.) Spreng. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of \textit{Leucas cephalotes} (Roth.) Spreng. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of \textit{Leucas cephalotes} (Roth.) Spreng. for various ailments by traditional practitioners. However,
isolation of individual phytochemical constituents may proceed to find a novel drug.
Leucas cephalotes (Roth.) Spreng.

Fig 19 A
Chapter-VII  Phytochemistry of plants

**Fig 19 B**

Hit 1: 9,12,15-Octadecatrienoic acid, (Z,Z)-

**Fig 19 C**

Hit 2: 9,12-Octadecadienoic acid (Z,Z)-
** Search Report Page 1 of 1 **

Unknown: MDT[CTR]30.0000...30.0000.10.Center,80,0,0.Area]:SMT[SA,3]] E87VSD.7lE87VSDi.7rw 20-6m

Compound in Library Factor = 994

Hit 1: 9,12,15-Octadecatrienoic acid, (Z.Z.Z):
C18H30O2; MF: 705; RMF: 741; Prob 7.67%; CAS: 463-40-1; Lib: mainlib; ID: 41695.

Fig 19 D

Hit 2: 8,11,14-Eicosatrienoic acid, (Z.Z.Z):
C20H34O2; MF: 694; RMF: 751; Prob 5.26%; CAS: 1783-84-2; Lib: replib; ID: 1033.

Fig 19 E

T.S

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Cruculigo orchioides* Gaerth. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 27

**Table No.27**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-Dichloro-4,5-dimethoxy-benzene</td>
<td><img src="image" alt="Structure" /></td>
<td>13.0</td>
<td>C₈H₇Cl₂O₂</td>
<td>207.05</td>
</tr>
<tr>
<td>1,2-Dichloro-3,5-dimethoxy-benzene</td>
<td><img src="image" alt="Structure" /></td>
<td>13.0</td>
<td>C₈H₇Cl₂O₂</td>
<td>207.05</td>
</tr>
<tr>
<td>Ethanone, 1-(3-Methyl-benzo[b]selenophen-2-yl)-</td>
<td><img src="image" alt="Structure" /></td>
<td>15.9</td>
<td>C₁₁H₁₀OSe</td>
<td>237.99</td>
</tr>
<tr>
<td>Ethanone, 1-(2-Methyl-benzo[b]selenophen-3-yl)-</td>
<td><img src="image" alt="Structure" /></td>
<td>15.9</td>
<td>C₁₁H₁₀OSe</td>
<td>237.99</td>
</tr>
<tr>
<td>2,4,6-Trichloro-3-methoxy-5-methyl-phenol</td>
<td><img src="image" alt="Structure" /></td>
<td>16.2</td>
<td>C₈H₇Cl₂O₂</td>
<td>239.95</td>
</tr>
<tr>
<td>1,2,3-Trichloro-4,5-dimethoxy-benzene</td>
<td><img src="image" alt="Structure" /></td>
<td>16.2</td>
<td>C₈H₇Cl₂O₂</td>
<td>239.95</td>
</tr>
<tr>
<td>Hexadecanoic acid</td>
<td><img src="image" alt="Structure" /></td>
<td>19.8</td>
<td>C₁₆H₃₂O₂</td>
<td>256.24</td>
</tr>
</tbody>
</table>
The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of 1,2-Dichloro-4,5-dimethoxy-benzene, 1,2-Dichloro-3,5-dimethoxy-benzene, ethanone, 1-(3-Methyl-benzo [b] selenophen-2-yl), ethanone, 1-(2-Methyl-benzo [b] selenophen-3-yl), 2,4,6-Trichloro-3-methoxy-5-methyl-phenol, 1,2,3-Trichloro-4,5-dimethoxy-benzene, hexadecanoic acid. The spectrum profile of GC-MS confirmed the presence of seven major components with the retention time 3.8, 11.4, 13.0, 14.9, 15.9, 13.2 and 19.8, respectively (Figure 20A). The individual fragmentation patterns of the components were illustrated in Figure 20B-H. The mass spectrum of the compound with retention time 13.0 (Hit 1) gave 10 major peaks (m/z) at 50, 63, 85, 99, 113, 128, 145, 163, 191 and 206 (Figure 20B). The mass spectrum of the compound with retention time 13.0 (Hit 2) gave 9 major peaks (m/z) at 50, 63, 75, 85, 99, 128, 163, 191 and 206 (Figure 20C). The mass spectrum of the compound with retention time 15.9 (Hit 1) gave 9 major peaks (m/z) at 51, 63, 77, 89, 115, 128, 195, 223 and 238 (Figure 20D). The mass spectrum of the compound with retention time 15.9 (Hit 2) gave 9 major peaks (m/z) at 51, 63, 75, 89, 115, 128, 195, 223 and 238 (Figure 20E). The mass spectrum of the compound with retention time 16.2 (Hit 1) gave 9 major peaks (m/z) at 51, 63, 75, 87, 133, 162, 197, 225 and 240 (Figure 20F). The mass spectrum of the compound with retention time 16.2 (Hit 2) gave 12 major peaks (m/z) at 61, 77, 84, 96, 109, 119, 133, 147, 162, 197, 225 and 240 (Figure 20G). The mass spectrum of the compound with retention time 19.8 gave 14 major peaks (m/z) at 57, 60, 73, 83, 97, 115, 129, 157, 171, 185, 213, 227, 239 and 256 (Figure 20H).
In the present study we characterized the chemical profile of *Cruculigo orchioides* Gaerth. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Cruculigo orchioides* Gaerth. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Cruculigo orchioides* Gaerth. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Cruculigo orchioides Gaerth.
**Search Report Page 1 of 1**

Unknown: MDTCTR30.0000..30.0000,10,Center,80,0,0,Area[SMT[SA,3]] E87VSD.7RE87VSDI.7w‘13.0^-
Compound in Library Factor = .905

**Fig 20 B**

Hit 1: 1,2-dichloro-4,5-dimethoxy-
C8H8Cl2O2, MF: 264, RMF: 810; Prob 52.4%; CAS: 2772-46-5; Lib: mainlib; ID: 148836.

**Fig 20 C**

Hit 2: 1,2-Dimethoxy-3,5-dichloro-benzene
C8H8Cl2O2, MF: 266, RMF: 769; Prob 13.1%; CAS: 90283-01-5; Lib: mainlib; ID: 140860.
**Search Report Page 1 of 1**

Unknown: MDT|CTR[30.0000...30.0000,0,Center,80.0,0,Area];SMT[S,A,3]|E87VSD.71\E87VSD.7w15.9a

Compound in Library Factor = -1116

Hit 1 : Ethanone, 1-(3-methylbenzo[b]selenophene-2-yl)-
C11H10OSe; MF: 648; RMF: 747; Prob 33.2%; CAS: 20984-18-3; Lib: mainlib; ID: 155798.

**Fig 20 D**

Hit 2 : Ethanone, 1-(2-methylbenzo[b]selenophene-3-yl)-
C11H10OSe; MF: 642; RMF: 740; Prob 26.1%; CAS: 28026-38-5; Lib: mainlib; ID: 155799.

**Fig 20 E**
Chapter-VII

Phytochemistry of plants

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Unknown: MDT[CTR]0.0000, 0.0000, 0, Center, 0.0, 0, Area: SMT[SA,3] E87VSD-78E87VSD-78w 16.9

Compound in Library Factor = 326

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** Fig 20 F **

** Fig 20 G **
**Search Report Page 1 of 1**

Unknown: MDT[CTR30.0000,30.0000,10,Center,80,0,0,Area]; SMT[SA,3] E87VSD.7R:E87VSD.7tw 19.8a

Compound in Library Factor = -285

**Fig 20 H**

Hit 1: n-Hexadecanoic acid
C18H32O2, MF: 781; RMF: 815; Prob 64.2%; CAS: 57-10-3; Lib: raplib; ID: 2558.

Hit 2: n-Hexadecanoic acid
C18H32O2, MF: 771; RMF: 828; Prob 64.2%; CAS: 57-10-3; Lib: mainlib; ID: 8479.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Drimia indica* (Roxb.) Jessop. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 28.

**Table No 28**

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandrost-8-en17-yl)</td>
<td><img src="structure.png" alt="Structure of Propanoic acid" /></td>
<td>31.7</td>
<td>C_{27}H_{42}O_{4}</td>
<td>430.62</td>
</tr>
<tr>
<td>3-Ethyl-5-(2-ethyl-butyl)-octadecane</td>
<td><img src="structure.png" alt="Structure of 3-Ethyl-5-(2-ethyl-butyl)-octadecane" /></td>
<td>31.7</td>
<td>C_{29}H_{54}</td>
<td>366.42</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandrost-8-en17-yl), 3-Ethyl-5-(2-ethyl-butyl)-octadecane. The spectrum profile of GC-MS
confirmed the presence of two major components with the retention time 30.8 and 31.7, respectively (Figure 21A). The individual fragmentation patterns of the components were illustrated in Figure 21B-C. The mass spectrum of the compound with retention time 31.5 (Hit 1) gave 17 major peaks (m/z) at 55, 69, 83, 121, 159, 173, 187, 213, 233, 247, 281, 309, 337, 355, 370, 415 and 430 (Figure 21B). The mass spectrum of the compound with retention time 31.5 (Hit 2) gave 9 major peaks (m/z) at 57, 71, 85, 97, 113, 141, 183, 281 and 364 (Figure 21C).

In the present study we characterized the chemical profile of *Drimia indica* (Roxb.) Jessop using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of *Drimia indica* (Roxb.) Jessop. using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Drimia indica* (Roxb.) Jessop.
for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Drimia indica (Roxb.) Jessop.

Fig 21 A
Chapter VII

Phytochemistry of plants
22. *Ledebouria revoluta* (L.f.) Jessop.

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanolic extract of *Ledebouria revoluta* (L.f.) Jessop. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table 29.

Table No.29

<table>
<thead>
<tr>
<th>Name of compound</th>
<th>Structure of compound</th>
<th>Retention time</th>
<th>Molecular formula</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>4,4,6a,6b,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one</td>
<td><img src="image1" alt="Structure" /></td>
<td>30.6</td>
<td>C_{30}H_{50}O</td>
<td>424.37</td>
</tr>
<tr>
<td>a-Amyrin</td>
<td><img src="image2" alt="Structure" /></td>
<td>30.6</td>
<td>C_{33}H_{56}O</td>
<td>478.73</td>
</tr>
<tr>
<td>Octadecane, 3-ethyl-5-(2-ethylbutyl)</td>
<td><img src="image3" alt="Structure" /></td>
<td>31.5</td>
<td>C_{26}H_{44}</td>
<td>366.42</td>
</tr>
</tbody>
</table>

The compound prediction is based on Dr. Duke’s Phytochemical and Ethnobotanical Databases. The results revealed that the presence of
Octadecane, 3-ethyl-5-(2-ethylbutyl) 4,4,6a,6b,8a,11,11,14b-Octamethyl 1,4,4a,5,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one, α-Amyrin. The spectrum profile of GC-MS confirmed the presence of five major components with the retention time 10.1, 30.9, 31.0, 31.4 and 31.6 respectively (Figure 22A). The individual fragmentation patterns of the components were illustrated in Figure 22B-D. The mass spectrum of the compound with retention time 30.6 (Hit 1) gave 11 major peaks (m/z) at 55, 69, 81, 95, 109, 135, 147, 203, 218, 232 and 424 (Figure 22B). The mass spectrum of the compound with retention time 30.6 (Hit 2) gave 8 major peaks (m/z) at 55, 69, 81, 95, 122, 147, 218 and 426 (Figure 22C). The mass spectrum of the compound with retention time 31.5 gave 9 major peaks (m/z) at 57, 71, 85, 97, 113, 141, 183, 281 and 364 (Figure 22D).

In the present study we characterized the chemical profile of Ledebouria revoluta (L.f.) Jessop. using GC-MS. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the chemical constituents of Ledebouria revoluta (L.f.) Jessop. using GC-MS. In addition to this, the results of the GC-MS
profile can be used as pharmacognostical tool for the identification of the plant.

GC-MS analysis showed the existence of various compounds with different chemical structures. The presence of various bioactive compounds confirms the application of *Ledebouria revoluta* (L.f.) Jessop. for various ailments by traditional practitioners. However, isolation of individual phytochemical constituents may proceed to find a novel drug.
Ledbouria revoluta (L.f.) Jessop.

Fig 22 A
** Search Report Page 1 of 1 **

Unknown: MDT[CTR]30.0000...30.0000,10,Center,80,0,0,Area].SMT[S,A,3] E87VSD.7ff[E87VSDk.7tw 31.5

Compound in Library Factor = 733

Hit 1: Octadecane, 3-ethyl-5-(2-ethylbutyl)
C26H54, MF: 673; RMF: 746; Prob 25.6%; CAS: 955282-12-7; Lib: replib; ID: 2152.

Fig 22 D

Hit 2: Octadecane, 3-ethyl-5-(2-ethylbutyl)
C26H54, MF: 658; RMF: 705; Prob 25.6%; CAS: 955282-12-7; Lib: mainlib; ID: 7340.