GC-MS ANALYSIS OF BIOACTIVE COMPOUNDS IN METHANOLIC EXTRACT OF *THESPESIA POPULNEA* (L.) SOL.EX CORREA

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**ABSTRACT**

The present investigation was carried out to characterize the bioactive compounds present in leaf extract of *Thespesia populnea* using Gas Chromatography-Mass Spectrum (GC-MS). The results of the GC-MS analysis provide different peaks determining the presence of 23 phytochemical compounds with different therapeutic activities. The major phytocompounds N,N-Dimethylglycine (49.0%), 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- (12.90 %), Sucrose (9.84 %), 11,14,17-Eicosatrienoic acid, methyl ester (7.85 %), n-Hexadecanoic acid (6.36 %) etc., other major and minor compounds were also present. Hence, this study offers base of using as herbal alternative for the synthesis and development to treat various infectious diseases.

**Keywords:** Phytocompounds, *Thespesia populnea*, GC-MS, Methanol, Infectious diseases.

**INTRODUCTION**

Natural products consist of complex mixtures of one or more plants that contain a range of therapeutically active ingredients arising from plant parts or crude plant extracts. The utilization of medicinal plants in the treatment of certain human diseases has become common place, particularly in developing countries (Chan, 2003). This is a result of the high costs and side effects of most modern drugs and the fact that medicinal plants are perceived as effective and safer alternatives. The efficacy of these drugs derived from medicinal plants depends on the use of proper plant part and its biological potency which in turn depends upon the presence of required quantity and nature of secondary metabolite in a raw drug (Vinoth et al., 2011). There is growing awareness in correlating the phytochemical constituents of a medicinal plant with its pharmacological activity. These are non-nutritive chemicals that have
protected human from various diseases. Phytochemical constituents are the basic source for the establishment of several pharmaceutical industries. The constituents are playing a significant role in the identification of crude drugs. Therefore, the present study is to identify the active phytocompounds of this plant and subjecting the methanol extract of the plant leaves to Gas chromatography – Mass Spectrum analysis.

*Thespesia populnea* (L.) Sol.ex Correa belongs to the family Malvaceae, commonly known as umbrella tree in English, porush in Hindi and Poovarasu in Tamil. It is found in the tropical regions and coastal forests of India. All the parts of the plant used in traditional system of medicine. The bark, leaves, flower and fruits are useful in cutaneous infection such as scabies, psoriasis, eczema, ring worm and guinea worm. The decoction of the bark is commonly used for the treatment of skin and liver diseases. A compound oil of bark and capsules is useful in urethritis and gonorrhea. The bark, root, fruits were also used in dysentery, cholera and haemorrhoids (Ilavarasan *et al.*, 2003). The phytochemical study of bark reveals the presence of gossypol, tannin and coloring matter and leaf extract indicates the presence of lupeol, lupenone, beta sistosterol and also acacetin, quercetin, vanillic, syringic, melilotic, and ferulic acid (Shirwaikar *et al.*, 1995).

**MATERIALS AND METHODS**

**Collection of plant material**

The leaves of *T.populnea* were collected from the Pachamalai, Eastern Ghats of Tamilnadu, South India. They were identified and authenticated by the Rabinat Herbarium, St. Joseph’s College, Tiruchirappalli, Tamilnadu, India.

**Preparation of extract**

Leaves of *T.populnea* (5g) was shade dried, powdered and extracted with methanol for 24 hours using cold maceration methods. The extract was then filtered through Whatmann filter paper No.41 along with 2g sodium sulfate to remove the sediments and traces of water in the filtrate. Before filtering, the filter paper along with sodium sulphate is wetted with absolute alcohol. The filtrate is then concentrated by bubbling nitrogen gas into the solution and reduce the volume to 1ml. The extract contains both polar and non-polar phytocomponents.

**GC-MS Analysis**

The GC-MS analysis of *T.populnea* powder leaves extract with in methanol, was performed using a Clarus 500 Perkin Elmer gas chromatography equipped with a Elite-5 capillary
column (5% phenyl 95% dimethyl polysiloxane) (30nm X 0.25mm ID X 0.25µm df) and mass detector turbomass gold of the company which was operated in EI mode. Helium was the carriers gas at a flow rate of 1ml/min. and the injector was operated at 290°C and the oven temperature was programmed as follows; 50°C at 8°C/min to 200°C (5min) at 7°C/min to 290°C(10min).

Identification of components
Interpretation on mass spectrum of GC-MS was done using the database of National Institute Standard and Technology (NIST), having more than 62,000 patterns. The mass spectrum of the unknown component was compared with the spectrum of the known components stored in the (NIST), library. The name, molecular weight and structure of the components of the test materials were ascertained (Nezhadali et al., 2010; Sathyaprabha et al., 2011).

RESULTS AND DISCUSSION
The side effects of allopathic drugs have led to look for products of natural origin to cure many diseases. Almost 8,000 species of medicinal plants are being used in India for betterment of health (Anon, 1996). The present study carried out on the methanol leaf extract of T. populnea revealed the presence of medicinally active constituents. The compounds present in the methanolic extract of T. populnea were identified by GC-MS analysis. The active principles with their Retention time (RT), Molecular formula, Molecular weight (MW) and peak area in percentage are presented in Figure 1. The result revealed the presence of 23 major compounds (Table 1). Similar observation was reported by Nishaa et al. (2013) in which the phyto-constituent rich ethanolic extract of Maranta arundinacea L subjected to GC-MS analysis revealed the presence of 49 compounds. Similar work was reported for chemical composition analysis of essential oil of Curcuma amada by Vishnupriya et al. (2012). The results of the GC-MS analysis provide 23 major peaks determining the presence of phytochemical compounds with different therapeutic activities.

The major compounds present in the leaves were N,N-Dimethylglycine (49.0%), 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- (12.90 %), Sucrose (9.84 %), 11,14,17-Eicosatrienoic acid, methyl ester (7.85 %), n-Hexadecanoic acid (6.36 %) etc., other major and minor compounds were also present (Table 1). Dimethylglycine (DMG) is a tertiary amino acid involved in a variety of biological processes because it is an intermediary metabolite in the cellular metabolism of choline and betaine. The amino acid, N, N-Dimethylglycine is found as major compound and is reported to have immune modulating properties (Graber et al., 1981). The
The second major compound in the present study was 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-. 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z) (RT 25.18) possesses anti-inflammatory, hypocholesterolemic, cancer preventive, hepatoprotective, nematicide insectifuge, antihistaminic antieczemic, antiacne, antiandrogetic, antiarthritic, anticoronary and insectifuge properties. Previously, 9(Z),12(Z),15(Z)-octadecatrienoic acid, methyl ester, also known as α-linolenic acid methyl ester known to inhibit proliferation of ER-positive and ER-negative breast cancer cells (Grossmann et al., 2009). n-Hexadecanoic acid can be an antioxidant, hypocholesterolemic, nematicide, pesticide, lubricant activities and hemolytic 5-alpha is a reductase inhibitors (Sermakkani and Thangapandian, 2012).

The present study concluded that the stronger extraction capacity of methanol could have produced number of active constituents which are responsible for many biological activities. So that it might be utilized for the development of traditional medicines and further investigation is in need to elute novel active compounds from the medicinal plants which may create a new way to treat many incurable diseases. And also this type of study may give information on nature of active principles present in the medicinal plants and to identify the plants from their adulterants using isolated compounds as biomarker.

Table 1. Phytocompounds present in the leaves of Thespesia populnea using GC-MS

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Peak Name</th>
<th>Retention time</th>
<th>Peak area</th>
<th>%Peak area</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>N,N-Dimethyl-3-methoxypropylamine</td>
<td>4.59</td>
<td>2254044</td>
<td>0.7536</td>
</tr>
<tr>
<td></td>
<td>C_{6}H_{15}NO</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>MW: 117</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>Propanamide, 2-hydroxy-N-methyl</td>
<td>5.16</td>
<td>2570530</td>
<td>0.8595</td>
</tr>
<tr>
<td></td>
<td>C_{4}H_{9}NO_{2}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>MW: 103</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.</td>
<td>2-Cyclopenten-1-one, 2-hydroxy</td>
<td>5.91</td>
<td>314511</td>
<td>0.1052</td>
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<tr>
<td></td>
<td>C_{5}H_{6}O_{2}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>MW: 98</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.</td>
<td>N,N-Dimethylglycine</td>
<td>8.00</td>
<td>146743328</td>
<td>49.0635</td>
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<tr>
<td></td>
<td>C_{4}H_{9}NO_{2}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>MW: 103</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.</td>
<td>4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl</td>
<td>10.54</td>
<td>1994383</td>
<td>0.6668</td>
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<tr>
<td></td>
<td>C_{6}H_{8}O_{4}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>MW: 144</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.</td>
<td>Benzoic acid, 2-butoxy-</td>
<td>11.33</td>
<td>576246</td>
<td>0.1927</td>
</tr>
<tr>
<td></td>
<td>Name</td>
<td>Formula</td>
<td>MW</td>
<td></td>
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<tr>
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<td>----------------------------------------------------------------------</td>
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<td>------</td>
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</tr>
<tr>
<td>7.</td>
<td>Gritto et al.</td>
<td>C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;16&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>208</td>
<td></td>
</tr>
<tr>
<td>8.</td>
<td>Ethanone, 1-(2-hydroxy-5-methylphenyl)-</td>
<td>C&lt;sub&gt;9&lt;/sub&gt;H&lt;sub&gt;10&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>150</td>
<td></td>
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<tr>
<td>9.</td>
<td>1-(3,6,6-Trimethyl-1,6,7,7a-tetrahydrocyclopenta[c]pyran-1-yl)ethanone</td>
<td>C&lt;sub&gt;13&lt;/sub&gt;H&lt;sub&gt;18&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>206</td>
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<tr>
<td>10.</td>
<td>2-(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;16&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>180</td>
<td></td>
</tr>
<tr>
<td>11.</td>
<td>2-Trimethyl-3-methylene-, (E)-</td>
<td>C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;24&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>200</td>
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<tr>
<td>12.</td>
<td>Sucrose</td>
<td>C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;22&lt;/sub&gt;O&lt;sub&gt;11&lt;/sub&gt;</td>
<td>342</td>
<td></td>
</tr>
<tr>
<td>13.</td>
<td>4-Methyl-2,5-dimethoxybenzaldehyde</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>180</td>
<td></td>
</tr>
<tr>
<td>14.</td>
<td>(E,E)-7,11,15-Trimethyl-3-methylene-hexadeca-1,6,10,14-tetraene</td>
<td>C&lt;sub&gt;20&lt;/sub&gt;H&lt;sub&gt;32&lt;/sub&gt;</td>
<td>272</td>
<td></td>
</tr>
<tr>
<td>15.</td>
<td>Tetradecanoic acid</td>
<td>C&lt;sub&gt;14&lt;/sub&gt;H&lt;sub&gt;28&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>228</td>
<td></td>
</tr>
<tr>
<td>16.</td>
<td>3,7,11,15-Tetramethyl-2-hexadecen-1-ol</td>
<td>C&lt;sub&gt;20&lt;/sub&gt;H&lt;sub&gt;40&lt;/sub&gt;O</td>
<td>296</td>
<td></td>
</tr>
<tr>
<td>17.</td>
<td>2-Pentadecanone, 6,10,14-trimethyl-</td>
<td>C&lt;sub&gt;18&lt;/sub&gt;H&lt;sub&gt;36&lt;/sub&gt;O</td>
<td>268</td>
<td></td>
</tr>
<tr>
<td>18.</td>
<td>Hexadecanoic acid, methyl</td>
<td>C&lt;sub&gt;14&lt;/sub&gt;H&lt;sub&gt;28&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>228</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Name</td>
<td>Formula</td>
<td>MW</td>
<td>Retention Time</td>
</tr>
<tr>
<td>---</td>
<td>--------------------------------------------------------</td>
<td>---------------</td>
<td>------</td>
<td>----------------</td>
</tr>
<tr>
<td>19</td>
<td>n-Hexadecanoic acid</td>
<td>C₁₇H₃₄O₂</td>
<td>270</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>9,12-Octadecadienoic acid (Z,Z)-, methyl ester</td>
<td>C₁₉H₃₄O₂</td>
<td>294</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>11,14,17-Eicosatrienoic acid, methyl ester</td>
<td>C₂₁H₃₆O₂</td>
<td>320</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>Octadecanoic acid, methyl ester</td>
<td>C₁₉H₃₈O₂</td>
<td>298</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>9,12,15-Octadecatrienoic acid, (Z,Z,Z)-</td>
<td>C₁₈H₃₀O₂</td>
<td>278</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 1. GC-MS profiles of leaves of Thespesia populnea**

**REFERENCES**


