

## GC-MS Profiling of *Borassus flabellifer* Linn. Tubers

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**ABSTRACT:** *Borassus flabellifer* is commonly known as palmyra palm, tala or tal palm, toddy palm, lontar palm, wine palm, or ice apple and is native to South Asia. The present work was undertaken to profile the components available in the tuber extract of *Borassus flabellifer* Linn. Around eighteen compounds were eluted which was distributed through 23 peaks having retention time ranging from 5.828 to 44.835 min. Among the eighteen compounds eluted, seven compounds were found to have medicinal properties. Three compounds- Dioxolane (Peak 2 at retention time 7.850 min.), N- Acetyltyramine (Peak 6 at retention time 24.387 min.) and 9, 10 – Anthracenedione (Peak 14 at retention time 39.562 min.) are known to have potent anticancer properties. In the wake of increasing number of cancer cases in the present time, the root tubers of the selected plant can be used as lead compounds to design new drugs to fight the dreadful disease- Cancer.

**Keywords:** *Borassus flabellifer*, GC-MS, Anticancer compounds.

### INTRODUCTION

Discovery of medicinal plants for therapeutic purposes is mainly based on the available traditional information from the local population (Ayoub *et al.*, 2014). The analysis of the medicinal properties of different plants have attracted higher interest recently due to their potent pharmacological activities, economic viability and low toxicity (Chew *et al.*, 2012). In the last few years, gas chromatography-mass spectrometry (GCMS) a combined analytical technique has become established as a key technological platform for secondary metabolite profiling in both plant and non-plant species (Fernie *et al.*, 2004). It has been shown that *in vitro* screening methods could provide the needed and necessary properties for further chemical and pharmacological investigations (Mathekga and Meyer 1998). *Borassus flabellifer* Linn. is a sturdy plant which is the state tree of Tamil Nadu in India and all parts used in one way or the another. Moreover the fruit and tuber of the plant is reported to have various pharmacological activities. This study investigated the detection of phytochemicals using GC-MS (gas chromatography and mass spectrometry) analysis of the methanolic extract of tuber sprouts of *B. flabellifer*. Earlier work by Vijayakumari *et al.* (2015) had analysed the fruit pulp by GCMS and found out the presence of ten compounds around 15 compounds by Kanthal *et al.* (2020).

### MATERIALS AND METHODS

In this present study tubers (sprouts), were collected from

parts of Madurai, Tamil Nadu authenticated by a taxonomist and subjected to various experiments. The collected samples are washed with distilled water, minced into small pieces, and dried in the sun and the parts dried were ground and stored in airtight containers. Extraction from dried plants parts was done by methanol using the direct hot extraction method

**GC-MS analysis.** GC-MS analysis of methanolic tuber extracts was performed on Thermo GC-TRACE ultra ver.: 5.0, Thermo MS DSQ II, (Thermo Fisher Scientific). Experimental conditions of the GC-MS analysis includes: TR 5-MS capillary standard non-polar column, dimension: 30Mts, ID: 0.25 mm, Film thickness: 0.25µm. The flow rate of the mobile phase carrier gas helium (He) was set at 1.0 mL/min. In the gas chromatography, the temperature programme (oven temperature) was set at 40°C raised and to 250°C at 5°C/min. The injection volume was 1 µL. Samples dissolved in methanol were run at a range of 50–650 m/z and the results were compared by using the Wiley Spectral library search programme (Rehman *et al.*, 2013).

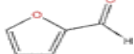
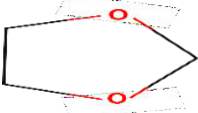
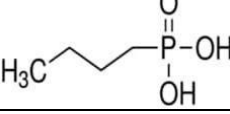
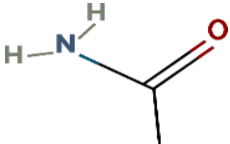
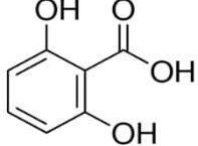
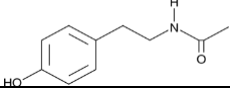
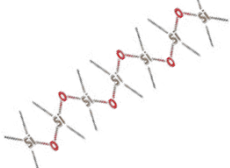

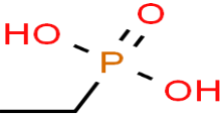
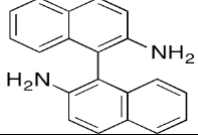
### RESULTS AND DISCUSSION

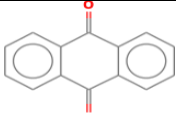
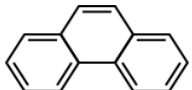
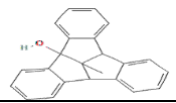
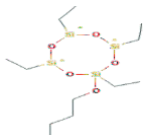
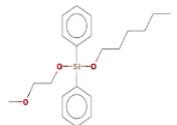
The phytochemicals found in the methanolic extract of *B. flabellifer* tubers were analysed using mass spectrometry in conjunction with GC-MS. The GC-MS chromatogram (Fig. 1) indicate the presence of various compounds obtained. The compounds were eluted at varying retention times indicating distinction in their structure and physicochemical properties. The

compounds corresponding to each peak was obtained using the data library. In the methanolic extract of *B. flabellifer* tuber, 18 biomolecules distributed through 23 peaks (Fig. 1) were identified and their molecular

weight and formula were determined. The list of phytoconstituents is tabulated in Table 1. The different pharmacological activities of compounds of *B. flabellifer* tuber extract was also described.

**Table 1: GCMS Profile of *Borassus flabellifer* Methanolic Extract of Tuber.**

Peak No.	Name of the Compound	Retention time (in min)	Molecular weight g/mol and Molecular Formula	Molecular structure
1	Furane - 2- Carboxaldehyde 5-(2,4,6 – trichloro 5 H <sub>4</sub> O <sub>2</sub> )	5.828	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	
2	1,3-Dioxolane 4-ethyl-2-penadecyl	7.850	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> 74.08 g/mol	
3	Butylphosphonic acid butyl 2-Phenylethy ester	13.359	C <sub>4</sub> H <sub>11</sub> O <sub>3</sub> P 138.10 g/mol	
4	Acetamide N-butyl-Phenyl	20.904	CH <sub>3</sub> CONH <sub>2</sub> 59.068 g/mol	
5	2,6-Dihydroxybenzoic acid 3TMS derivative	21.600	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub> 154.12 g/mol	
6	N-Acetyltyramine	24.387	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> 179.22g/mol	
7	Heptasiloxane hexadecamethyl	25.681	O <sub>6</sub> Si <sub>7</sub> 292.59 g/mol	
8	Cyclotetrasiloxane octamethyl	29.314	C <sub>23</sub> H <sub>30</sub> O <sub>4</sub> Si <sub>4</sub> 482.8 g/mol	
12	Ethylphosphonic acid bis(tert-butyl dimethylsilyl) ester	39.045	C <sub>2</sub> H <sub>7</sub> O <sub>3</sub> P 110.05 g/mol	
13	(1,1' - Binaphthalene)-2,2'-diamine	39.259	C <sub>20</sub> H <sub>16</sub> N <sub>2</sub> 284.4 g/mol	
14	9,10 - Anthracenedione 1,8-dihydroxy-3-methoxy-6-methyl	39.562	C <sub>14</sub> H <sub>8</sub> O <sub>2</sub> 208.2121	

				
15	Phenanthrene 9-ethyl-3,6-dimethoxy-10 methy	40.619	C <sub>14</sub> H <sub>10</sub> 178.23 g/mol	
16	Methyltribenzocentrotriquinanol	40.994	C <sub>23</sub> H <sub>18</sub> O 310.4 g/mol	
17	Pyrazolo[3,4-b]thiopyrano[4,3-d]Pyridin-1-amine	41.203		
18	1-[2,4-Bis(trimethylsiloxy)Phenyl]-2-[(4-trimethyl)	41.298		
19	Ether bis(P-tert-butylphenyl)	41.499		
20	1,3,5,7-Tetraethyl-1- butoxycyclotetrasiloxane	42.178	C <sub>12</sub> H <sub>29</sub> O <sub>5</sub> Si <sub>4</sub> 365.70 g/mol	 et al., 2007:
21	Silane diphenylhexyloxy(2-methoxyethoxy)	44.835	SiH <sub>4</sub> 32.12 g/mol	

Eighteen bioactive compounds were identified from the methanolic extract of *B. flabellifer* based on retention time, peak area percentage. Early reports intimated that GC/MS is the first line information about phytochemical composition of living system. Arirudran *et al.* (2022) have revealed thirty-six bioactive compounds in ethanolic extracts from the root of *B. flabellifer*. Vijayakumari *et al.* (2015) reported the presence of Furace - 2- Carboxaldehyde and ten other bioactive compounds in the Palmyra fruit pulp. In this investigation, Furace - 2- Carboxaldehyde was the first compound eluted at a retention time of 5.823 min with a peak area of 2175 sq. Unit and with a peak height of 333. Sahni *et al.* (2014) reported thirty-nine bio-compounds in the hexane fraction of dried roots forty-four compounds in the chloroform fraction of dried roots and eight compounds in the methanol fraction of dried roots. A total of four bioactive compounds in *B. flabellifer* male flower ethanolic extract were identified and characterized by Tunit *et al.* (2022), while even volatile fatty acid compositions of toddy palm nectar detected by Pammi *et al.* (2021).

In this study, the highest peak identified was peak number 22, at retention time of 42.178 min and the compound identified is Tetraethyl-1-butoxycyclotetrasiloxane with a molecular formula C<sub>12</sub>H<sub>29</sub>O<sub>5</sub>Si<sub>4</sub>, and its molecular weight is 365.70 g/mol. The next highest is peak number 17 at retention time of 40.994 min, the compound was identified as Methyltribenzocentrotriquinanol (C<sub>23</sub>H<sub>18</sub>O), with molecular weight 310.4 g/mol, followed by the compound 1,3-Dioxolane at peak number 2 at retention time of 7.850 min (Table 1). According to Kucuk *et al.* (2011), Dioxolane is a potent anticancer

against leukaemia and also has antibacterial and antifungal properties and also inhibits the herpes simplex viruses. Many compounds showing medicinal properties has been synthesized that confer antifungal, antibacterial, antineoplastic, antiviral and anticonvulsant (Baji *et al.*, 1997; Genta *et al.*, 2002; Shirai *et al.*, 1998; Bera *et al.*, 2003; Zapata-Sudo *et al.*, 2007).

Butylphosphonic acid (C<sub>4</sub>H<sub>11</sub>O<sub>3</sub>P) molecular weight 138.10 g/mol. is a reactive and unstable chemical compound. It has been shown to have inhibitory properties in the treatment of inflammatory bowel disease. The compound was eluted as the third compound at 3rd peak. Acetamide (CH<sub>3</sub>CONH<sub>2</sub>) at the retention time of 20.904 min (Table 1). was the fourth compound eluted has anti-arthritis and antibiotic properties (Yalcin *et al.*, 1997; Jawed *et al.*, 2010). The molecular weight of this compound was 59.068 g/mol. 2,6-Dihydroxybenzoic (C<sub>7</sub>H<sub>6</sub>O<sub>4</sub>) acid with a molecular weight of 154.12 g/mol was eluted at a retention time of 21.600 min from peak 5, is an iron-chelating drug (Graziano *et al.*, 1974) and has antibacterial properties (George *et al.*, 2011). N-Acetyltyramine (C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>), molecular weight 179.22g/mol eluted at 24.387 min is a promising anti-cancer agent eluted from peak 6. It is reported by Zhao *et al.* (2010) that N-Acetyl tyramine had many bioactivities, such as fungi toxic activity against *Cladosporium sphaerospermum*, antitumor activity against A375 human melanoma cells and K562 human leukaemia cells, it is an IL-1R antagonist and inhibitor of factor XIIIa. According to the National Institute of Standards and Technology Heptasiloxane (O<sub>6</sub>Si<sub>7</sub>) is effective in habiting growth of fungi like *Candida albicans* and *Trichophyton*

*mentagrophytes*, and can be used for the treatment of these fungal infections. Heptasiloxane was detected from peak 7.

Cyclotetrasiloxane (C<sub>23</sub>H<sub>30</sub>O<sub>4</sub>Si<sub>4</sub>), was eluted at a retention time of 29.314 min ORM PEAK 8, is a skin-conditioning, and hair-conditioning agent, and is used as a solvent in cosmetics. It is a 'volatile silicone,' meaning it evaporates off the skin and hair rather than remaining there. It has amazing silkiness and excellent spreading characteristics. It is used to make cleaning solutions, surfactants, cosmetic products, and polishes. The twelfth peak number corresponds to the compound Ethylphosphonic acid (C<sub>2</sub>H<sub>7</sub>O<sub>3</sub>P), is used in the synthesis of nucleotide analogues.

The thirteenth peak corresponds to 1,1'-Binaphthalene]-2,2'-diamine (C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>) molecular weight 284.4 g/mol is corresponding to a retention time of 39.259 min. It is the reagent used for the synthesis of various ligands. 9,10 – Anthracenedione (C<sub>14</sub>H<sub>8</sub>O<sub>2</sub>), molecular weight 208.2121g/mol was eluted at the retention time of 39.562 min. Anthraquinone, also called anthracenedione is an aromatic organic compound and is a chemotherapy and antimalarial drug. According to Malik and Muller (2016), anthraquinones exhibit a unique anticancer activity. Since their discovery, medicinal chemists have made several structural modifications, resulting in the design and synthesis of a large number of novel anthraquinone compounds with different biological activities. In general, anthraquinone compounds have been considered to have anticancer activity mainly through DNA damage, cycle arrest and apoptosis. However, recent studies have shown that novel anthraquinone compounds may also inhibit cancer through paraptosis, autophagy, radiosensitising, overcoming chemoresistance and other methods Tian *et al.* (2020). The anthraquinone-rich dichloromethane fraction displayed the highest anticancer activity when evaluated in a human hepatoma cancer cell line (HepG2), in which it induced increased apoptosis mediated by p53 and caspase activation (Eom *et al.*, 2020).

Phenanthrene (C<sub>14</sub>H<sub>10</sub>), molecular weight 178.23 g/mol is used to make bile acids, cholesterol and steroids. The peak number 18 corresponds to the compound Pyrazolo [3,4- b]thiopyrano[4,3-d] Pyridin-1-amine eluted at a retention time 41.203 min (Table 1). 1-[2,4-Bis(trimethylsiloxy)Phenyl]-2-[(4-trimethyl was the compound eluted at the retention time of 41.298 min, with a peak height of 298 and with peak area 3127 sq. Unit. The next compound was identified as bis (P-tert-butylphenyl – an ether eluted at the retention time of 41.728 min Silane (SiH<sub>4</sub>) with molecular weight 32.12g/mol was eluted at 44.835 min was the last compound eluted from the methanolic tuber extract of *B. flabellifer* which is used as a waterproofing agent in construction projects and prevents corrosion. Silane can also be used as an adhesive for bonding as well as metal-based components.

Previous reports said that GCMS analysis of *Borassus flabellifer* Linn. roots is well known for its medicinal properties and curative agents for many

diseases (Akerle and Synge 1991). Extracts of *Borassus flabellifer* using GCMS stated that they contain fatty acids, alkanes, alkenes, ketones, aldehydes, diterpenes, phytols, and sterols, which can regulate blood pressure, coagulation and lipid levels (Arirudran *et al.*, 2022). It is documented that the roots of *Borassus flabellifer* Linn. was found to possess an enriched amount of nutritious ingredient, curative agents and drugs (Meechaona *et al.*, 2007). The present work has again stressed the medicinal importance of this plant which is least exploited of its medicinal importance.

## CONCLUSIONS

Medicinal plants, which form the backbone of traditional medicine, in the last few decades, have been the subject of very intense pharmacological studies. Due to the undesirable side effects of synthetic drugs, phytochemicals of plants may be useful for drug discovery and development against various diseases. The presence of 18 phytoconstituents in the plant extract was confirmed through GC-MS analysis. The tubers of *Borassus flabellifer* contains plenty of bioactive compounds. It is believed to possess medicinal values, frequently associated with chronic diseases and also certain types of malignancy. Therefore, it seems reasonable to consider the tubers of *Borassus flabellifer* as a valuable ingredient which can improve and enhance our health. From this study, it can be concluded that *Borassus flabellifer* may serve as a new potential source of anticancer medicines due to the presence of these phytochemicals and bioactive compounds which confer the medicinal properties. However *in silico* works of these compounds can pave the way for new anticancer drug discoveries from these natural source of phytochemicals.

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**Conflict of Interest.** None.

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