

## Full Length Article

# Gas chromatography and mass spectrometric analysis of *Padina pavonia* (L.) Lamour

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### ABSTRACT

The present investigation aims to identify phyco-components and metal chelating components of methanol extract of *Padina pavonia* (L.) Lamour from Hare Island, Thoothukudi Coast, Gulf of Mannar. Eighteen chemical compounds were identified by gas chromatography and mass spectrometric analysis. Most of the compounds were assumed to have antioxidant, antimicrobial, anti-inflammatory, antitumour and cancer preventive properties. Compounds with metal chelating ability like phenol, myristic acid ester, myristic acid, palmitic acid ester, palmitic acid, linoleic acid ester and oleic acid were identified by their functional groups.

**Key Words:** *Padina pavonia*, GC-MS analysis, antimicrobial, anti-inflammatory, antitumour, anticancer.

### INTRODUCTION

Brown algae represent a rich and easily regenerated resource of polysaccharides of structural and biological interests: laminarins, fucoidans, and also alginic acids (Percival and McDowell, 1967; Painter, 1983). Laminarins are known as anticancer substances (Bohn and Bemiller, 1995; Shin *et al.*, 2009). Brown algae contain 5-20% fucoidan (Chapman, 1980), about 40% of which are sulphate esters. Sulphonic groups are present in the three algal divisions typically play roles in metal binding (Davis *et al.*, 2003). Fucoidans have activity against hepatitis viruses (Venkateswaran *et al.*, 1989), anti-HIV infection (Shaeffer and Krylov, 2000), and have antitumour (Dias *et al.*, 2005) and anticoagulant (De Azevedo *et al.*, 2009) properties. It is assumed that carboxyl (-COOH) groups of alginic acid found in brown algae play a key role in metal ion binding (Kuyucak and Volesky, 1989; Davis *et al.*, 2003). Alginic acid usually constitutes about 10-40% of brown algal dry weight (Percival and McDowell, 1967). Schiewer and Wong (2000) reported that in certain brown algae the carboxyl groups of alginic acid are more abundant than either carboxyl or amino

groups of the protein and are therefore likely to be the main binding sites. These chemical sites are naturally present and functional even when the biomass is dead (Volesky, 2001). Alginic acids are successfully used in various areas of industry as gel-forming materials in medicine and cosmetology for preparation of non-fatted ointments, etc. (Lewis *et al.*, 1988). Phenols are another important seaweed constituent act as metal chelator due to their hydroxyl groups (Wu and Hansen, 2008; Sushanto Gouda *et al.*, 2013). *Padina pavonia* is the one of the most abundant brown alga in Hare Island, Thoothukudi coast, Gulf of Mannar (Mary Josephine *et al.*, 2013). To our knowledge, no chemical analysis of *P. pavonia* has been reported from this region. Hence, the present communication deals with the GC-MS analysis of methanol extract of *P. pavonia*.

### MATERIALS AND METHODS

The brown alga, *Padina pavonia* (L.) Lamour collected from Hare Island, Thoothukudi Coast, Gulf of Mannar. They were washed twice with fresh water to remove the entire sand particle.

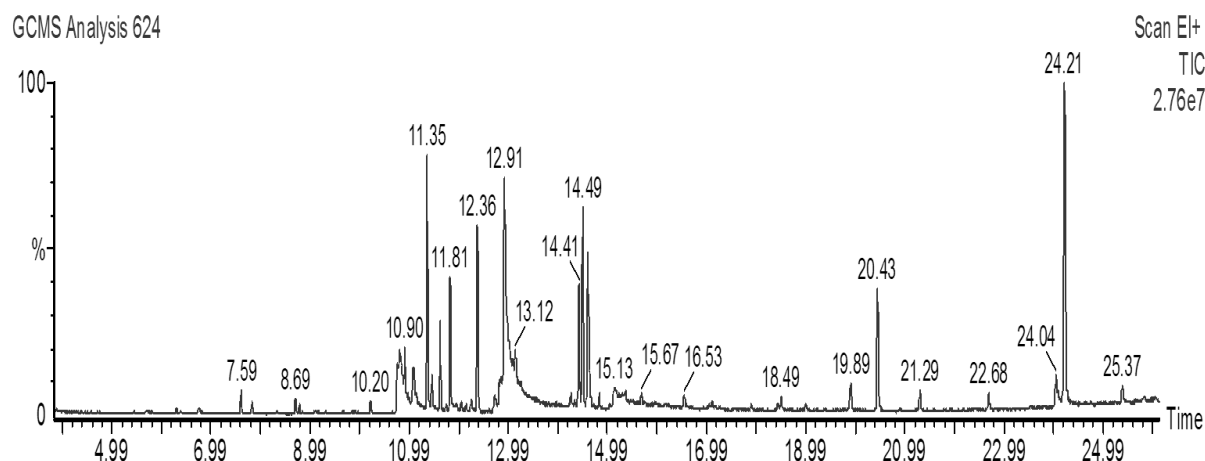


Fig. 1 GC-MS Chromatogram of the methanol extract of *Padina Pavonia*

Table 1: Phycocomponents detected in the methanol extract of *Padina pavonia* by GC-MS analysis

S. No.	Retention Time	Name of the compound*	Molecular Formula	Molecular Weight	Peak Area (%)
1.	7.59	Nonane, 3,7-dimethyl-	C <sub>11</sub> H <sub>24</sub>	156	0.75
2.	7.82	Phenol,3,5 bis(1,1 dimethylethyl)-	C <sub>14</sub> H <sub>22</sub> O	206	0.45
3.	8.69	3-Undecene,9-methyl-,(E)-	C <sub>12</sub> H <sub>24</sub>	168	0.45
4.	8.77	Octane, 3,4,5,6-tetramethyl-	C <sub>12</sub> H <sub>26</sub>	170	0.30
5.	10.20	Tetradecanoic acid, methyl ester	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	242	0.45
6.	10.80	Tetradecanoic acid	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	228	7.92
7.	10.90	1,7 Dimethyl-4-(1-methylethyl) cyclodecane	C <sub>15</sub> H <sub>30</sub>	210	2.99
8.	11.07	3,3-Dimethyl-hepta-4,5 dien-2-ol	C <sub>9</sub> H <sub>16</sub> O	140	2.84
9.	11.35	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	296	7.32
10.	12.36	Hexadecanoic acid, methyl ester	C <sub>20</sub> H <sub>40</sub> O	270	5.98
11.	12.91	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256	27.20
12.	14.41	9,12 Octadecadienoic acid, methyl ester	C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>	294	4.33
13.	14.49	9-Octadecenoic acid(Z)-,methyl ester	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>	296	7.32
14.	14.59	6,10,14-Trimethyl Pentadecan-2-ol	C <sub>18</sub> H <sub>38</sub> O	270	7.17
15.	20.43	1,2 Benzene dicarboxylic acid diisooctyl ester	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	390	6.28
16.	21.29	Tridecane, 1- Iodo-	C <sub>13</sub> H <sub>27</sub> I	310	1.05
17.	24.21	Squalene	C <sub>30</sub> H <sub>50</sub>	410	16.14
18.	25.37	Eicosane, 7-hexyl-	C <sub>26</sub> H <sub>54</sub>	368	1.05

\* Compounds were identified from the database stored in the National Institute of Standard Technology (NIST – Version, 2005)

The samples were shade-dried and powdered. About 25g of powder was extracted with 250ml of methanol in the ratio of 1:10 in Soxhlet apparatus. The extract was allowed to dry and the final residue was subjected to GC-MS analysis.

#### GC-MS ANALYSIS

GC-MS analysis was carried out by following the method of Hema *et al.*, (2010) using a Perkin-Elmer GC Clarus 500 system and Gas Chromatograph interfaced to a Mass Spectrophotometer (GC-MS) equipped with a

**Table 2: Chemical nature and activity of phycocomponents identified in the methanol extract of *Padina pavonia* by GC-MS analysis**

S.No.	Name of the compound	Molecular Formula	Chemical nature	Activity
1.	Phenol,3,5 bis(1,1 dimethylethyl)-	C <sub>14</sub> H <sub>22</sub> O	Phenolic compound	Antimicrobial, Antioxidant , Anti-inflammatory.
2.	Tetradecanoic acid, methyl ester	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	Myristic acid ester	Antioxidant, Cancer preventive, Nematicide.
3.	Tetradecanoic acid	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	Myristic acid	Antioxidant, Cancer preventive, Nematicide.
4.	3,3-Dimethyl-hepta-4,5 dien-2-ol	C <sub>9</sub> H <sub>16</sub> O	Alcoholic compound	Antimicrobial.
5.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	Terpene alcohol	Antimicrobial, Anti-inflammatory.
6.	Hexadecanoic acid, methyl ester	C <sub>20</sub> H <sub>40</sub> O	Palmitic acid ester	<b>Antioxidant, Nematicide, Pesticide, Antiandrogenic, Flavor.</b>
7.	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	Palmitic acid	<b>Antioxidant, Nematicide, Pesticide, Antiandrogenic, Flavor.</b>
8.	9,12 Octadecadienoic acid, methyl ester	C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>	Linoleic acid ester	Anti-inflammatory, Cancer preventive.
9.	9-Octadecenoic acid(Z)-,methyl ester	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>	Oleic acid ester	Anti-inflammatory, Antiandrogenic, Cancer preventive.
10.	6,10,14-Trimethyl Pentadecan-2-ol	C <sub>18</sub> H <sub>38</sub> O	Alcoholic compound	Antimicrobial.
11.	1,2 Benzene dicarboxylic acid diisooctyl ester	C <sub>24</sub> H <sub>38</sub> O	Plasticizer compound	Antimicrobial, Antifouling.
12.	Tridecane, 1- Iodo-	C <sub>13</sub> H <sub>27</sub> I	Iodine compound	Antimicrobial.
13.	Squalene	C <sub>30</sub> H <sub>50</sub>	Triterpene	<b>Antibacterial, Antioxidant, Diuretic, Antitumor, Cancer preventive, Immunostimulant, Chemo preventive, Lipoxygenase-inhibitor, Pesticide.</b>

Elite-5MS fused silica capillary column (30m x 0.25mm x 0.25µm) composed of 5% diphenyl / 95% dimethyl polysiloxane.

For GC-MS detection, an electron ionization system with ionizing energy of 70eV was used. Helium gas (99.999%) was used as the carrier gas at constant flow rate 1ml/min and an injection volume of 2µl was employed split ratio of 10:1; injector temperature 250°C. The oven temperature was programmed from 110°C (isothermal for 2min) with an increase of 10°C /min to 200°C, then 5°C/min to 280°C, ending with a 9min isothermal at 280°C. Mass spectra were taken at 70eV; 200°C of inlet line source temperature a scan interval of 0-2min and mass scan from 45 to 450 (m/Z). Total GC running time was 36 minutes. The relative % amount was calculated by comparing its peak area to the total areas. Software adopted to handle mass spectra and chromatogram was Turbomass (Version 5.2).

#### IDENTIFICATION OF COMPOUNDS

Interpretation on mass spectrum (GC-MS) was done using the database of National Institute of Standard and Technology (NIST) having more than 62,000 patterns. The spectrum of the unknown compounds was compared with the spectrum of the known compounds stored in the

NIST Library (Version, 2005). The name, molecular weight and peak area of the compounds of the test material was ascertained.

#### RESULTS AND DISCUSSION

Eighteen compounds were identified in the methanol extract of *P. pavonia* by GC-MS analysis (Fig. 1). The active principles in *P. pavonia*, their retention time, molecular formula, molecular weight and peak area (%) were presented in Table 1. The study indicated that there were thirteen compounds having significant biological functions that were showed in Table 2. Most of the compounds had antimicrobial, antioxidant, anti-inflammatory, antitumour and cancer preventive properties. It was in agreement with the results of Mayer and Lehmann (2001), Mayer and Hamann (2004), Smit (2004), Flora and Maria Victorial Rani (2013), Gihan *et al.*, (2014-2015). Seven compounds such as phenol, myristic acid ester, myristic acid, palmitic acid ester, palmitic acid, oleic acid ester and linoleic acid were identified in *P. pavonia* extract. Some of these compounds (Table 3) were reported to have metal chelating ability (Kamenarska *et al.*, 2005). The data gathered from this study suggested that *P. pavonia* could be utilized for future studies.

**Table 3: Metal chelating compounds identified in *Padina pavonia* by GC-MS analysis**

S. No.	Name of the compound	Functional groups
1.	Phenol	Phenolic group[-OH ]
2.	Myristic acid,ester	Carboxylic group [-COOH]
3.	Myristic acid	Carboxylic group [-COOH]
4.	Palmitic acid	Carboxylic group [-COOH]
5.	Palmitic acid ester	Carboxylic group [-COOH]
6.	Oleic acid ester	Carboxylic group [-COOH]
7.	Linoleic acid ester	Carboxylic group [-COOH]

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