GAS CHROMATOGRAPHY – MASS SPECTROSCOPY (GC - MS) ANALYSIS OF BIOACTIVE PHYTOCHEMICAL COMPOUNDS IN *PADINA BOERGESENII* ALLENDER & KRAFT

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ABSTRACT

The work was to characterize the bioactive constituents present in three extracts such as ethanol, ethyl acetate and chloroform using GCMS analysis. The compounds recorded were carbohydrate, protein, saponins, alkaloids, and flavanoids, terpenoids, phenols, fatty acids. The identification of different biologically active compounds in these three solvents were made by correlating their peak areas and the retention times with literation and interpretation made by mean of mass spectra. The ethanol extracts showed the presence of a greater number of compounds.

Key words: Bioactivity, Gas chromatography, Ethanol extracts, *Padina boergesenii*

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INTRODUCTION

Seaweeds are considered as an attractive avenue for the screening of biologically active compounds (Ahmed *et al*., 2014; Mohamed *et al*., 2012). It contains diverse phenolic compounds such as flavonoids, phenolic acid, tannins (Grassman *et al*., 2004). These compounds were found to show antibacterial, antifungal, antiviral and antioxidant effects (Faulkner, 2002; Schwartsmann *et al*., 2000; Mayer *et al*., 2007; Zhang *et al*., 2010).

In the previous studies *P. boergesenii* showed the presence of valuable source of bioactive compounds (Kalasariya *et al*., 2023). *P. boergesenii* control urinary risk factors of stones and found to have hypoglycemic effects, it also found to show antibacterial and antioxidant activity, anti-inflammatory, cytotoxic activities (Prieto *et al*., 1999) So the importance of this seaweed is vital, as there is increasing demand for natural therapeutic drugs (Holdt and Kraan, 2011). GC - MS is one of the best fast and accurate techniques to detect various compounds that includes alkaloids, nitro compounds, long chain hydrocarbons, organic acids, steroids, esters and amino acids. (Razack *et al*., 2015). Very few studies were carried out in this plant extract. Hence the present study was designed to detect the phytochemical compounds from *Padina boergesenii* by GC-MS analysis which is collected from Kovalam, Kanniyakumari district.

MATERIALS AND METHODS

Preparation of Seaweed Powder

The collected seaweed samples were washed thoroughly to remove all the attached debris, epiphytes, sediments, sand and salt particles. water followed the sample were shade dried grounded to fine powder using an electric mixer. The fined powdered samples were then stored in an airtight container in the refrigerator at 4°C for further use. Preparation of seaweed extracts was done by following the method of (Abdelrheem *et al*., 2020).

Identification of Phytocompounds using GC-MS Analysis

GC-MS analysis of the extracts was carried out by the following method of Hema *et al*., (2010) using a GC- MS Clarus 500 Perkin Elmer system and gas chromatography interfaced to mass spectrometer The detection employed with the NIST (National Institute of Standards and Technology). 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 Phytocompounds was done using the database of National Institute of Standard and Technology (NIST). The mass spectrum of the unknown compounds was compared with the spectrum of the known compounds stored in the NIST Library (Version, 2005),

RESULTS AND DISCUSSION

The chemical constituents of different extracts were characterised by GC-MS analysis (Table 1) The GC -MS chromatogram of ethanol, ethyl acetate and chloroform plant extracts of *Padina boergesenii* Allender & Kraft recorded a total of 27 peaks corresponding to the bioactive compounds that were recognized by relating their peak retention time, peak area (%), height (%) and mass spectral fragmentation patterns to that of the known compounds described by the National Institute of Standards and Technology (NIST) library.

The ethanol extract showed the presence of broad range of compounds such as 1-(4-Methoxy-phenyl)-5,5-dioxo-hexahydro-5.lambda.(6)-thieno[3,4-b]pyrrol-2-one (R.T.17.194), Isothiocyanic acid, (p-phenylazo)phenyl ester (R.T. 15.213), trans-3-Ethoxy-b-methyl-b-nitrostyrene (R.T.15.109), Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl (R.T. 15.033), 2-(Acetoxymethyl)-3-(methoxycarbonyl) biphenylene (R.T. 14.527), 1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isopropyl ester (R.T. 14.867), 9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester (R.T. 13.586), 3,5-Dimethylbenzaldehyde thiocarbamoylhydrazone (R.T. 13.458), Octasiloxane, 1,1,3,3,5,5,7,7,9,9, 11,11,13,13,15,15-hexadecamethyl (R.T. 13.416), 2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4a.alpha.,7.beta.,8a.beta.)- (R.T. 13.112), 8-Bromooctanoic acid, ethyl ester (R.T. 11.972), n-Hexadecanoic acid (R.T. 11.720). 7-Octadecyne, 2-methyl- (R.T. 10.880), Cyclohexane, 1-methyl-4-(1-methylethenyl)-, trans (R.T. 10.443). The maximum peak was found to be 17.194 which is a phenolic compound. The other compounds identified were terpenoids, fatty acids and indole derivatives.

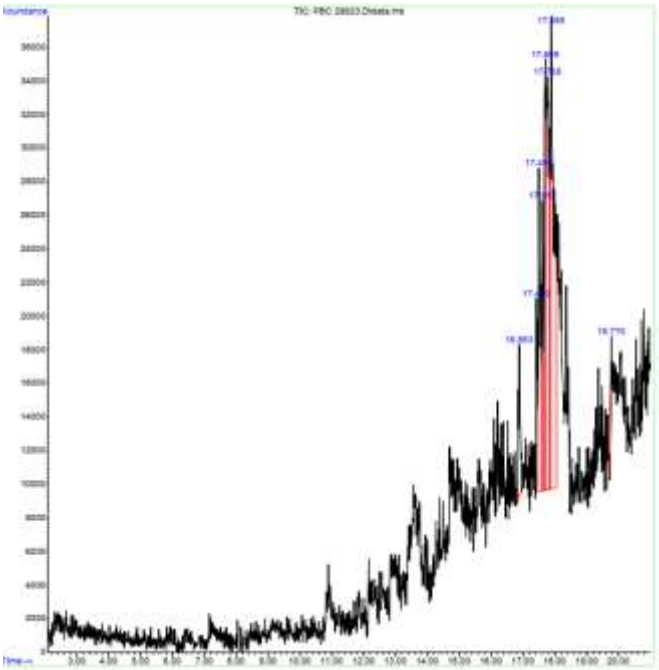
Table 1 Active phytocompounds Identified in the ethanol extracts GCMS analysis by *Padina boergesenii* Allender & Kraft

Peak No	Name of the compounds	Retention Time (Min.)	Peak Area %	Molecular Formula	Molecular Weight (m/Z) (g/mol)
1	Cyclohexane, 1-methyl-4-(1-methylethenyl)-, trans	10.443	6.50	$C_{10}H_{18}$	138.2499
2	7-Octadecyne, 2-methyl-	10.880	3.88	$C_{19}H_{36}$	264.5
3	n-Hexadecanoic acid	11.720	38.54	$C_{16}H_{32}O_2$	256.4241
4	8-Bromooctanoic acid, ethyl ester	11.972	8.42	$C_{10}H_{19}BrO_2$	251.16
5	2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4a.alpha.,7.beta.,8a.beta.)-	13.112	7.29	$C_{14}H_{24}O$	208.34
6	Octasiloxane, 1,1,3,3,5,5,7,7,9,911,11,13,13,15,15-hexadecamethyl	13.416	7.43	$C_{16}H_{48}O_7Si_8$	577.2
7	3,5-Dimethylbenzaldehyde thiocarbamoylhydrazone	13.458	3.34	$C_{10}H_{13}N_3S$	207.30
8	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	13.586	4.07	$C_{21}H_{40}O_4$	356.54
9	2-(Acetoxymethyl)-3-(methoxycarbonyl)biphenylene	14.527	1.22	$C_{17}H_{14}O_4$	282.29
10	1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isopropyl ester	14.867	2.59	$C_{21}H_{25}$	355.43
11	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl	15.033	6.63	$C_{14}H_{42}O_6Si_7$	503.07
12	trans-3-Ethoxy-b-methyl-b-nitrostyrene	15.109	2.19	$C_{11}H_{13}NO_3$	207.23
13	Isothiocyanic acid, (p-phenylazo)phenyl ester	15.213	2.32	$C_{13}H_9N_3S$	239.296
14	1-(4-Methoxy-phenyl)-5,5-dioxo-hexahydro-5.lambda.(6)-thieno[3,4-b]pyrrol-2-one	17.194	5.58	$C_{13}H_{15}NO_4S$	281.072

The chloroform extracts of seaweeds indicated the presence of various types of phytocompounds namely tert-Butyl 2-aminophenylcarbamate ditms (R.T. 19.770), 1-(4-Methoxy-phenyl)-5,5-dioxo-hexahydro-5.lambda.(6)-thieno[3,4-b]pyrrol-2-one (R.T. 17.885), Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl- (R.T. 7.768), Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl- (R.T. 17.698). Cyclohexa-2,5-diene-1,4-dione, 2-methyl-5-(4-morpholinyl)- (R.T. 17.612), Purine-2,6-dione, 8-(3-ethoxypropylamino)-1,3-dimethyl-3,9-dihydro- (R.T. 17.498), 4-(3-Hydroxy-2,6,6-trimethylcyclohex-1-enyl)pent-3-en-2-one (R.T. 17.420), 2-Hydroxychalcone (R.T. 16.883). The identified compounds were flavonoids, phenols and fatty acids

Table 2 Active phytocompounds Identified in the chloroform extracts GCMS analysis by *Padina boergesenii* Allender & Kraft

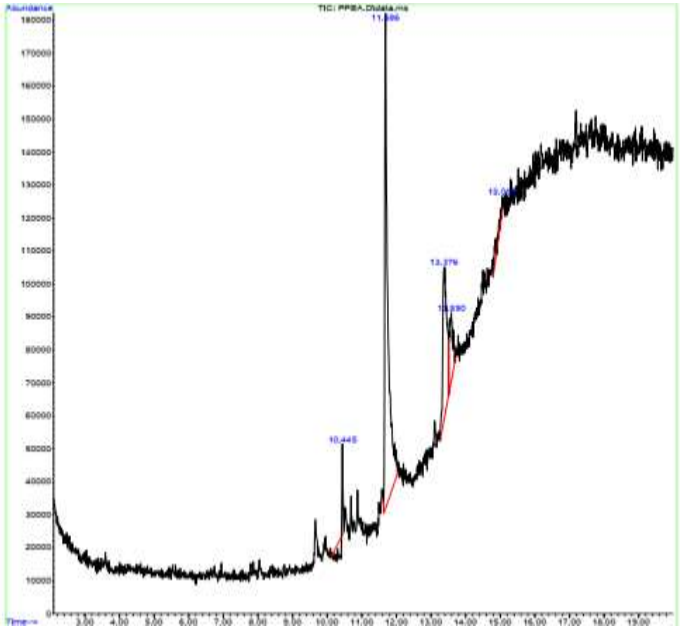
Peak No	Name of the compounds	Retention Time (Min.)	Peak Area %	Molecular Formula	Molecular Weight (m/Z) (g/mol)
1	2-Hydroxychalcone	16.883	5.18	$C_{15}H_{12}O_2$	224.25
2	4-(3-Hydroxy-2,6,6-trimethylcyclohex-1-enyl)pent-3-en-2-one	17.420	4.94	$C_{14}H_{22}O_2$	222.32
3	Purine-2,6-dione, 8-(3-ethoxypropylamino)-1,3-dimethyl-3,9-dihydro-	17.498	11.14	$C_{15}H_{13}N_5O_4$	327.29
4	Cyclohexa-2,5-diene-1,4-dione, 2-methyl-5-(4-morpholinyl)-	17.612	7.51	$C_{11}H_{13}NO_3$	207.23
5	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	17.698	13.26	$C_{14}H_{42}O_6Si_7$	503.07
6	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	17.768	22.94	$C_{16}H_{48}O_7Si_8$	577.2
7	1-(4-Methoxy-phenyl)-5,5-dioxo-hexahydro-5.lambda.(6)-thieno[3,4-b]pyrrol-2-one	17.885	33.88	$C_{13}H_{15}NO_4S$	281.072
8	tert-Butyl 2-aminophenylcarbamate ditms	19.770	1.15	$C_{17}H_{32}N_2O_2Si_2$	208.26



The ethyl acetate extracts of seaweeds indicated the presence of various phytocompounds namely 1,4-Bis(trimethylsilyl)benzene (R.T. 15.057), Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl (R.T. 13.590), 9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester (R.T. 13.376), n-Hexadecanoic acid (R.T. 11.686), 1,4-Eicosadiene (R.T. 10.445). The total number of compounds recorded was 5. The highest peak was found to be 15.057 which is an organosilicon compound. Other compounds detected were terpenoids, fatty acids etc.

Table 3 Active phytocompounds Identified in the ethyl acetate extracts GCMS analysis by *Padina boergesenii* Allender & Kraft

Peak No	Name of the compounds	Retention Time (Min.)	Peak Area %	Molecular Formula	Molecular Waight (m/Z) (g/mol)
1	1,4-Eicosadiene	10.445	0.03	$C_{20}H_{38}$	278.5
2	n-Hexadecanoic acid	11.686	62.65	$C_{16}H_{32}O_2$	256.4241
3	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	13.376	24.72	$C_{21}H_{40}O_4$	356.54
4	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl	13.590	10.36	$C_{16}H_{48}O_7Si_8$	577.2
5	1,4-Bis(trimethylsilyl)benzene	15.057	2.24	$C_{12}H_{22}Si_2$	222.47



In all the three extracts Terpenoids, Flavonoids, fatty acid, phenols, Heterocyclic Organic compound and Indole derivative,

The fatty acids present in marine seaweed extracts play an important role in the formation of many other bioactive secondary metabolites since some fatty acids have been shown to possess antibacterial activities (Barbosa *et al*., 2007; Oh *et al*., 2008). Marine seaweeds exhibit a high level of fatty acids compounds which show potential bioactivity (Manilal *et al*., 2010).

Presence of phenols, flavonoids, terpenoids, sterols etc. are reported to have antimicrobial (Zbakh *et al*., 2012), anti-inflammatory (Jaswir and Monsur, 2011), antiviral (Bouhlal *et al*., 2011), antioxidant (Devi *et al*., 2011), anticancer activities (Kim *et al*., 2011). Hence the presence study showed that all the plant extracts possess phytochemical compounds and the use of these plant extract might help in the preparation of novel medicine.

CONCLUSION

The present data offers great insight with the latest report of the biological activity of *P. boergesenii*. Various bioactive compounds present in *P. boergesenii* was naturally identified as a potential source of many bioactive compounds. From the result, we suggest that *P. boergesenii* could be effectively beneficial to pharmaceutical and therapeutic applications.

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