

## GC-MS Assisted Phytoactive Chemical Compounds Identification and Profiling with Mineral Constituents from Biologically Active Extracts of *Aerva javanica* (Burm. f) Juss. ex Schult.

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### Abstract

*Aerva javanica* (Burm. f) Juss. ex Schult. (Family: Amaranthaceae) family is one of the traditional medicinal plant growing in the United Arab Emirates. Apart from studies related to some medicinal properties, phytochemical, GC MS compound characterization and biological activities still to be investigated. An experiment was conducted to determine the possible bioactive components with their chemical structures and elucidation of phytochemicals from the aerial parts of the plant. The macro and micro-mineral constituents and antioxidant activities were also evaluated. Aerial parts of *A. javanica* were extracted sequentially with hexane, chloroform, ethyl acetate, acetone, methanol by cold percolation method. Free radical scavenging and antioxidant properties of methanolic extract were evaluated by using *in vitro* antioxidant assays such as hydroxyl radical scavenging activity, 1,1-diphenyl-2-picrylhydrazyl (DPPH) radicals, superoxide radical scavenging activity and ABTS radical scavenging activity. Primary phytochemical and micro-macro element was tested using standard protocol. The chemical characterization was done with the help of Gas Chromatography-Mass Spectrometry (GC-MS), and the mass spectra of the total compounds in the extract were matched with the National Institute of Standard and Technology (NIST) library. Mineral constituents were identified and estimated by ICP-OES. Ninety-nine metabolites were obtained by GC-MS analysis; indole was found to be major components followed by 2-Chlorallyl diethylthiocarbamate (CDEC), Carbaril, Bis(2-ethylhexyl) phthalate, Quinoline, 4H-Cyclopenta[def]phenanthrene, 2-[Bis(2-chloroethylamino)]-tetrahydro-2H-1,3,2-oxazaphosphorine-2-oxide, Phenobarbital, 1H-Indole, 2-methyl-, 2,3,7,8-Tetrachlorodibenzo-p-dioxin Disulfide, diphenyl. The presence of various bioactive compounds in the extract validates the traditional medicinal uses of this plant.

**Keywords:** *Aerva javanica*; antioxidant; GC-MS; piperidine; Phenobarbital; phytochemical

### Introduction

Day by day new drugs are being developed from different plant species. Highly significant anticancer drugs and different antimicrobial agents are the need of the day. The potential of herbal agents should be analyzed for their candidature in treatment of various ailments (Malongane *et al.*, 2017). With the all the benefits of modern synthetic

medicine, still people prefer plant based natural medicines due to the side effects of synthetic medicines (de Oliveira *et al.*, 2017). Plants deliver dynamic molecule, develop at different degrees in many nations of the world, and are the premise of nearby traditional herbal medicine and drug in their particular societies (Teschke and Zhang, 2015). The synthetic additives and antioxidants are widely used in the current industries and health systems. In modern times, there are many food antioxidant substances and are

harmless if used in minor quantities but in large quantities they have risks to human health like skin rashes and itching, and many other ailments (Lidon and Silva, 2016).

In the search for new compounds, and also for quality control, the suitable methods of screening are very important (Keskes *et al.*, 2017). The selection of accurate medicinal plants, the extract screening within vitro methods for estimation of its biological activities will lead to the discovery of potentially useful compounds (Mathekaga and Meyer, 1998). In traditional medical systems, almost all the plants used may contain potential substances which are responsible for their biological activities and can be utilized for various diseases (Duraipandiyar *et al.*, 2006). History reveals that plants are sources of successful drugs, and will continuously be important for screening of new lead compounds (Atanasov *et al.*, 2015).

*Aerva javanica* (Burm. f) Juss. ex Schult. is one among the important plants in Amaranthaceae family. This plant is widely seen many countries (Judd *et al.*, 2008). Many phytochemical compounds have been isolated from this plant (Emam, 1999). *A. javanica* has been widely used for many diseases in traditional and modern medical systems (Deshmukh *et al.*, 2008). There are various reports stating the medicinal properties of *A. javanica* like antioxidant, antiviral, antiparasitic, antibacterial (Baltina *et al.*, 2003; Al-Fatimi *et al.*, 2007; El-Hadi *et al.*, 2010; Singh *et al.*, 2010; Srinivas and Reddy, 2012). There are traditional uses for this plant (Samejo *et al.*, 2012). The leaves of plant are used for fodder to goats and whole plant is used as a fuel. The whole *A. javanica* plant is used for the purpose of chest pain, ascariis and diarrhea with blood (Teklehaymanot and Giday, 2010).

In this study, there was analyzed the metabolic profile of *A. javanica* using gas chromatography-mass spectrometry (GC-MS) with their chemical structures and elucidation of phytochemicals from the aerial parts of the plant. The macro and micro-mineral constituents and antioxidant activities were also evaluated.

## Materials and Methods

### Plant material

Samples of *Aerva javanica* (Burm. f) Juss. ex Schult. were collected from the Emirate of Abu Dhabi (UAE). The plant material collects in all collection site was authorized by the Department of Biology (College of Science, UAE University). The field studies did not involve endangered or protected species.

### Preparation of plant extracts

The coarsely powdered the aerial parts of *A. javanica* were extracted sequentially with hexane, chloroform, ethyl acetate, acetone, methanol by cold percolation method. All the organic extract extracts were filtered using rotary evaporator. The residues were dissolved in Dimethyl Sulfoxide (DMSO) and these crude extracts were subjected to *in-vitro* assays. Different organic extract of samples for metabolomics analysis.

### Antioxidant activity of extracts

ABTS<sup>•+</sup> radical (Wolfenden and Willson 1982) DPPH<sup>•</sup> assay (Brand-Williams *et al.*, 1995), Superoxide anion scavenging activity (Nishimiki *et al.*, 1972) and hydroxyl radical scavenging activity (Halliwell, 1982) were determined from the extracts.

### Phytochemical screening test for the extracts

The dried extracts were subjected to the preliminary phytochemical screening by using Harbourne (Harborne, 1998) methods to test for alkaloids, flavonoids, tannins, terpenoids, steroids, saponins, protein, cardiac glycosides and anthraquinones.

### Microelements and macroelements

Samples were prepared as explained previously (Ameri *et al.*, 2014). The percentages of each element in this sample was determined by plotting the absorbance of each element versus the element concentration by using standard AR grade solutions of the elements, for example K, Mg, Ca, Na, Fe, Mn, Zn, P and S. The elemental analysis was done for aerial parts of the plant species (ICP-OES - Agilent Technologies, 710).

### Sample preparation for GCMS

Different solvents (methanol, acetone, ethyl acetate, chloroform and Hexane) separately received and stored at -20 °C for further use. For GCMS, each extract was prepared separately by dissolving 1 mg of each extract dissolved in 1ml of fresh HPLC grade solvent and, vortexes for 2 min and the extract was filtered by 0.2 µl filter. The 25 ng/µl concentration each extract made with HPLC grade solvents was added 1 ml of extract in respective GC tube for analysis. Methanol, acetone and chloroform samples were completely dried using Nitrogen gas. Sample was derivatised using 30 µl pyridine and 60µl of BSTFA: TMCS (99:1) and incubated at 60 °C for 60 min. Derivatised samples were subjected 1 µLin to GC-MS (Lisec *et al.*, 2006).

### GC-MS analysis

GC-MS measurements were performed with a Shimadzu instrument equipped with GC: Aligent 7890 A, MS: MS detector 5975C, Ionization for MS: Electron Impact Ionization, Mass Analyzer: Single Quadrupole, Software: Data Analysis, AMDS, Library: NIST 2011, column: DP 5 ms, Dimensions: 30 m L X 0.25 mm ID × 0.25 µm film thickness, initial temperature is 240 °C 2 min hold time, ram temperature is 50 °C to 280 °C 5 min is the hold time, total time is 40 min, carrier gas is helium, flow (13 ml/min) is 1.0, split flow: 1.5 ml/min, injection volume: 1µl, Scan mass range: 30 m/z-600 m/z and polarity + ve. GC-MS performed based on the database having more than many patterns. The spectrum of the unknown compound was compared with the spectrum of the known compounds in library.

### Data analysis

Raw GC-MS data were analysed as explained by Jin *et al.* (2016) and following the method of Jumtee *et al.* (2009).

## Results and Discussion

### Antioxidant assays of methanolic extract

The extracts showed significant antioxidant potential when compared to standard gallic acid (Table 1). In ABTS+ scavenging activity the values are varied significantly ( $P < 0.05$ ) and ranged from 10 to 160  $\mu\text{g}$  GAE/g extract. The hydrogen-donating ability is revealed by this assay. The antioxidant activity was almost comparable directly to the standard gallic acid (IC50 value 7.94  $\mu\text{g}/\text{mL}$ ) (Table 1). Gallic acid was used as reference standard in DPPH method. In comparison with gallic acid, the methanolic extracts of *A. javanica* showed high scavenging activity *in vitro* (Table 1).

*javanica* was 39.1-76.4% and that of the standard gallica was 37.2-58.3%. The methanolic extract of *A. javanica* exhibited concentration-dependent radical scavenging activity, that is, percentage inhibition increased with sample concentration (Table 1).

### Phytochemical screening of methanolic extract

Phytochemical screening for the methanolic extracts of *A. javanica* reveals the active phytochemical constituents of the plant under study in which flavonoids, tannins, alkaloids, steroids, protein, terpenoid, phenols, cardiac glycosides were present. However, the extract tested showed the absence of saponin and anthraquinones (Table 2).

Table 1. *In vitro* free radical scavenging activities of methanolic extract from *Aerva javanica*

Concentration ( $\mu\text{g}/\text{ml}$ )	Inhibitory activity (%)							
	Hydroxyl radical scavenging activity		Superoxide radical scavenging activity		DPPH radical scavenging activity		ABTS radical scavenging activity	
	<i>Gallic acid</i> (GAE)	<i>A. javanica</i>	<i>Gallic acid</i> (GAE)	<i>A. javanica</i>	<i>Gallic acid</i> (GAE)	<i>A. javanica</i>	<i>Gallic acid</i> (GAE)	<i>A. javanica</i>
10	41.0 $\pm$ 2.8	27.3 $\pm$ 1.4	37.2 $\pm$ 1.6	39.1 $\pm$ 1.2	38.2 $\pm$ 2.8	46.2 $\pm$ 1.1	36.5 $\pm$ 2.8	52.3 $\pm$ 2.3
20	42.3 $\pm$ 1.3	36.2 $\pm$ 2.1	50.4 $\pm$ 1.8	44.6 $\pm$ 1.7	43.1 $\pm$ 1.4	57.5 $\pm$ 2.6	40.4 $\pm$ 1.9	55.2 $\pm$ 2.0
40	48.9 $\pm$ 1.5	46.1 $\pm$ 1.6	53.1 $\pm$ 2.9	59.4 $\pm$ 2.5	56.2 $\pm$ 2.9	65.8 $\pm$ 3.3	43.9 $\pm$ 3.4	66.6 $\pm$ 1.9
80	51.0 $\pm$ 2.4	56.4 $\pm$ 2.9	55.3 $\pm$ 1.2	65.2 $\pm$ 3.6	62.4 $\pm$ 1.6	74.1 $\pm$ 2.8	48.0 $\pm$ 2.5	68.2 $\pm$ 1.2
160	54.0 $\pm$ 3.2	62.1 $\pm$ 2.4	58.3 $\pm$ 3.2	76.4 $\pm$ 3.3	67.5 $\pm$ 2.1	83.1 $\pm$ 1.6	60.3 $\pm$ 3.2	78.5 $\pm$ 2.5
IC50	36.8 $\pm$ 1.1	35.5 $\pm$ 1.4	33.96 $\pm$ 1.1	28.96 $\pm$ 0.5	31.25 $\pm$ 0.8	25.69 $\pm$ 1.4	7.94 $\pm$ 0.1	5.35 $\pm$ 0.3

Data represented as means  $\pm$  SD (n = 5).

Both *A. javanica* and GAE showed significant inhibitory activity in a concentration-dependent manner to inhibit hydroxyl-radical-mediated deoxyribose damage was assessed at a concentration of 10-160  $\mu\text{g}/\text{mL}$ . In the present investigation, the hydroxyl radical scavenging activity observed was in the range of 27.3-62.1% at the concentration of 160  $\mu\text{g}/\text{ml}$ . While scavenging hydroxyl radical, the ability of methanol extract (62.1%) was found to be higher than reference standard gallic acid (54.0%) (Table 1). Superoxide radical reduced NBT to a blue-colored formation that was measured at 560 nm. At 10-160  $\mu\text{g}$ , the superoxide scavenging activity of methanolic extract of *A.*

### Mineral compositions

Nutritional composition of the aerial plant parts of *A. javanica* was presented in Table 3. Ca, Cr, Cu, K, Mg, Mn, Ni, P, S and Zn were presented in appreciable quantities. Low concentrations of Cd, Co, Fe, N, and Pb were observed in the methanolic extract of *A. javanica*.

Table 2. Preliminary phytochemical constituents of *Aerva javanica* plants

Constituent	Concentration
Flavonoid	++
Tannin	+
Alkaloid	+
Steroids	+
Protein	+
Terpenoids	+
Saponin	-
Phenols	++
Cardiac glycoside	+

Legend:

+ = Low concentration;

++ = Moderate concentration;

+++ = High concentration;

- = Absent.

Table 3. Mineral composition of *Aerva javanica* plants (mg/kg (ppm))

Mineral composition	Content (mg/kg (ppm))
Ca	17.34
Cd	<0.001
Co	0.58
Cr	5.2
Cu	3.29
Fe	0.38
K	11.58
Mg	10.7
Mn	23.3
Ni	6.57
Na	0.83
Pb	<0.011
P	1.64
S	2.6
Zn	15.6

Table 4. Biologically active chemical compounds of hexane extract of the aerial parts of *A. javanica*

No	CAS	RT (min)	Name of the compound	Molecular formula	Molecular weight	Peak area (%)
1	591-78-6	4.3073	2-Hexanone	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> COCH <sub>3</sub>	100.16	0.39
2	1678-91-7	5.1103	Cyclohexane, ethyl- - incomplete name		112.21	1.00
3	110-89-4	5.4264	Piperidine	C <sub>5</sub> H <sub>11</sub> N	85.15	3.60
4	95-47-6	6.1992	o-Xylene	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	106.17	2.50
5	98-82-8	6.8798	Benzene, (1-methylethyl)- - incomplete name	C <sub>6</sub> H <sub>5</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	120.19	8.50
6	103-65-1	7.5958	Benzene, propyl- - incomplete name	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	120.19	4.70
7	611-14-3	7.7825	Benzene, 1-ethyl-2-methyl- - incomplete name	C <sub>9</sub> H <sub>12</sub>	120.19	3.30
8	108-67-8	8.6278	Benzene, 1,3,5-trimethyl- - incomplete name	C <sub>6</sub> H <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub>	120.19	5.70
9	629-50-5	8.7567	Tridecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>11</sub> CH <sub>3</sub>	184.36	5.70
10	124-18-5	8.7635	Decane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> CH <sub>3</sub>	142.28	0.01

#### GC-MS Analysis of different solvents extract

From five batches of approximately 1 kg of air dried powdered leaves, mean percentage yields of 4.78% of n-hexane extract, 5.12% of chloroform ethyl acetate extract, 3.52% of Ethyl acetate, 2.74 % of acetone extract and 8.47% of methanol extract were obtained. Methanol extract gave the highest percentage yield. Most of the constituents were polar in nature.

There are many unknown compounds in the polar extracts from the plant material of *A. javanica*. Comprehensive coverage showed similar discrimination as when using the 155 known and putative metabolites and solely the 99 identified features.

It is for the first time that the composition of the five extracts of the aerial parts of *A. javanica* has been investigated through GC / MS analysis. The mass spectra were compared with those of the known compounds stored in the National Institute of Standards and Technology (NIST) research library. The bioactive compounds present in n-hexane, chloroform, ethyl acetate, acetone and methanol extracts obtained from *A. javanica* aerial parts are shown in Tables 1-5. The prevailing compounds were 2-Chloroallyl diethylthiocarbamate (CDEC), Carbaril, Bis(2-ethylhexyl) phthalate, Quinoline, 4H-Cyclopenta[def]phenanthrene, 2-[Bis(2-chloroethylamino)]-tetrahydro-2H-1,3,2-oxazaphosphorine-2-oxide, Phenobarbital, 1H-Indole, 2-methyl-, 2,3,7,8-Tetrachlorodibenzo-p-dioxin, Disulfide, diphenyl.

As whole Hexane extract of the aerial parts of *A. javanica* was found to be rich in benzene metabolites. On comparison of the mass spectra of the constituents with the NIST library, the ten phytochemicals were characterized and identified (Table 4). The results revealed that Piperidine was found as the one major component in the hexane extract and the nine minor components are Tridecane, o-Xylene, 2-Hexanone and other benzene derivatives were also present.

The chloroform extract of *A. javanica* pertaining to the GC-MS analysis were given in Table 5. Thirty-eight compounds were detected in the chloroform extract of the

aerial parts of *A. javanica* and Piperidine, Carbaril, Bis(2-ethylhexyl) phthalate, Quinoline were found to be the major compounds followed by Dimethyl phthalate, Propanedinitrile, 5-Fluorouracil, 1,3-Dioxolane, Eicosane and various benzene and propenoic acid were also identified.

The ethyl acetate extracts showed twenty chemical compounds in the GC MS analysis (Table 6) which were detected according to their retention time on fused silica capillary column. These compounds mainly comprised of o-Xylene, Dimethyl sulfon, Undecane, Pentadecane was identified as a major chemical constituent followed by Propanoic acid, Ethylbenzene Tridecane, Dibutyl phthalate etc.

The most polar methanol extract of the aerial parts of *A. javanica* led to the identification of nineteen chemical compounds by GC MS analysis (Table 7). 1H-Indole, 2-methyl-, CDEC, 2,3,7,8-Tetrachlorodibenzo-p-dioxin, Disulfide, diphenyl and Benzothiazole, 2-methyl- were identified as the main chemical constituents followed fourteen minor components are Naphthalene, 1,2-dimethyl, Thiotepa, Sulfur tetrafluoride-2-Imidazolidinethione and other benzene derivatives were also identified.

The acetone ether crude extract of the aerial parts of *A. javanica* were analysed by GC-MS which leads to the identification of 17 organic compounds. The chemical compounds were identified according to their retention time on a fused silica capillary column. The list of the compounds with their retention time, molecular formula, molecular weight, area and area (%) were presented in Table 8. The identified major compounds are 4H-Cyclopenta[def]phenanthrene, CDEC, 2-[Bis(2-chloroethylamino)]-tetrahydro-2H-1,3,2-oxazaphosphorine-2-oxide, Phenobarbital along with other minor constituents were also present.

The antioxidant properties of this plant extracts can be attributed to the presence of different phytochemicals. In this context, the presence of phytochemicals such as alkaloids, flavonoids, tannins, steroids, terpenoids, reducing sugar, saponins and glycosides are to be mentioned, as they

have a prominent role in plant antioxidant responses (Robert and Lin, 1994). The presence of flavonoid itself function acts as scavenger of free radicals by rapid donation of a hydrogen atom affording a phenoxy radical intermediate that is relatively stable (Bors *et al.*, 1990). Similar antioxidant actions and phytochemicals were reported previously from *A. lanata* (Yamunadevi *et al.*, 2001; Kumar *et al.*, 2013). Crude extracts of different parts of *A. javanica* made with hexane, chloroform and methanol showed the presence of phytochemicals (Srinivas and Reddy, 2012).

Different extracts were obtained from the aerial parts of *A. javanica* through selective sequential extraction with solvents of increasing polarity, namely, n-hexane, chloroform, ethyl acetate, acetone and methanol. GC-MS analysis of the n-hexane, ethyl acetate and methanol extracts revealed the presence of various bioactive compounds.

The major compound of Piperidine is present both in Hexane and chloroform extracts but in different quantities. In addition, Phenobarbital is present both acetone and the polar methanol extract. Piperidine are significant as they are

Table 5. Biologically active chemical compounds of chloroform extract of the aerial parts of *A. javanica*

No	CAS	RT (min)	Name of the compound	Molecular formula	Molecular weigh	Peak area (%)
1.	110-86-1	4.0984	Pyridine	C <sub>5</sub> H <sub>5</sub> N	79.10	0.01
2.	106-46-7	4.2902	Benzene, 1,4-dichloro- - incomplete name	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.002	9.40
3.	107-20-0	5.3032	Acetaldehyde, chloro- - incomplete name	C <sub>2</sub> H <sub>3</sub> ClO	78.498	0.00
4.	131-11-3	5.3148	Dimethyl phthalate	C <sub>6</sub> H <sub>4</sub> -1,2-(CO <sub>2</sub> CH <sub>3</sub> )	194.18	0.27
5.	556-64-9	5.3148	Thiocyanic acid, methyl ester	C <sub>2</sub> H <sub>3</sub> NS	73.12	0.01
6.	109-77-3	8.1947	Propanedinitrile	CH <sub>2</sub> (CN) <sub>2</sub>	66.06	16.00
7.	83-34-1	8.557	1H-Indole, 3-methyl- - incomplete name	C <sub>9</sub> H <sub>9</sub> N	131.17	0.07
8.	51-21-8	8.5577	5-Fluorouracil	C <sub>4</sub> H <sub>3</sub> FN <sub>2</sub> O <sub>2</sub>	130.08	0.09
9.	56-04-2	8.5832	Myethylthiouracil	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> OS	142.18	2.60
10.	2097-19-0	8.6349	2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane, 1-phenyl- - incomplete name	C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub> Si	251.35	0.01
11.	4170-30-3	8.6454	2-Butenal	C <sub>4</sub> H <sub>6</sub> O	70.09	0.11
12.	61-82-5	8.8386	3-Amino-s-triazole	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub>	84.08	11.00
13.	2437-56-1	8.8716	1-Tridecene	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> CH=CH <sub>2</sub>	182.35	0.68
14.	104-76-7	8.8754	1-Hexanol, 2-ethyl- - incomplete name	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH <sub>2</sub> OH	130.23	0.62
15.	141-79-7	8.9026	3-Penten-2-one, 4-methyl- - incomplete name	C <sub>6</sub> H <sub>10</sub> O	98.15	4.80
16.	98-00-0	9.1111	2-Furanmethanol	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	98.09	6.20
17.	203-64-5	9.1431	4H-Cyclopenta[def]phenanthrene	C <sub>15</sub> H <sub>10</sub>	190.24	5.50
18.	123-38-6	9.1699	Propanal	CH <sub>3</sub> CH <sub>2</sub> CHO	58.08	3.10
19.	767-59-9	9.2468	1H-Indene, 1-methyl-	C <sub>10</sub> H <sub>10</sub>	130.19	6.90
20.	2682-20-4	9.4785	3(2H)-Isothiazolone, 2-methyl- - incomplete name	C <sub>4</sub> H <sub>5</sub> NOS	115.15	0.04
21.	624-83-9	9.7424	Methane, isocyanato-	C <sub>2</sub> H <sub>3</sub> NO	57.05	2.60
22.	78-93-3	9.9186	2-Butanone	C <sub>2</sub> H <sub>3</sub> COCH <sub>3</sub>	72.11	0.04
23.	621-82-9	9.973	2-Propenoic acid, 3-phenyl- - incomplete name	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	148.16	0.66
24.	121-44-8	10.0356	Triethylamine	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	101.19	7.20
25.	259-79-0	12.7068	Biphenylene	C <sub>12</sub> H <sub>8</sub>	152.19	1.80
26.	606-20-2	13.1986	Benzene, 2-methyl-1,3-dinitro- - incomplete name	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	182.13	1.70
27.	63-25-2	13.7694	Carbaril	C <sub>10</sub> H <sub>7</sub> OCONHCH <sub>3</sub>	201.22	20.00
28.	135-19-3	13.7694	2-Naphthalenol	C <sub>10</sub> H <sub>7</sub> OH	144.17	20.00
29.	646-06-0	14.9272	1,3-Dioxolane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.08	0.64
30.	883-20-5	15.5789	Phenanthrene, 9-methyl- - incomplete name	C <sub>15</sub> H <sub>12</sub>	192.26	10.00
31.	91-08-7	16.1419	Benzene, 1,3-diisocyanato-2-methyl- - incomplete name	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	174.16	25.00
32.	1910-42-5	20.7712	Paraquat dichloride	C <sub>12</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> · xH <sub>2</sub> O	257.16	7.70
33.	91-20-3	20.7712	Naphthalene	C <sub>10</sub> H <sub>8</sub>	128.17	36.00
34.	1490-04-6	29.6864	Menthol	C <sub>10</sub> H <sub>16</sub> O	160.29	33.00
35.	629-59-4	35.1042	Tetradecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>12</sub> CH <sub>3</sub>	198.39	20.00
36.	91-59-8	36.0457	2-Naphthalenamine	C <sub>10</sub> H <sub>7</sub> NH <sub>2</sub>	143.19	9.50
37.	117-81-7	41.8833	Bis(2-ethylhexyl) phthalate	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	390.56	1.30
38.	91-22-5	42.2789	Quinoline	C <sub>8</sub> H <sub>7</sub> N	129.16	12.00

Table 6. Biologically active chemical compounds of ethyl acetate extract of the aerial parts of *A. javanica*

No	CAS	RT (min)	Name of the compound	Molecular formula	Molecular weigh	Peak area (%)
1.	67-66-3	4.2399	Trichloromethane	CHCl <sub>3</sub>	119.38	0.00
2.	64-19-7	4.2658	Acetic acid	CH <sub>3</sub> CO <sub>2</sub> H	60.05	0.00
3.	71-43-2	4.2964	Benzene	C <sub>6</sub> H <sub>6</sub>	78.11	0.61
4.	79-09-4	4.3716	Propanoic acid	CH <sub>3</sub> CH <sub>2</sub> COOH	74.08	0.84
5.	108-24-7	4.4855	Acetic anhydride	(CH <sub>3</sub> CO) <sub>2</sub> O	102.09	0.26
6.	103-81-1	4.892	Benzeneacetamide	C <sub>8</sub> H <sub>9</sub> NO	135.16	0.13
7.	100-41-4	6.1151	Ethylbenzene	C <sub>8</sub> H <sub>5</sub> C <sub>2</sub> H <sub>5</sub>	106.17	3.00
8.	108-38-3	6.1151	Benzene, 1,3-dimethyl- - incomplete name	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	106.17	3.00
9.	95-47-6	6.2631	o-Xylene	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	106.17	4.10
10.	67-71-0	6.972	Dimethyl sulfone	(CH <sub>3</sub> ) <sub>2</sub> SO <sub>2</sub>	94.13	3.60
11.	1120-21-4	11.7129	Undecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>9</sub> CH <sub>3</sub>	156.31	5.60
12.	112-42-5	19.545	1-Undecanol	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> OH	172.31	2.50
13.	128-37-0	22.2767	Butylated Hydroxytoluene	[(CH <sub>3</sub> ) <sub>3</sub> C] <sub>2</sub> C <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> )OH	220.35	0.35
14.	96-76-4	22.34	Phenol, 2,4-bis(1,1-dimethylethyl)- - incomplete name	C <sub>14</sub> H <sub>22</sub> O	206.32	0.95
15.	36653-82-4	28.8017	1-Hexadecanol	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> OH	242.44	1.60
16.	84-74-2	31.982	Dibutyl phthalate	C <sub>6</sub> H <sub>4</sub> -1,2-[CO <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub> ] <sub>2</sub>	278.34	1.20
17.	57-10-3	32.1447	n-Hexadecanoic acid	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOH	256.42	2.00
18.	544-76-3	41.4625	Hexadecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>	226.44	2.30
19.	629-62-9	41.471	Pentadecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>13</sub> CH <sub>3</sub>	212.41	2.60
20.	112-95-8	44.4415	Eicosane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> CH <sub>3</sub>	282.55	1.40

Table 7. Biologically active chemical compounds of methanol extract of the aerial parts of *A. javanica*

No	CAS	RT (min)	Name of the compound	Molecular formula	Molecular weight	Peak area (%)
1.	101-55-3	9.648	Benzene, 1-bromo-4-phenoxy- - incomplete name	C <sub>12</sub> H <sub>9</sub> BrO	249.1	14.00
2.	74-85-1	9.9249	Ethylene	CH <sub>2</sub> =CH <sub>2</sub>	28.05	0.42
3.	96-45-7	10.0933	2-Imidazolidinethione	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S	102.16	0.90
4.	608-27-5	12.8294	Benzenamine, 2,3-dichloro- - incomplete name	C <sub>6</sub> H <sub>5</sub> Cl <sub>2</sub> N	162.02	11.00
5.	7783-60-0	13.8345	Sulfur tetrafluoride	F <sub>4</sub> S	108.06	12.00
6.	120-72-9	14.8213	Indole (antioxidant)	C <sub>8</sub> H <sub>7</sub> N	117.15	8.50
7.	1634-04-4	14.9315	Propane, 2-methoxy-2-methyl- - incomplete name	C <sub>5</sub> H <sub>12</sub> O	88.14	0.57
8.	52-24-4	15.5451	Thiotepa	C <sub>6</sub> H <sub>12</sub> N <sub>3</sub> PS	189.22	0.97
9.	613-12-7	15.5631	Anthracene, 2-methyl- - incomplete name	C <sub>15</sub> H <sub>12</sub>	192.26	11.00
10.	95-83-0	16.9513	1,2-Benzenediamine, 4-chloro- - incomplete name	ClC <sub>6</sub> H <sub>3</sub> (NH <sub>2</sub> ) <sub>2</sub>	142.59	6.00
11.	95-06-7	17.7567	CDEC	C <sub>8</sub> H <sub>14</sub> ClNS <sub>2</sub>	223.79	4.70
12.	573-98-8	20.7874	Naphthalene, 1,2-dimethyl- - incomplete name	C <sub>12</sub> H <sub>12</sub>	156.22	8.00
13.	1746-01-6	29.6141	2,3,7,8-Tetrachlorodibenzo-p-dioxin	C <sub>12</sub> H <sub>4</sub> Cl <sub>4</sub>	321.97	0.95
14.	882-33-7	31.6179	Disulfide, diphenyl	C <sub>6</sub> H <sub>5</sub> SSC <sub>6</sub> H <sub>5</sub>	218.34	1.50
15.	79-92-5	36.7619	Camphene	C <sub>10</sub> H <sub>16</sub>	136.23	7.10
16.	7005-72-3	37.1718	Benzene, 1-chloro-4-phenoxy- - incomplete name	C <sub>12</sub> H <sub>9</sub> ClO	204.65	9.60
17.	120-75-2	46.0812	Benzothiazole, 2-methyl-	C <sub>8</sub> H <sub>7</sub> NS	149.21	8.80
18.	84-76-4	46.3526	1,2-Benzenedicarboxylic acid, dinonyl ester	C <sub>26</sub> H <sub>42</sub> O <sub>4</sub>	418.61	7.10
19.	84-69-5	46.353	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	278.34	7.00

Table 8. Biologically active chemical compounds of acetone extract of the aerial parts of *A. javanica*

No	CAS	RT (min)	Name of the compound	Molecular formula	Molecular weight	Peak area (%)
1.	460-19-5	5.09	Ethanedinitrile	C <sub>2</sub> N <sub>2</sub>	52.036	0.29
2.	107-13-1	5.243	2-Propenenitrile	CH <sub>2</sub> =CHCN	53.06	0.04
3.	75-64-9	9.3547	2-Propanamine, 2-methyl-	C <sub>4</sub> H <sub>11</sub> N	73.14	2.70
4.	75-55-8	9.753	Aziridine, 2-methyl- - incomplete name	C <sub>3</sub> H <sub>7</sub> N	57.09	6.70
5.	208-96-8	12.6993	Acenaphthylene	C <sub>12</sub> H <sub>8</sub>	152.19	2.10
6.	1752-30-3	12.9541	Hydrazinecarbothioamide, 2-(1-methylethylidene)-	C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> S	131.19	0.31
7.	95-06-7	13.6721	CDEC	C <sub>8</sub> H <sub>14</sub> ClNS <sub>2</sub>	223.78	10
8.	646-06-0	14.9154	1,3-Dioxolane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.08	0.90
9.	883-20-5	15.566	Phenanthrene, 9-methyl-	C <sub>15</sub> H <sub>12</sub>	192.26	20.00
10.	140-29-4	16.8838	Benzyl nitrile	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CN	117.15	11.00
11.	50-18-0	17.4712	2-[Bis(2-chloroethylamino)]-tetrahydro-2H-1,3,2-oxazaphosphorine-2-oxide	C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> P	261.08	0.36
12.	88-89-1	21.1417	Phenol, 2,4,6-trinitro-	C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>	229.1	19.00
13.	128-37-0	30.9725	Butylated Hydroxytoluene	[(CH <sub>3</sub> ) <sub>3</sub> C] <sub>2</sub> C <sub>6</sub> H <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> )OH	220.35	27.00
14.	112-53-8	32.7943	1-Dodecanol	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>11</sub> OH	186.33	47.00
15.	112-63-0	36.6648	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>	294.47	0.65
16.	50-06-6	39.6006	Phenobarbital	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	232.24	0.59
17.	103-23-1	39.6591	Hexanedioic acid, bis(2-ethylhexyl) ester	C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>	370.56	3.20

drug intermediates (Lin *et al.*, 2010; de Sa *et al.*, 2009; Meth-Cohn, 2000). Several tryptophan and tryptamine derivatives of prenylated indole compounds, and their scavenging activity for reactive oxygen species (ROS) and reactive nitrogen species (RNS) showing good activity (Estevão *et al.*, 2010). In present study showing that methanolic extract and chloroform extract showed indole compounds and its derivative.

## Conclusions

In conclusion, the methods revealed several new constituents, while one of the *A. javanica* extracts displayed comparative antioxidant activity to that of the bioactive molecule of Indole, 1H-Indole, 2-methyl-, 2,3,7,8-Tetrachlorodibenzo-p-dioxin Disulfide, diphenyl. Finally, statistical analysis demonstrated certain correlations among the variables selected. The studies on phytochemical constituents of *A. javanica* are scanty. Identification of these compounds in the plant serves as the basis in determining the possible health benefits of the plant leading to further biologic and pharmacologic studies.

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