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## Evaluation of antioxidant activity, untargeted metabolite profile and elemental analysis of *Euphorbia hirta* L

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**Abstract**

Antioxidant is a new hype in naturopathy and at present it has huge demand in cosmetic, nutritional supplementation and pharmacological industry. It reduces cell damages caused by free-radical which are responsible for various ailments like ageing, cancer, diabetes mellitus, atherosclerosis, cataracts and inflammation. Therefore, antioxidant activity of a popular medicinal plant *Euphorbia hirta* was determined. Different parts *viz.* leaves, roots, stems of *Euphorbia hirta* were successively extracted with n-hexane, ethyl acetate, methanol and water by Soxhlet apparatus. All the extracts were studied for total phenol content using folin-ciocalteu reagent and 2,2 diphenyl 1-picrylhydrazyl (DPPH) free radical scavenging capacity was determined. Metabolites profile were identified in methanolic and water extracts of all the parts of plant by Q-TOF LC/MS. Different elements were studied in all the parts of plant by inductively coupled plasma mass spectrometry (ICP-MS). The results of study showed that methanolic extract of leaves had more amount of total phenol content (360 mg/g of extract). Methanolic extract of leaves was found to be good antioxidant activity (IC<sub>50</sub> value-26 µg/ml). Heavy metals were not found in any extracts of parts of plant. Therefore, study was suggested that *Euphorbia hirta* leaves, roots and stems has a huge potential in terms of commercial use as source of antioxidant.

**Keywords:** *Euphorbia hirta*, total phenol, antioxidant, ICP-MS, Q-TOF LC/MS, metabolite analysis

**Introduction**

*Euphorbia hirta* (asthma-plant) is a pantropical weed, possibly native to India. It belongs to *Euphorbiaceae* family. It is a hairy herb that grows in open grasslands, roadsides and pathways. It is widely used as a medicinal herb. The *Euphorbiaceae* is mostly monoecious herbs, shrubs, and trees, sometimes succulent and cactus-like. It comprises about 300 genera and 5,000 species, distributed in the temperate, sub-tropical and tropical regions of the world (Gupta and Srivastava 2007) [6]. The *Euphorbiaceae* is characterized by the frequent occurrence of milky sap and in many members of the family, including the genus *Euphorbia*, the milky latex or sap is poisonous and skin contact may cause inflammation and a blistering rash.

In south India, it is used as ear drops, in the treatment of boils, sores and wounds. The latex of the plant is often used as warts and cuts to prevent pathogen infection. A decoction of leaves induces milk flow and the leaf chewed with palm kernel for restoration of virility. It is also effective in treating ulcers. The plant is also eaten as vegetables (Asha *et al.* 2014) [2].

*Euphorbia hirta* contains flavonoids, terpenoids, phenols, essential oil and other compounds. The plant parts are widely used in traditional system of medicines, in the treatment of respiratory diseases, gastrointestinal disorders, wound healing, pulmonary disorders, urinogenital disorders, tumors, lactation in women etc. The plant has also been used as anti-inflammatory, antioxidant, antitumour, antidiabetic, free radical scavenging, anti allergic, analgesic and antianaphylactic, antioxytic, sedative, antiarthritic, antidiarrhoeal, spasmogenic, antithrombocytopenic, diuretic, burn wound healing, immune stimulatory, sperm motility, genotoxic, synergic, antiviral, antihelmentic, immunoprophylactic, antimalarial, antimicrobial, herbicidal, antimolluscidal, larvicidal property and so on. In this report we explore investigations related to phytochemistry uses and pharmacological uses of the plant (Asha *et al.* 2014) [2].

## Material and Methods

### Plant Collection

*Euphorbia hirta* was collected in January (2018), from campus of Junagadh Agricultural University, (Plate 1). The collected different parts of plant materials (*viz.* leaves, stem and root) were washed under running tap water (Plate 2). They were shade dried for 2-3 days at room temperature. Dried plant parts were grind to make fine powder. Powders of different plant parts were used for extraction using different solvents with respect to their polarities.

### Chemicals

- Lists of solvents were used in study: ethyl acetate, n-hexane, methanol, 0.1 % formic acid in water, acetonitrile and nitric acid.
- Lists of chemicals were used in study: Gallic acid, sodium carbonate, Folin-Ciocalteu's reagent, 2,2 diphenyl 1-picrylhydrazyl (DPPH).

### Plant Extraction

Different powder of various parts of plant were successively extracted in soxhlet apparatus using different polarities of various solvents like hexane, ethyl acetate methanol and water (Tiwari *et al.* 2011)<sup>[10]</sup> respectively. The 15 g powder was weigh and used for extraction. Percent yield (% yield) was calculated by following formula

$$\% \text{ yield} = (\text{wt of dry extract} / \text{wt of sample}) \times 100$$

### Total Phenol Content

The total phenol content can be determined by Folin-Ciocalteu reagent method (McDonald *et al.*, 2001)<sup>[7]</sup>. The 0.5 ml of extract and 0.5 ml of Folin-Ciocalteu reagent (10%) were mixed and incubated at room temperature for 5 min. Then 2.5 ml saturated sodium carbonate was added and further incubated for 15 min at room temperature and absorbance was measured at 765 nm. Gallic acid (McDonald *et al.* 2001; Wolfe *et al.* 2003)<sup>[7, 11]</sup> was used as positive controls. The total phenol content was expressed in terms of standard equivalent (mg g<sup>-1</sup> of extracted compound) (Chanda and Dave 2009)<sup>[5]</sup>.

### DPPH Free Radical Scavenging Activity

DPPH free radical scavenging activity was measured by Liyana-Pathirana and Shahidi, 2005. The reaction mixture (3.0 ml) consists of 1.0 ml of DPPH in methanol (0.270 mM), 1.0 ml of the extract and 1.0 ml of methanol. It was incubated for 10 min in dark, and then the absorbance was measured at 517 nm. Ascorbic acid was used as standards. The percentage of inhibition can be calculated using the formula:

$$\text{Inhibition \%} = [(A_{\text{control}} - A_{\text{sample}}) / (A_{\text{control}})] \times 100$$

where,

$A_{\text{control}}$  = Absorbance of DPPH radical + methanol

$A_{\text{sample}}$  = Absorbance of DPPH radical + sample extract/standard

### Elemental Analysis by ICP-MS

Different powder of plant parts (0.5 g) were pre digested for 1 hrs in nitric acid, than heated gradually up to 180 °C for 1.5 hrs. The digested plant parts were subsequently cooled and brought up to volume 50.0 ml with distilled water. These solutions were used for analysis by ICP-MS.

Instrument Condition for ICP-MS

No.	ICP-MS Parameter	Instrument condition
1	Power	1.2 kW
2	Plasma flow	15 l/ min
3	Auxiliary flow	1.50 l/ min
4	Nebulizer flow	0.85 l/min
5	Raplicate read time	10 s
6	Number of Raplicates	3
7	Instrument stabilization delay	30 s
8	Rince time	15 s
9	Sample uptake delay	10 s
10	Pump rate	15 rpm
11	Sample cone	1.0 mm nickel
12	Sample uptake rate	0.85 ml/min
13	Skimmer cone	0.7 mm nickel

### Metabolites profile of Different Solvent Extracts by Q-TOF LC/MS

In the LC condition mobile phase were 0.1 % Formic acid in water (solvent A) and acetonitrile (solvent B) were used. Total run time was 30 min. Flow rate was 0.600 ml/min. column temperature was 40 °C.

### LC Condition

Sr. no.	Time(min)	A (%)	B (%)
1	0	95	5
2	7	95	5
3	12	5	95
4	20	95	5
5	30	95	5

### Q-TOF (MS) Condition

Sr. no.	Parameter	Condition
1	Mode MS scan	Positive (+)
2	Ion source	dual AJS ESI
3	Mass range	(100-1700) m/z
4	Collision Gas	N(nitrogen)
5	Gas temp.	325 °C
6	Drying gas	8 (l/min)
7	Nebulizer	45 psi
8	Sheath gas temp.	350°C
9	Sheath gas flow	11 (l/min)
10	Capillary voltage	4000 v
11	Fragmenter voltage	150 v
12	Skimmer cone	65 mm
13	Nozzel voltage	1000 v

## Results and Discussion

### The % yield of various extracts of different parts of *Euphorbia hirta*

The maximum yield (13.70%) was found in water extract of stem as compared to other solvents extracts (Table 1). Minimum yield (0.061%) was found in ethyl acetate extract of root. Among all methanolic extracts, methanol extracts of leaves was found high content of % yield as compared to other methanolic extracts of different parts of plant. Methanolic extract of root showed low content of yield as compared to other methanolic extract. Among all ethyl acetate and n-hexane extracts of leaves showed high content of yield as compared to other ethyl acetate and n-hexane extracts of various parts of plant respectively. Ethyl acetate and n-hexane extracts of root showed low content of % yield as compared to ethyl acetate and n-hexane extracts.

### Total Phenol Content

Stems had higher amount of phenol content as compared to leaves and roots in water extract. Leaves had high amount of phenol content as compared to stem and root in water extract (Table 2). Methanol extract of stems had more phenol content as compared to other solvents extracts of different parts of plant. Methanol extract of stem had low phenol content as compared to methanol extract of leaves and root. Ethyl acetate extract of stems had more phenol content as compared to ethyl acetate extract of leaves and roots. Hexane extract of roots had no found phenol content. Gallic acid was used as standard. All the extracts were determined by equivalent to gallic acid standard. Hexane extracts of all the parts of plant had low amount of phenol as compared to other extracts. High polarities contain more amount of phenol *viz.* methanol and water as compared to low polarity contains solvent *viz.* ethyl acetate and n-hexane (Chanda and Dave, 2007). So, it can be concluded that highly polar solvent can use for extraction of phenolic compounds. High solubility of phenols in polar solvents provides high concentration of these compounds in the extracts obtained using polar solvents for the extraction (McDonald *et al.* 2001) [7].

### Antioxidant Activities

The antioxidant activity of the methanolic extracts was determined using the method of DPPH free radical scavenging activity (Blois 1958). The DPPH stable free radical method is an easy, rapid and sensitive way to survey the antioxidant activity of a specific compound or plant extracts (Blois, 1958). The antioxidant activity of *Euphorbia hirta* was showed in Table 3 and Figure 1 to 10. The results of study showed that water extract of leaves showed more amount of total phenol (170 mg/g of extract) and it showed very good DPPH radical scavenging activity (155µg extract/ml), so it can be concluded from the results that their positive correlation was found between the total phenol content and DPPH free radical scavenging activity (Salazar *et al.* 2008).

### Elements Analysis by ICPMS of Different Parts of *Euphorbia hirta*

Inductively coupled plasma mass spectrometry (ICP-MS) is a type of mass spectroscopy that is highly sensitive and capable of the determination of a range of metals and several non-metals at concentrations below part per billion (ppb). Inductively coupled plasma mass spectrometry is a method used for separating and detecting the ions. In trace elemental analysis, the method has advantages of high speed, precision and sensitivity compared to atomic absorption technique (Montaser *et al.* 1992) [8]. One of the great advantages to ICP-MS is extremely low detection limits for a wide variety of elements. Some elements can be measured down to part per quadrillion ranges while most can be detected at part per trillion levels. Shows some common detection limits by element. Element U, Cs and Bi is Detection Limit (ppt) like less than 10. Ag, Be, Cd, Rb, Sn, Sb and Au is Detection Limit (ppt) like 10-50. Ba, Pb, Se, Sr, Co, W, Mo and Mg are Detection Limit (ppt) like 50-100. Cr, Cu and Mn is Detection Limit 100-200ppt. Zn, As and Ti is detected in 400-500ppt. Li and P is detected in 1-3 ppb and Ca is less than 20 ppb (Batsala *et al.* 2012) [13].

Total 20 elements were analyzed in *Euphorbia hirta* leaves, roots and stems (Table 4). Aluminum, sodium, strontium, arsenic were not found in leaves, roots and stems. Total 15 elements *viz.* Ag, B, Ba, Cd, Co, Cr, Cu, Fe, K, Li, Mn, Mo,

Ni, Pb, Hg and Zn were found at different concentration in leaves, roots and stems. The potassium was maximum (>1000 µg/g) found in all parts. Iron content was highest in leaves, roots and stems. but it was within the limit as per Ayurveda pharmacopeia The recommended permissible limits for mercury, lead, cadmium and arsenic are 1 mg/kg, 10 mg/kg, 0.3 mg/kg and 3 mg/kg respectively (Anonymous2005)[1]. Among all the elements, Boron was highest in leaves (71.86 µg/g) followed by roots (22.69 µg/g) and stems (17.72 µg/g) Nickel was highest in roots (61.43 µg/g) followed by leaves (7.48 µg/g) and stems (6.15 µg/g). Manganese was highest in stems (29.05) followed by leaves (0.17) but in roots have more manganese content (51.73) as compared to stems. ). Except other elements like Ag, B, Cd, Co, Cr, Cu, Li, Mg, Mo, Ni, and Pb were showed different level of content in all parts of plant. Iron showed good content in all parts as compared to other elements it can conclude that leaves can be used as good source of important nutrients.

### Metabolites profile of various extracts of three different parts of *Euphorbia hirta* by Q-TOF LC/MS

Total 43 metabolite were identified in methanolic extracts of leaves compounds by Q-TOF LC/MS analysis (Table 5). Among many compounds are important for human and animal health. Different compounds *viz.* Cytarabine, Vidarabine, 4-(2-hydroxy-3-isopropyl-aminopropyl) benzoic acid, Pinacidil-N-Oxide etc have different biological activities. It contains activity like anticancer drug, anti-viral, Beta-adrenoreceptor blocking drug, Vasodilator respectively. Mass spectrum of methanolic of leaves of *Euphorbia hirta* was shown in figure 11.

Total 35 metabolite were identified in methanolic extracts of root compounds by Q-TOF LC/MS analysis (Table 6). Total 41 metabolite compounds were identified in methanolic extracts of stems (Table 7) by Q-TOF LC/MS analysis. Among many compounds are important for human and animal health. Different compounds had different biological activities *viz.* Euphornin, (beta)-Warfarin, Cytarabine, Nafrolyl and Viscutin 1, etc. and it contains activity like antineoplastic agent, Anticoagulant Drug, anticancer drug, Inhibits vasoconstrictor and Insect growth inhibitory activity respectively. Mass spectrum of methanolic of roots and mass spectrum of methanolic of stems of *Euphorbia hirta* were shown in figure 12-13.

Total 37 metabolite compounds were identified in water extracts of leaves by Q-TOF LC/MS analysis (Table 8). Among many compounds are important for human and animal health. Different compounds had different biological activities *viz.* acarbose, (beta±)-Warfarin, C24 Sulfatide 1, Viscutin 2, etc. and it contains activity like Therapeutic Drugs, Anticoagulant Drug, CST activity in the brain is normal in alzheimer's disease, Insect growth inhibitory activity respectively. Mass spectrum of water of leaves of *Euphorbia hirta* was shown in figure 14.

Total 23 metabolite compounds were identified in water extract of roots (Table 9) while total 36 metabolite compounds were identified in water extract of stems by Q-TOF LC/MS analysis (Table 10). Among many compounds are important for human and animal health. Different compounds had different biological activities *viz.* mycobactin S, vitamin E succinate (tocopherol succinate), Lycoperside D, Methyl-2-pyrrolidinone etc. and it contains activity like, homeopathic medicine, vitamin, alkaloid, organic compound consisting 5-membered lactam respectively. Mass spectrum of

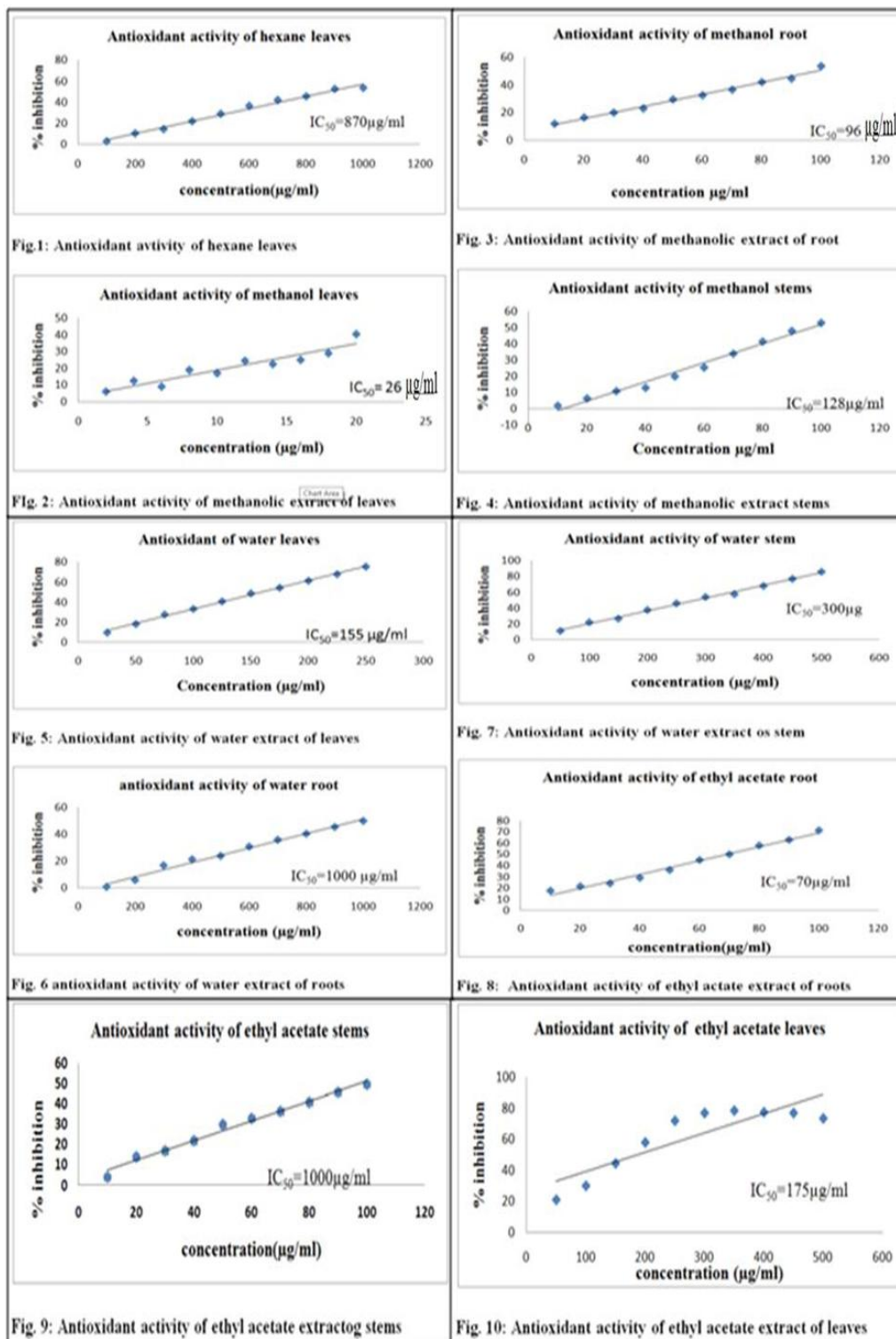
water of roots and mass spectrum of water of stems of *Euphorbia hirta* were shown in figure 14-16.

Methanolic extracts of leaves had higher contain metabolites as compare to roots and stems. Different groups of compounds like flavones, flavonols, alkaloids, and fatty acyl, were found in methanolic extract of leaves, stems and roots. Various compounds of alkaloid group were found in methanolic extract of leaves.

### Conclusions

The QTOF/LCMS results showed that antioxidants like flavones, flavonols were found in all the parts of plant. Methanolic extracts of leaves had more DPPH free radical

scavenging activity because it had more amounts of various metabolite of different groups of flavones and flavonols. Also, methanolic extracts of leaves had more content of total phenol. The results of antioxidant and total phenol showed that there was positive correlation between total phenol and antioxidant activities. So it can be conclude that methanolic extracts of leaves had good source for antioxidant followed by water extract of leaves. Also trace level of few heavy metal were found within the permissible limit and some important elements like B, Fe and Zn were found in good quantity in leaves. Further study will require for isolation of antioxidant from methanolic extract of leaves.



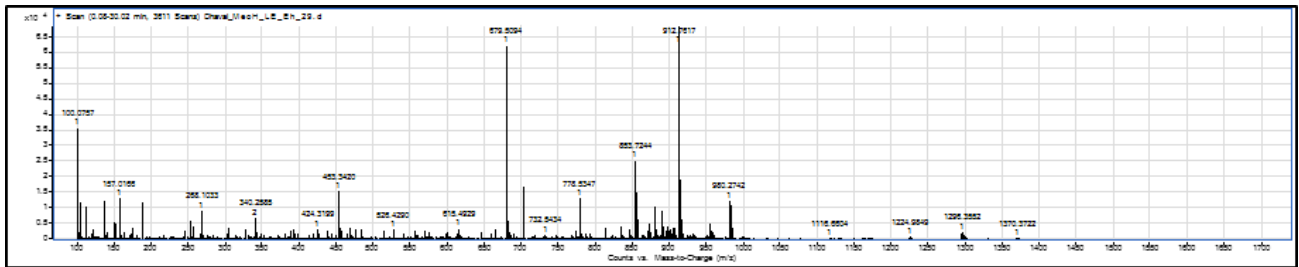


Fig 11: Mass spectrum of methanolic extract of leaves

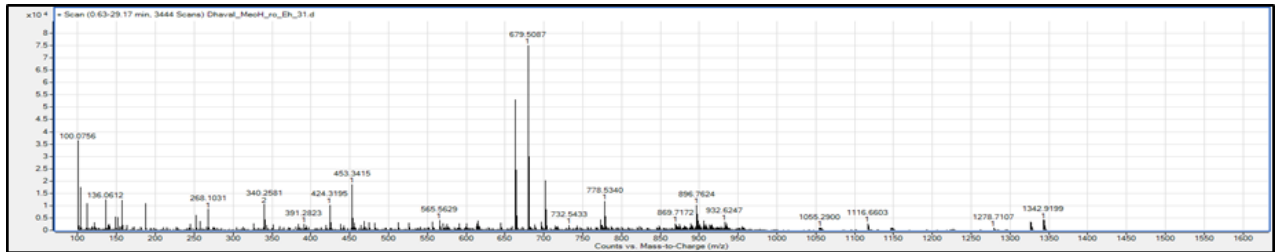


Fig 12: Mass spectrum of methanolic extract of roots

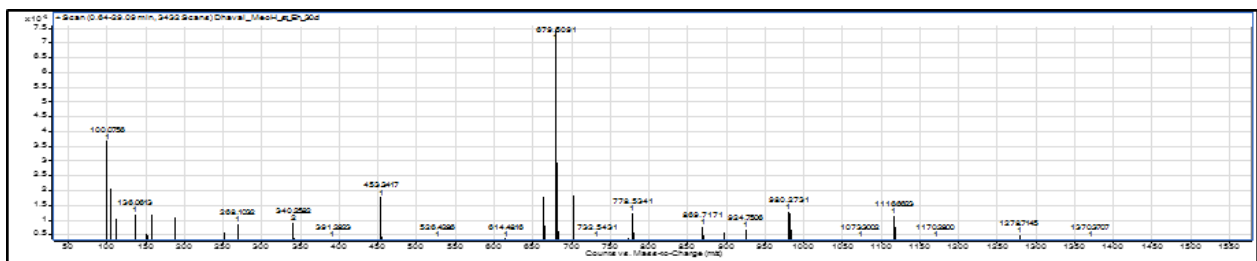


Fig 13: Mass spectrum of methanolic extract of stem



Fig 14: Mass spectrum of water extract of leaves

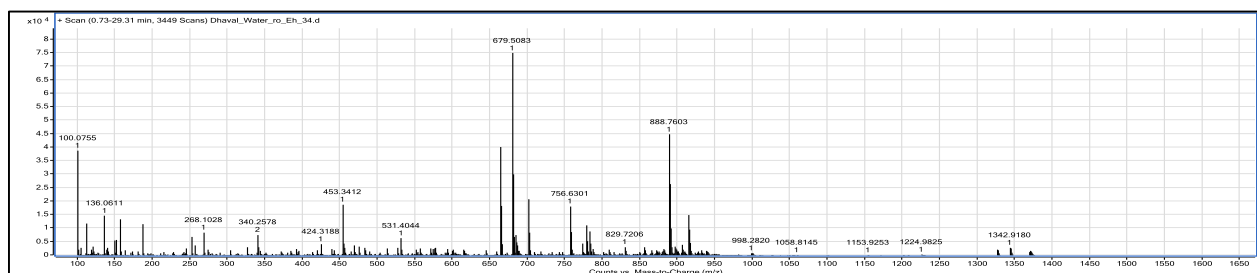


Fig 15: Mass spectrum of water extract of roots

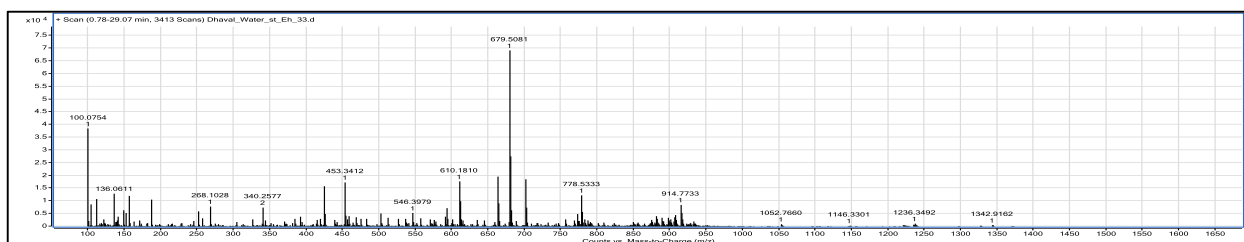


Fig 16: Mass spectrum of water extract of stem





Plate 1: Photograph of *Euphorbia hirta* L.



Plate 2: Photographs of Leaves, Roots and Stem of *Euphorbia hirta* L.

Table 1: Percent (%) yields of different solvents extracts of various parts of *Euphorbia hirta*

Parts	Extracts	Total phenol content (mg/g)
leaves	n hexane	5
	ethyl acetate	22
	methanol	360
	water	170
roots	n hexane	Absent
	ethyl acetate	28
	methanol	100
	water	62
stems	n hexane	3
	ethyl acetate	31
	methanol	68
	water	90

Table 2: Total phenol content of different plant extracts

Extract	Parts of plant	% yield
n-hexane	leaves	2.09
	roots	0.51
	stems	1.12
ethyl acetate	leaves	1.81
	roots	0.06
	stems	0.94
methanol	leaves	12.59
	roots	5.54
	stems	8.02
water	leaves	12.39
	roots	3.65
	stems	13.70

Table 3: Antioxidant activity (IC<sub>50</sub> value) of different extracts of plants

Parts of plant	Extracts	Antioxidant IC <sub>50</sub> (µg/ml)
Leaves	n-hexane	870
	ethyl acetate	175
	Methanol	26
	Water	155
Roots	n-hexane	>1000
	ethyl acetate	70
	Methanol	96
	Water	1000
Stems	n-hexane	>1000
	ethyl acetate	1000
	Methanol	128
	Water	300

Table 4: Elemental analysis of different parts of *Euphorbia hirta*

Sr. No.	Metals	Mass	Concentration mean (µg/g)		
			Leaves	Roots	Stems
1	Silver (Ag)	107	2.69	2.21	0.97
2	Aluminum (Al)	27	0	0	0
3	Boron (B)	11	71.86	22.69	17.72
4	Barium (Ba)	138	13.43	13.81	16.39
5	Cadmium (Cd)	111	0.04	0.32	0.03
6	Cobalt (Co)	59	0.63	1.97	0.19
7	Chromium (Cr)	52	5.80	15.17	3.32
8	Copper (Cu)	63	14.83	0.838	6.561
9	Iron (Fe)	57	421.41	553.17	106.98
10	Potassium (K)	39	> 1000	> 1000	> 1000
11	Lithium (Li)	7	0.26	0.32	0.05
12	Manganese (Mn)	55	0.17	51.73	29.05
13	Molybdenum (Mo)	98	0.59	0.24	0.18
14	Sodium (Na)	23	ND	ND	ND
15	Nickel (Ni)	60	7.48	61.43	6.15
16	Lead (Pb)	208	2.40	0.11	1.27
17	Strontium (Sr)	88	ND	ND	ND
18	Zinc (Zn)	66	45.78	0.19	22.13
19	Mercury (Hg)	202	0.090	0.27	ND
20	Arsenic (As)	75	ND	ND	ND

**Table 5:** Metabolites analysis of methanolic extract of leaves of *Euphorbia hirta* by Q-TOF LC/MS

Sr.no	RT	Area	Height	Name of compound	mass	Formula	Note
1	12.158	223513	34418	Asn-Trp-OH	426.117	C <sub>20</sub> H <sub>18</sub> N <sub>4</sub> O <sub>7</sub>	Peptide consists two amino acids
2	5.296	914975	29901	13,14-dihydro-16,16-difluoro Prostaglandin F <sub>2</sub> $\alpha$	392.238	C <sub>20</sub> H <sub>34</sub> F <sub>2</sub> O <sub>5</sub>	Treatment of hepatobiliary disease
3	11.74	129956	16804	Vidarabine	267.0961	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>	Antiviral, Treatment of herpes simplex Drug Dollery, Colin Therapeutic Drugs
4	20.315	2570639	65666	Guanine	151.049	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	amino acid,base of DNA
5	13.132	147875	34828	A 80987	653.3215	C <sub>37</sub> H <sub>43</sub> N <sub>5</sub> O <sub>6</sub>	HIV1 protease inhibitors
6	12.659	5869958	261550	PE(17:2(9Z,12Z)/20:1(11Z))	755.5453	C <sub>42</sub> H <sub>78</sub> N O <sub>8</sub> P	Diacylglycerophosphoglycerols
7	29.229	964371	20586	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5582	C <sub>46</sub> H <sub>81</sub> O <sub>10</sub> P	Diacylglycerophosphoglycerols
8	8.779	258205	17191	Ethyl 3-(N-butylacetamido)propionate	215.1514	C <sub>11</sub> H <sub>21</sub> N O <sub>3</sub>	Insect repellent.
9	11.912	957448	62617	Melanoxetin	302.0418	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	aturally occurring flavonoid compounds
10	12.642	401992	92537	Tributyl phosphate	266.1639	C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P	Extractant and plastiizer
11	21.131	546826	12268	C16 Sphinganine	273.2658	C <sub>16</sub> H <sub>35</sub> N O <sub>2</sub>	Lipid products
12	8.339	702510	26185	4-(2-hydroxy-3-isopropyl-aminopropyl)benzoic acid	253.1305	C <sub>13</sub> H <sub>19</sub> N O <sub>4</sub>	B-adrenoreceptor blocking drug. It is highly b1 adrenoreceptorselective.metabolite of BisoprololDollery,Colin Therapeutic Drugs, 2nd Ed. 1999 p. B64
13	20.63	96870		PE-Cer(d14:2(4E,6E)/20:1(11Z)(2OH))	672.4845	C <sub>36</sub> H <sub>69</sub> N <sub>2</sub> O <sub>7</sub> P	Lipid compound
14	11.891	42920	4904	Mycobactin S	827.5054	C <sub>44</sub> H <sub>69</sub> N <sub>5</sub> O <sub>10</sub>	Homeopathic medicine
15	12.707	226144	28959	Glycerol 1,3-dihexadecanoate	568.5066	C <sub>35</sub> H <sub>68</sub> O <sub>5</sub>	Aliphatic acyclic compound found in tea
16	20.334	342219	13284	Cytarabine	243.0847	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub>	Anticancer Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. C373.
17	7.128	580888	29527	Corchoionol C 9-glucoside	386.1926	C <sub>19</sub> H <sub>30</sub> O <sub>8</sub>	Found in capers. it is stabilizer,nutrient,surfactant and emulsifier
18	15.237	147566	17287	N-Cyclohexanecarbonylpentadecylamine	337.333	C <sub>22</sub> H <sub>43</sub> N O	use potential treatment for obesity and chronic pain
19	20.309	112405	4767	C24 Sulfatide	891.6471	C <sub>48</sub> H <sub>93</sub> N O <sub>11</sub> S	CST activity in the brainis normal inAlzheimer's disease
20	11.915	193245	12626	Apigenin 7-O-glucoside	432.1039	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>	Antioxidant activity
21	12.588	17688	4845	Triphenyl phosphate	326.0694	C <sub>18</sub> H <sub>15</sub> O <sub>4</sub> P	It is a plasticizer and fire retardant
22	13.804	1627186	49170	PE-NMe2(18:1(9Z)/16:0)	745.5593	C <sub>41</sub> H <sub>80</sub> N O <sub>8</sub> P	Lipid compound
23	12.714	47011	5962	all-trans-heptaprenyldiphosphate	654.3811	C <sub>35</sub> H <sub>60</sub> O <sub>7</sub> P <sub>2</sub>	synthase activity
24	7.593	993534	36663	Styrene	104.0624	C <sub>8</sub> H <sub>8</sub>	Colourless oily liquids. sweet smell,easylevoprate,use in polymerization
25	14.797	5310484	252734	3-hexanoyl-NBD Cholesterol	662.4439	C <sub>39</sub> H <sub>58</sub> O <sub>5</sub>	Derivative
26	11.899	43404	5602	Lycoposide D	739.4529	C <sub>39</sub> H <sub>65</sub> N O <sub>12</sub>	Alkaloid from tomato
27	11.817	997203	484636	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5597	C <sub>46</sub> H <sub>81</sub> O <sub>10</sub> P	Lipid compound
28	3.542	198564	28079	N-Methyl-2-pyrrolidinone	99.0683	C <sub>5</sub> H <sub>9</sub> N O	Organic compound consisting 5-membered lactam
29	20.205	2520862	83203	Cytosine	111.0431	C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	It is main base found in DNA,RNA
30	13.495	27316	3637	5 $\alpha$ -Androst-3-en-17-one	272.213	C <sub>19</sub> H <sub>28</sub> O	Endogenous steroid hormone and week androgen
31	3.476	221381	32722	N-Acryloylglycine	129.0423	C <sub>5</sub> H <sub>7</sub> N O <sub>3</sub>	Vinyl monomer containing amino acid and carboxylic acid
32	24.28	67143	5840	PE-Cer(d16:1(4E)/22:1(13Z))	714.5706	C <sub>40</sub> H <sub>79</sub> N <sub>2</sub> O <sub>6</sub> P	Lipid compound
33	7.037	1635162	43713	Pinacidil-N-Oxide	261.1593	C <sub>13</sub> H <sub>19</sub> N <sub>5</sub> O	Vasodilator, Treatment of hypertension Metabolite of PinacidilDollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. P127
34	11.746	40425	3668	Promecarb	207.1254	C <sub>12</sub> H <sub>17</sub> N O <sub>2</sub>	insecticide
35	3.621	61139	6856	Viscutin 1	526.1494	C <sub>27</sub> H <sub>26</sub> O <sub>11</sub>	Insect growth inhibitory activity
36	3.589	92427	13096	DMPO	113.0836	C <sub>6</sub> H <sub>11</sub> N O	Water soluble nitric oxide
37	11.796	62747	6479	2-Propenyl 2-aminobenzoate	177.0786	C <sub>10</sub> H <sub>11</sub> N O <sub>2</sub>	Flavour ingredient
38	3.786	60355	11779	N-Methyl-2-pyrrolidinone	99.0682	C <sub>5</sub> H <sub>9</sub> N O	Organic compound consisting 5 membered lactam
39	14.472	31207	4260	cis-1,2-dimethylcyclohexane	112.1249	C <sub>8</sub> H <sub>16</sub>	Toxic compound
40	3.459	172994	14648	Calystegin B2	175.0839	C <sub>7</sub> H <sub>13</sub> N O <sub>4</sub>	Alkaloid, glycosidase inhibitors
41	13.057	47416	8253	4-Hydroxyphenylglyoxylate	166.0261	C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>	Inter mediate. obtain from olive oil

42	12.339	72180	13765	1,3,8-Naphthalenertriol	176.0468	C10 H8 O3	Chemical comp
43	12.44	10299	2060	Juglone	174.0314	C10 H6 O3	leaves and nuts of Juglans spp., Caryaspp and Pterocarya spp.

**Table 6:** Metabolites analysis of methanolic extract of roots of *Euphorbia hirta* by Q-TOF LC/MS

Sr.no	RT	Area	Height	Name of compound	Mass	Formula	Note
1	20.63	118968	18603	PE-Cer(d14:2(4E,6E)/20:1(11Z)(2OH))	672.4842	C36H69N2O7 P	Lipid compound
2	11.77	145857	17501	N-(1-Deoxy-1-fructosyl)alanine	251.1009	C9 H17 N O7	mixer of diastereomers
3	11.817	474673	229620	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5583	C46 H81 O10 P	lipid compound
4	11.74	164071	14434	Miserotoxin	267.0957	C9 H17 N O8	A toxin found in manyspaces of Astragalus
5	13.05	2540178	390007	Nafronyl	383.2448	C24H33NO3	Inhibits vasoconstrictor and platelet aggregant effects of serotonin Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. N11
6	12.659	10590704	275399	PE(17:2(9Z,12Z)/20:1(11Z))	755.5446	C42 H78 NO8P	Lipid compound
7	12.441	110086	23610	(beta±)-Warfarin	308.1038	C19 H16 O4	Anticoagulant Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. W1
8	10.048	681779	31100	Leu Tyr	294.1567	C15 H22 N2 O4	dipeptide
9	14.699	80887	11718	Euphornin	584.2986	C33 H44 O9	antineoplastic agent
10	13.041	41380	8671	12-hydroxyjasmonic acid	226.1202	C12 H18 O4	tuber-inducing properties
11	21.131	955624	20541	C16 Sphinganine	273.2655	C16 H35 N O2	lipid compound
12	14.747	981584	28243	PG(20:4(5Z,8Z,11Z,14Z)/20:1(11Z))	824.5569	C46 H81 O10 P	lipid compound
13	20.334	474447	16691	Cytarabine	243.0845	C9 H13 N3 O5	Anticancer Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. C373.
14	3.922	291559	12396	Viscutin 1	526.1482	C27 H26 O11	Insect growth inhibitory activity
15	15.697	222609	11294	CerP(d18:1/20:0)	673.5403	C38 H76 N O6 P	Ceramide 1-phosphates
16	14.316	935050	157053	PE(P-16:0/0:0)	437.2909	C21 H44 N O6 P	Monoacylglycerophosphoglycerols
17	12.969	112533	21535	Anandamide (18:3, n-6)	321.2659	C20 H35 N O2	use to treat anxiety and depression
18	14.41	1052644	52371	3-O-Sulfogalactosylceramide	907.6393	C48 H93 N O12 S	glycosphingolipids
19	12.705	171121	38579	Dideoxymycobactin	837.5598	C47 H75 N5 O8	antigens
20	12.588	17996	5374	4-methyl-n-(2-oxo-2,5,6,7-tetrahydro-1h-cyclopenta[b]pyridin-4-yl)benzenesulfonamide	304.0878	C15 H16 N2 O3 S	Corrosion inhibitor, used to water treatment cooling tower
21	4.833	13296992	424388	2-Amino-3-methyl-1-butanol	103.0997	C5 H13 N O	antibiotics
22	20.175	54201	7842	OlmesartanMedoxomil	558.2202	C29 H30N6 O6	synthetic
23	14.269	127829	11337	PI(O-20:0/18:0)	880.6407	C47 H93 O12 P	lipid compound
24	4.142	95500	10631	N-Methyl-2-pyrrolidinone	99.0681	C5 H9 N O	Organic compound consisting 5-membered lactam
25	3.841	262107	44439	DMPO	113.0836	C6 H11 N O	Water soluble nitric oxide
26	4.035	482643	37176	4-Methylaminobutyrate	117.0785	C5 H11 N O2	peptide
27	11.908	42307	4532	PE(18:4(6Z,9Z,12Z,15Z)/20:3(5Z,8Z,11Z))	761.4965	C43 H72 N O8 P	lipid compound
28	14.797	3640855	1111225	3-hexanoyl-NBD Cholesterol	662.444	C39H58N4 O5	derivative
29	12.812	159596	23785	Progesterone 3-biotin	697.4225	C38 H59 N5 O5 S	sex hormones
30	3.773	62400	10792	Hydroxyatrazine	197.1278	C8 H15 N5 O	Pesticide property
31	3.786	306788	38195	N-Methyl-2-pyrrolidinone	99.0681	C5 H9 N O	Organic compound consisting 5-membered lactam
32	4.006	656643	57878	4-Hydroxy-6-methylpyran-2-one	126.0312	C6 H6 O3	Pennicilliumstipitatum
33	3.753	482921	48513	N-Acryloylglycine	129.0421	C5 H7 N O3	Vinyl monomer containing amino acid and carboxylic acid
34	4.03	332042	28334	2-amino-heptanoic acid	145.1096	C7 H15 N O2	Amino acid
35	3.581	139633	11745	Cytosine	111.0429	C4 H5 N3 O	amino acid,base of DNA



**Table 7:** Metabolites analysis of methanolic extract of stems of *Euphorbia hirta* by Q-TOF LC/MS

Sr.no	RT	Area	Height	Name of compound	Mass	Formula	Note
1	13.132	166790	37317	A 80987	653.321	C37 H43 N5 O6	HIV1 protease inhibitors
2	14.699	2750177	425264	Euphornin	584.2991	C33 H44 O9	antineoplastic agent
3	11.879	38586	4564	Rhodocladonic Acid	318.0369	C15 H10 O8	Cladoniaspp
4	13.804	1786627	53771	PE-NMe2(18:1(9Z)/16:0)	745.5612	C41 H80 N O8 P	Lipid compound
5	12.659	10468144	259330	PE(17:2(9Z,12Z)/20:1(11Z))	755.5448	C42 H78 N O8 P	Lipid compound
6	20.109	1385396	37671	Miserotoxin	267.096	C9 H17 N O8	A toxin found in manyspeaces of Astragalus
7	12.441	45247	8854	(beta±)-Warfarin	308.1043	C19 H16 O4	Anticoagulant Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. W1
8	12.273	143120	28491	(R)-Pterosin B	218.13	C14 H18 O2	Antidiabetic activity
9	11.817	410664	212129	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5586	C46 H81 O10 P	lipid compoud
10	21.131	827138	18711	C16 Sphinganine	273.2656	C16 H35 N O2	lipid products
11	15.858	174664	18692	Galalpha1-3(Fucalpha1-2)Galbeta1-4Glcbeta-Cer(d18:1/20:0)	1225.79	C62 H115 N O22	Lipid compound
12	20.63	71346	10414	PE-Cer(d14:2(4E,6E)/20:1(11Z)(2OH))	672.4842	C36 H69 N2 O7 P	Lipid compound
13	2.228	64177	9095	3-hexanoyl-NBD Cholesterol	662.4424	C39 H58 N4 O5	Derivative
14	14.747	482404	22611	PG(20:4(5Z,8Z,11Z,14Z)/20:1(11Z))	824.5569	C46 H81 O10 P	lipid products
15	12.995	23435	5462	Stigmatellin Y	484.281	C29 H40 O6	chromones
16	12.812	64986	11431	Progesterone 3-biotin	697.423	C38 H59 N5 O5 S	sex hormones
17	13.05	357171	64070	Nafronyl	383.2445	C24 H33 N O3	Inhibits vasoconstrictor and platelet aggregant effects of serotonin Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. N11
18	12.705	260000	52880	Dideoxymycobactin	837.5608	C47 H75 N5 O8	Antigens
19	12.413	52289	11545	O-hexanoyl-adenosine monophosphate	445.1358	C16 H24 N5 O8 P	Lipid compound
20	14.797	31511661	1827066	3-hexanoyl-NBD Cholesterol	662.4434	C39 H58 N4 O5	Derivative
21	15.029	1170023	163501	PI(20:4(5Z,8Z,11Z,14Z)/0:0)	620.296	C29 H49 O12 P	Lipid compound
22	13.338	161653	26834	Sphinganine	301.2987	C18 H39 N O2	amino acid,base of DNA
23	16.039	198769	21301	Prostaglandin A1-biotin	646.412	C35H58N4O5 S	Anti proliferative activity
24	15.364	213528	27133	PI(20:4(5Z,8Z,11Z,14Z)/0:0)	620.2958	C29 H49 O12 P	Lipid compound
25	20.89	228745	19642	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5598	C46 H81 O10 P	Lipid compound
26	11.915	131124	18029	Apigenin 7-O-glucoside	432.1039	C21 H20 O10	Antioxidant activity
27	13.957	87830	13660	Hematoporphyrin	598.2784	C34 H38 N4 O6	Pubchem 11103
28	12.476	31494	5327	Viscutin 2	568.1573	C29 H28 O12	Insect growth inhibitory activity
29	4.241	7046296	431041	2-Amino-3-methyl-1-butanol	103.0998	C5 H13 N O	antibiotics
30	3.786	95701	12407	N-Methyl-2-pyrrolidinone	99.0683	C5 H9 N O	Organic compound consisting 5-membered lactam
31	3.476	428759	60791	N-Acryloylglycine	129.0423	C5 H7 NO3	Vinyl monomer containing amino acid and carboxylic acid
32	3.589	261379	56194	DMPO	113.0837	C6 H11 N O	Water soluble nitric oxide
33	20.205	2774134	83070	Cytosine	111.0431	C4 H5 N3 O	Amino acid
34	14.41	306056	15847	3-O-Sulfogalactosylceramide	907.64	C48 H93 N O12 S	giycoosphingolipids
35	11.754	1500876	78775	3-Isochromanone	148.0519	C9 H8 O2	Alicyclic hydrocarbon
36	3.542	363069	50633	N-Methyl-2-pyrrolidinone	99.0683	C5 H9 N O	Organic compound consisting 5-membered lactam
37	12.023	10454	4164	1-Arachidonoyl Glycerol-d5	383.3094	C23 H33 D5 O4	Ligand bindind affinity and agonist activity
38	20.315	2620678	64883	Guanine	151.049	C5 H5 N5 O	amino acid,base of DNA
39	11.746	2881365	179636	Promecarb	207.1253	C12 H17 N O2	insecticide
40	11.899	48446	4434	Lycoperoside D	739.453	C39 H65 N O12	Alkaloid from tomato
41	12.3	106987	19761	C10:1n-7	170.1302	C10 H18 O2	Alkyl derivative

**Table 8:** Metabolites analysis of water extract of leaves of *Euphorbia hirta* by Q-TOF LC/MS

Sr.no	RT	Area	Height	Name of compound	Mass	Formula	Note
1	11.74	115007	12311	Miserotoxin	267.0955	C9 H17 N O8	A toxin found in manyspeaces of Astragalus
2	11.191	113143	15036	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5566	C46 H81 O10 P	Diacylglycerophosphoglycerols
3	11.77	191900	19441	N-(1-Deoxy-1-fructosyl)alanine	251.1008	C9 H17 N O7	Mixture of diastereomers
4	12.441	1029464	343377	(beta±)-Warfarin	308.1038	C19 H16 O4	Anticoagulant Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. W1
5	20.315	2688098	67451	Guanine	151.0487	C5 H5 N5 O	Amino acid
6	20.63	120609	19891	PE-Cer(d14:2(4E,6E)/20:1(11Z)(2OH))	672.4837	C36 H69 N2 O7 P	lipid compound
7	11.879	15434	2633	cis-Coutaric acid	296.054	C13 H12 O8	Found in wine,pomace, grape
8	11.899	46217	5687	Lycoperoside D	739.4507	C39 H65 N O12	Alkaloid from tomato
9	13.132	144856	33260	A 80987	653.3206	C37 H43 N5 O6	HIV1 protease inhibitors
10	12.569	429624	116793	Furano[2",3":6,7]aurone	262.0617	C17 H10 O3	metabolite
11	13.064	112807	14788	Dihydro-beta-Tubaic Acid	236.1037	C13 H16 O4	derivative mundulone
12	3.495	117313	16649	Acarbose (component 1)	303.131	C13 H21 N O7	hydrolase inhibitor used in regulating intestinal carbohydrate digestion and absorption metabolite of AcarboseDollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. A7.
13	13.05	2362506	334602	Nafronyl	383.2444	C24 H33 N O3	Inhibits vasoconstrictor and platelet aggregant effects of serotonin Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. N11
14	12.659	8924276	278465	PE(17:2(9Z,12Z)/20:1(11Z))	755.544	C42 H78 N O8 P	Lipid compound
15	11.891	45314	5206	Mycobactin S	827.5029	C44 H69 N5 O10	Siderophore
16	3.915	658801	103589	D-1-[(3-Carboxypropyl)amino]-1-deoxyfructose	265.1152	C10 H19 N O7	Aliphatic heteromonocycliccompound,Nutrient
17	20.334	445477	14449	Cytarabine	243.0843	C9 H13 N3 O5	Anticancer Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. C373.
18	24.28	206199	7225	PE-Cer(d16:1(4E)/22:1(13Z))	714.5698	C40 H79 N2 O6 P	Lipid compound
19	14.797	1646474	477347	3-hexanoyl-NBD Cholesterol	662.4434	C39 H58 N4 O5	derivative
20	12.413	27643	6340	p-Hydroxytriamtereneglucuronide	445.1348	C18 H19 N7 O7	Potassium-conserving diuretic Metabolite of TriametereneDollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. T169
21	12.509	49757	11664	Mangostenone B	462.2032	C28 H30 O6	Metabolite
22	14.316	1112416	179398	PE(P-16:0/0:0)	437.2909	C21 H44 N O6 P	Lipid compound
23	13.804	1943883	58372	PE-NMe2(18:1(9Z)/16:0)	745.5618	C41 H80 N O8 P	Lipid compound
24	20.309	113507	4240	C24 Sulfatide	891.646	C48 H93 N O11 S	CST activity in the brainis disease
25	4.311	202650	9293	Esprocarb	265.1512	C15 H23 N O S	metabolite
26	14.699	42303	4731	Euphornin	584.2984	C33 H44 O9	Toxic compound
27	3.922	27556	3342	Viscutin 1	526.1474	C27 H26 O11	Insect growth inhibitory activity
28	12.995	89030	12065	PG(16:0/0:0)	484.2804	C22 H45 O9 P	lipid compound
29	13.491	8368246	183207	PE(16:0/22:2(13Z,16Z))	771.5809	C43 H82 N O8 P	lipid compound
30	4.035	757727	115000	4-Methylaminobutyrate	117.0785	C5 H11 N O2	ester copound
31	20.205	2499470	76832	Cytosine	111.0429	C4 H5 N3 O	Amino acid
32	3.786	212387	25206	N-Methyl-2-pyrrolidinone	99.0681	C5 H9 N O	Organic compound consisting 5-membered lactam
33	3.954	114622	11942	3-Hydroxycoumarin	162.0313	C9 H6 O3	Alyxialucida
34	3.841	124001	21196	DMPO	113.0835	C6 H11 N O	Water soluble nitric oxide
35	12.588	20273	5204	4-methyl-n-(2-oxo-2,5,6,7-tetrahydro-1h-cyclopenta[b]pyridin-4-yl)benzenesulfonamide	304.0873	C15 H16 N2 O3 S	Hetero cyclic compound
36	3.753	321068	45346	N-Acryloylglycine	129.042	C5 H7 N O3	Vinyl monomer containing amino acid and carboxylic acid
37	16.27	615789	66628	episterylpalmitoleate	634.5712	C44 H74 O2	metabolite

**Table 9:** Metabolites analysis of water extract of roots of *Euphorbia hirta* by Q-TOF LC/MS

Sr.no	RT	Area	Height	Name of compound	Mass	Formula	Note
1	11.74	10004	5183	Miserotoxin	267.0954	C9 H17 N O8	A toxin found in manyspaces of Astragalus
2	12.413	21531	6007	p-Hydroxytriamterene glucuronide	445.1345	C18 H19 N7 O7	Potassium-conserving diuretic Metabolite of Triameterene Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. T169
3	12.569	6998	1855	Furano[2",3":6,7]aurone	262.0626	C17 H10 O3	metabolite
4	12.865	6476904	1417217	Dihydrocelastrol	452.2938	C29 H40 O4	derivative
5	20.63	187084	24584	PE-Cer(d14:2(4E,6E)/20:1(11Z)(2OH))	672.484	C36 H69 N2 O7 P	lipid compound
6	12.923	252264	38310	C18 Sulfatide	807.5524	C42 H81 N O11 S	CST activity in the brainis normal inAlzheimer's disease
7	11.891	37490	4123	Mycobactin S	827.5037	C44 H69 N5 O10	Homeopathic medicine
8	14.747	934500	29172	PG(20:4(5Z,8Z,11Z,14Z)/20:1(11Z))	824.5565	C46 H81 O10 P	lipid compound
9	12.441	108735	24554	Latifolin	286.1214	C17 H18 O4	metabolite
10	21.131	2224808	45766	C16 Sphinganine	273.2654	C16 H35 N O2	Lipid products
11	14.797	40014310	3978027	3-hexanoyl-NBD Cholesterol	662.4431	C39 H58 N4 O5	derivative
12	12.659	1027169	124492	PE(17:2(9Z,12Z)/20:1(11Z))	755.544	C42 H78 N O8 P	lipid compound
13	6.629	140388	7909	Ethyl 3-(N-butylacetamido)propionate	215.1509	C11 H21 N O3	Insect repellent.
14	13.05	1261921	188630	Nafrolyl	383.2443	C24 H33 N O3	Inhibits vasoconstrictor and platelet aggregant effects of serotonin Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. N11
15	20.877	2722051	92667	Vitamin E succinate(tocopherol succinate)	530.3969	C33 H54 O5	vitamin use full for humen body
16	13.909	207704	38863	Avermectin A1b monosaccharide	728.4147	C41 H60 O11	carbohydrates
17	11.899	48579	4544	Lycoperside D	739.4507	C39 H65 N O12	Alkaloid from tomato
18	24.28	211630	13475	PE-Cer(d16:1(4E)/22:1(13Z))	714.5701	C40 H79 N2 O6 P	lipid compound
19	14.316	667231	111881	PE(P-16:0/0:0)	437.2906	C21 H44 N O6 P	lipid compound
20	21.229	468725	15359	Arachidonoyl amine	303.2568	C20 H33 N O	N-acyl amines or Fatty amides
21	20.89	1188475	25667	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5589	C46 H81 O10 P	Glycerophospholipids
22	3.786	287466	38316	N-Methyl-2-pyrrolidinone	99.068	C5 H9 N O	Organic compound consisting 5-membered lactam
23	13.491	8352733	199660	PE(16:0/22:2(13Z,16Z))	771.5808	C43 H82 N O8 P	lipid compound

**Table 10:** Metabolites analysis of water extract of stems of *Euphorbia hirta* by Q-TOF LC/MS

Sr.no	RT	Area	Height	Name of compound	Mass	Formula	Note
1	5.296	245587	18378	13,14-dihydro-16,16-difluoro Prostaglandin F2 <sub>1±</sub>	392.2373	C20H34 F2 O5	Treatment of hepatobiliary disease
2	12.569	18818	4584	Furano[2",3":6,7]aurone	262.0626	C17 H10 O3	Flavonoid,hetero cyclic compound
3	11.817	581070	229285	PG(18:4(6Z,9Z,12Z,15Z)/22:1(11Z))	824.5573	C46 H81 O10 P	Glycerophospholipids
4	20.336	1097729	36109	Miserotoxin	267.0955	C9 H17 N O8	A toxin found in manyspaces of Astragalus
5	11.77	152887	15045	N-(1-Deoxy-1-fructosyl)alanine	251.1008	C9 H17 N O7	mixer of diastereomers
6	3.922	53718	5436	Viscutin 1	526.148	C27 H26 O11	Flavones and Flavonols and Leucoanthocyanidins Insect growth inhibitory activity
7	12.242	297595	45732	Symlandine	381.2156	C20 H31 N O6	metabolite
8	12.413	22864	4673	p-Hydroxytriamterene glucuronide	445.1344	C18 H19 N7 O7	Potassium-conserving diuretic Metabolite of Triameterene Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. T169
9	13.804	1667851	61749	PE-NMe2(18:1(9Z)/16:0)	745.5617	C41 H80 N O8 P	lipid compound

10	12.476	22887	5219	Viscutin 2	568.1569	C29 H28 O12	Insect growth inhibitory activity
11	12.158	51140	8191	Asn-Trp-OH	426.1164	C20 H18 N4 O7	Peptide consists two amino acids
12	11.891	44531	5448	Mycobactin S	827.504	C44 H69 N5 O10	Homeopathic medicine
13	13.132	243746	55909	A 80987	653.3211	C37 H43 N5 O6	pyridine HIV1 protease inhibitors
14	12.441	69442	12383	(beta±)-Warfarin	308.1034	C19 H16 O4	Anticoagulant Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. W1
15	12.659	1967351	157341	PE(17:2(9Z,12Z)/20:1(11Z))	755.5441	C42 H78 N O8 P	lipid compound
16	13.05	2122210	308059	Nafrolyl	383.2445	C24 H33 N O3	Inhibits vasoconstrictor and platelet aggregant effects of serotonin Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999 p. N11
17	14.316	1731790	280079	PE(P-16:0/0:0)	437.2908	C21 H44 N O6 P	lipid compound
18	24.28	187441	10751	PE-Cer(d16:1(4E)/22:1(13Z))	714.5697	C40 H79 N2 O6 P	lipid compound
19	14.747	549634	26854	PG(20:4(5Z,8Z,11Z,14Z)/20:1(11Z))	824.5569	C46 H81 O10 P	lipid compound
20	12.588	19399	5657	Triphenyl phosphate	326.0693	C18 H15 O4 P	Phosphoric acid and phenol, Extractant and plastiizer
21	14.797	46760858	2518012	3-hexanoyl-NBD Cholesterol	662.4433	C39 H58 N4 O5	Derivative
22	5.184	103884	7729	Risperidone	410.2112	C23 H27 F N4 O2	Antipsychotic, Treatment of schizophrenia Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. R43
23	11.899	45355	5077	Lycoperside D	739.452	C39 H65 N O12	Alkaloid from tomato
24	14.699	85900	10896	Euphornin	584.2982	C33 H44 O9	antineoplastic agent
25	12.995	32344	10160	Stigmatellin Y	484.2805	C29 H40 O6	Potent inhibitor of the quinol oxidation chromones
26	14.305	225176	35054	Trihexyphenidyl	301.2415	C20 H31 N O	Anticholinergic, Treatment of Parkinsons Drug Dollery, Colin Therapeutic Drugs, 2nd Ed. 1999p. T183
27	19.981	8934641	144878	N-Methyl-2-pyrrolidinone	99.0682	C5 H9 N O	Organic compound consisting 5-membered lactam
28	3.954	274365	26177	3-Hydroxycoumarin	162.0315	C9 H6 O3	Alyxialucida
29	15.195	177858	25316	CB-52	417.3244	C26 H43 N O3	metaboite
30	13.275	495112	50028	Debenzoylzucchini factor B	559.4043	C37 H53 N O3	Phosphoric acid and phenol
31	3.755	214637	30269	3,5-Dihydroxy-phenylglycine	183.0535	C8 H9 N O4	amino acid
32	3.841	249589	35414	DMPO	113.0835	C6 H11 N O	Water soluble nitric oxide
33	23.717	41442	3247	PE-Cer(d16:1(4E)/22:1(13Z))	714.5688	C40 H79 N2 O6 P	lipid compound
34	14.41	416421	21957	3-O-Sulfogalactosylceramide	907.6386	C48 H93 N O12 S	glycosphingolipids
35	13.053	387100	49282	Phenylacetaldehyde	120.057	C8 H8 O	derivative of acid
36	5.085	81968	8237	Deoxycoformycin	268.1178	C11 H16 N4 O4	metabolite

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