



GC-MS Analysis of Bioactive Compounds from Whole Plant Chloroform Extract of *Ageratum conyzoides*

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Abstract: Most of the drug industries depend on medicinal plants for the production of pharmaceutical compounds, most herbal medicines and their derivatives products were often prepared from crude extracts from plants; which comprise a complex mixture of different phytochemical constituents (plant secondary metabolites). The aim of the work is to identify the bioactive compounds present in the chloroform extract of *Ageratum conyzoides* whole plant using Gas Chromatography and Mass spectroscopy. The GC-MS revealed seventy one phytochemicals ranging from high and low molecular weight chemical entities with varying quantities present. The major compounds present include 9,12-Octadecadienoic acid (12.48%), cis-4-Acetoxy-trans-1-(m-methoxyphenyl)cyclohexanecarbonitrile (11.52%), Octadecanoic acid (4.97%), Tetratetracontane (1.35%), 1H-Indole-3-carboxaldehyde (3.68%), 5-methoxy-19-Hydroxy-3-alpha,5-cyclo-5alpha-androstan-17-one (1.44%), cis-4,4-Dimethylbicyclo(6.3.0) undecane-2,6-dione (1.89%), 2-Heptenoic acid (1.23%), Kaur-16-ene (1.04%), Bicyclo [11.3.0] hexadecane-2,14-dione (0.45%), 3,3,6,6-Tetramethyl-1,2,3,4,5,6,7,8-octahydroacridine (1.61%). The minor ones such as Benzenemethanol, 4-(1,1-dimethylethyl)- (0.28%), Benzaldehyde, 2-hydroxy-4-methoxy-(0.22%), 2,3,4,7-Tetrahydro-1H-indene (0.18%), 7-Oxabicyclo [4.1.0] heptanes (0.16%), 2-Undecanone, 6,10-dimethyl- (0.96%), Diazoacetic acid, 2-isopropyl-5-methylcyclohexyl ester (0.54%), Bicyclo[11.3.0]hexadecane-2,14-dione (0.45%), are also present. These chemical compounds are considered biologically and pharmacologically important.

Keywords: *Ageratum conyzoides*, herbal medicine, *Osu angweri ngwa*, GC-MS analysis, bioactive compounds

1. INTRODUCTION

Medicinal plants are sources of herbal and synthetic drugs, a lot of medicine if not all, have bioactive constituents which are responsible for biological and pharmacological activities they exhibit.

Most of the activities can be attributed to secondary metabolites (phytochemical constituents) that are bioactive and present in the plant. Secondary metabolites are organic compounds that are not directly involved in the normal growth development and reproduction of the plant [1] and through to result from the evolutionary defense put up by plants [2]. Examples include alkaloids, tannins, terpenoids, flavonoids, saponins, phenolics, coumarins, glycosides and steroids.

They are of paramount importance in the treatment of diseases for man. South Eastern Nigeria is endowed with many of such vegetative plants and they are used as food and in herbal medicine to cure diseases and heal injuries; this implies that treatment of diseases in this region is not limited to synthetic drugs, as most people still depend on botanical preparations as medicine. These are always available in form of infusions, decoctions, macerations and concoctions. Most of these people even believe that herbal preparations are more effective than conventional synthetic drugs but are more effective than conventional synthetic drugs but are skeptical about its use since there is no clear cut dosage hence making it a major constraint

Ageratum conyzoides is among the medicinal plants that have effect against disease and may contain those biologically active compounds, which are effective against ailments. It belongs to the family and tribe of *Asteraceae* and *Eupatoriae* respectively. The plant is native to Central America, Caribbean, Florida (USA), South- East Asia, South China, India, West Africa (including Nigeria), Australia and South America [3,4]. The plant is traditionally called "Ufu Opioko" and "Otogo" by the Igedes in Benue

State, Nigeria [5]; in South Western Nigeria, it is known as “Imi esu” [6]; in South Western Nigeria, it is known as “Imi esu” [7]; while in the South East part of Nigeria, billygoat weed is called “Akwukwo nwa osi n’aka” or “Osu angweri ngwa”. *Ageratum conyzoides* has been known since ancient times for its curative properties and has been utilized for the treatment of various ailments, such as typhoid, anaemia, malaria, headache, burns and wounds, analgesic, inflammation, asthma, spasmodic arthrosis, dysnea, pneumonia and haemostatic effects, stomach ailments, gynecological diseases, leprosy and other skin diseases. [8,9]. A large percentage of the publications on the photochemistry has to do with the essential oil of this plant.

The oil content varies randomly from 0.11 to 0.58% for leaves and from 0.03 to 0.18% for the roots depending on times of the year [10]. From water distillation of the fresh flowers, the oil content was found to be 0.2%. The yield of oil from the petroleum ether extract of the seed was 26% [4].

A large number of constituents have been identified from the GC-MS analysis of the essential oil of *A. conyzoides*. The largest so far, a total of 51 constituents have been reported from the analysis of an oil sample of the plant collected from a university environment in Nigeria. [11]. Group of compounds like monoterpenes, sesquiterpenes, triterpenes, sterols, chromene, chromone, benzofuran, coumarins, flavonoids, alkaloids, tannins, saponins, precocene I and II and other miscellaneous compounds have been identified in *Ageratum conyzoides*.

2. MATERIALS AND METHODS

2.1. Sample Collection and Preparation

Fresh plant materials were collected from a nearby farmland within Michael Okpara University of Agriculture, Umudike in the month of March, 2018 and was taxonomically identified by Mr. I. Ndukwe in plant taxonomy section of the Forestry Department of Michael Okpara University of Agriculture Umudike, Nigeria. A voucher specimen (AC 7344) was deposited at Department of Botany School of biological sciences.

The Fresh leaves, stems and roots were harvested washed with tap water and rinsed with sterile distilled water, then dried under shade to prevent interference of UV-radiation from the sun. Dried plant materials were powdered using electric blender. The powdered materials were preserved in an air-tight container, ready for extraction.

2.2. Extraction of Plant Materials

The powdered plant sample (500g) was extracted with 2L of chloroform (8hrs/3 times/30 °c). The extract was concentrated under reduced pressure using Digital Heidolph Rotary evaporator (4000 series) and the supernatant plant extract (6.54g) was decanted after complete removal of the solvent. The extract was centrifuged at 10,000 ppm for 20 minutes and tract was then subjected to systematic GC – analysis.

2.3. GC – MS Analysis Conditions

The GC-MS analysis of the extract was carried out using a HP 7890 GC instrument integrated with an Agilent 5975C MSD mass spectrometer (Aligent, Santa Clara, CA, USA). The capillary column was an Agilent HP-5MS (30.m x 0.25mm i.d. x 0.25 NM film thickness), helium (Purity > 99.999%) was used as the carrier gas, and the flow rate was 1 ML/min. The injector temperature was 250°C, and the injection mode was splitless. The G.C oven temperature was held at 50°C for 5min, which was increased to 210°C at a rate of 3°C/min, maintained at 210°C for 3 min, and finally increased to 230°C at 150C/min. The mass spectrometer conditions were as follow: [12, 13, 14] ionization energy, 70 Ev; ion Source temperature, 230°C; quadrupole temperature, 150°C; quadrupole mass spectrometer scan range 30 – 500 atomic mass units (amu); solvent delay time 2.8min.

2.4. Components Identification

The components of the chloroform extract of *Ageratum conyzoides* was identified by matching the peaks with computer Wiley Ms. libraries and confirmed by comparing mass spectra of the peaks and those from literature [15].

3. RESULTS AND DISCUSSIONS

The chloroform extract of the whole plant of *Ageratum conyzoides* on GC-MS analysis showed seventy one peaks indicating the presence of seventy one compounds in the plant as shown in figure 1.

The molecular formula, the molecular weight, the retention time and the percentage constituents of the compounds are shown in Table 1.

The mass spectrometer analyzes the compounds eluted at different times help to identify the nature and structures of the compounds. The large compounds fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compounds which can be identified from the data library. The GC-MS study of the chloroform extract of the whole plant of *Ageratum conyzoides* had shown the presence of lots of photochemical which strongly contribute to the medicinal activity of the whole plant. The identified major compounds possess some important biological potential for future drug development

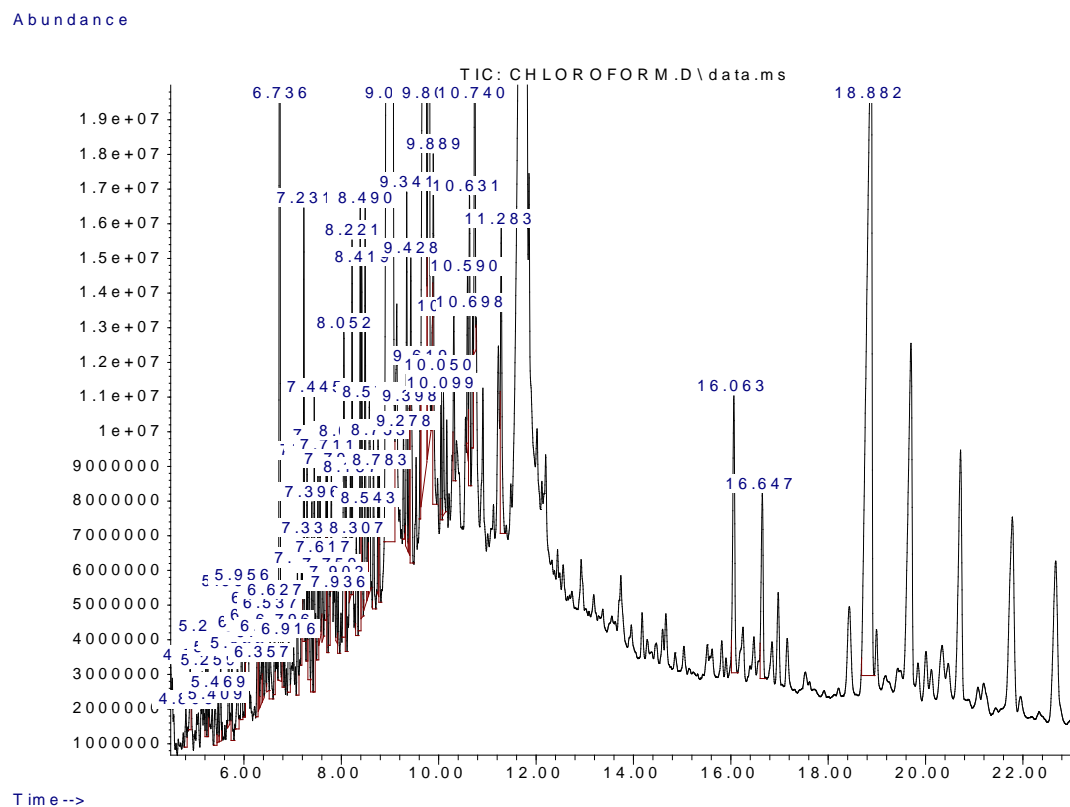
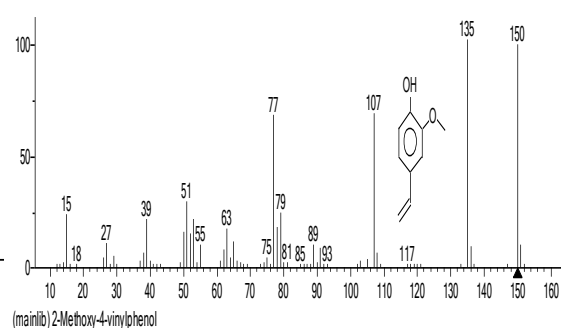
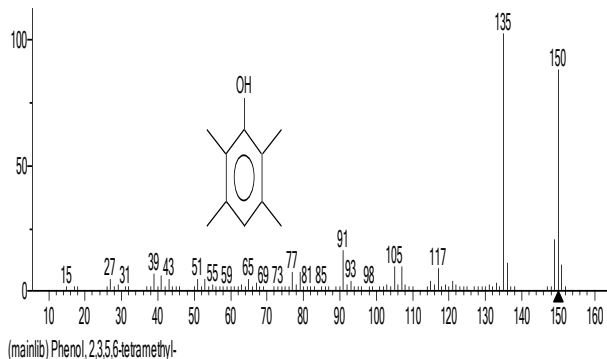
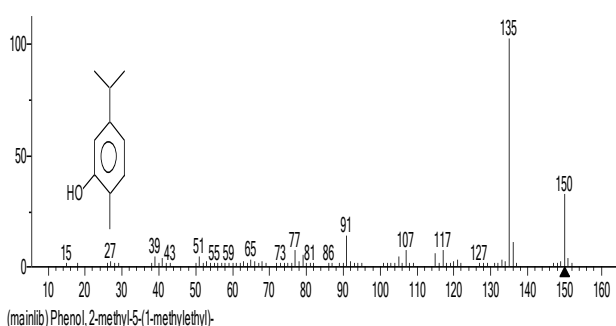
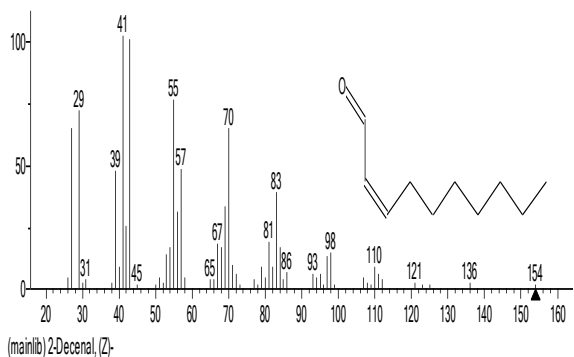
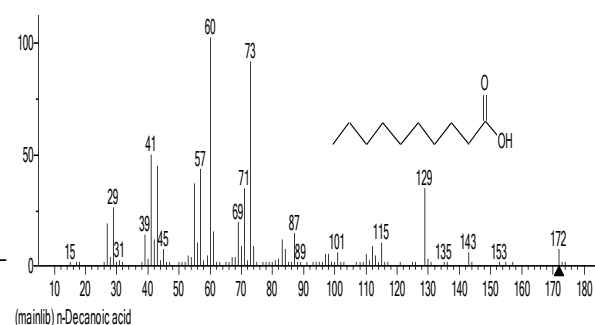
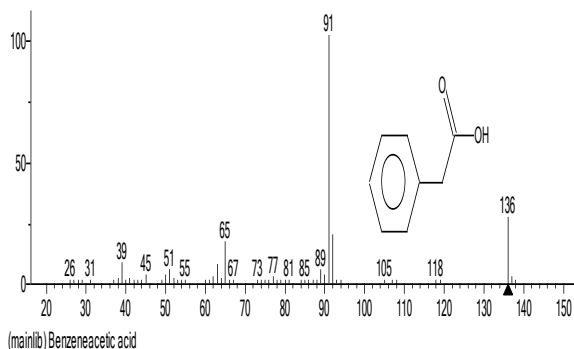
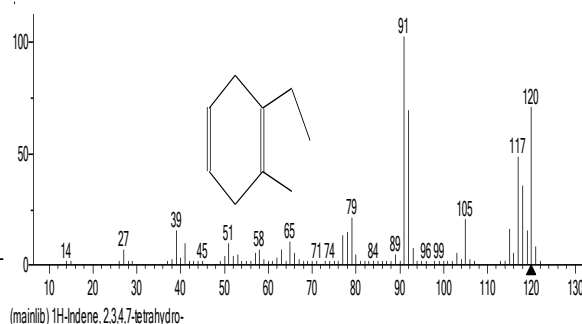
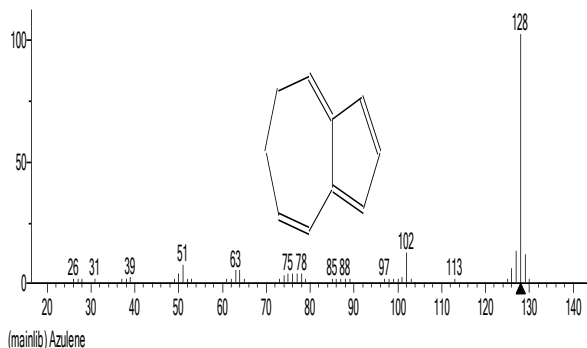
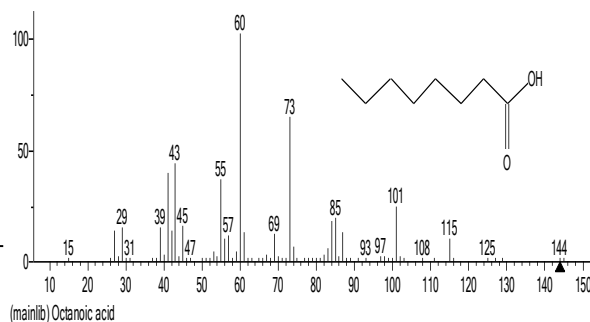
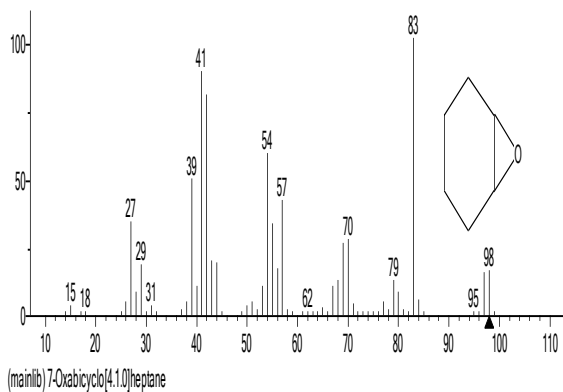


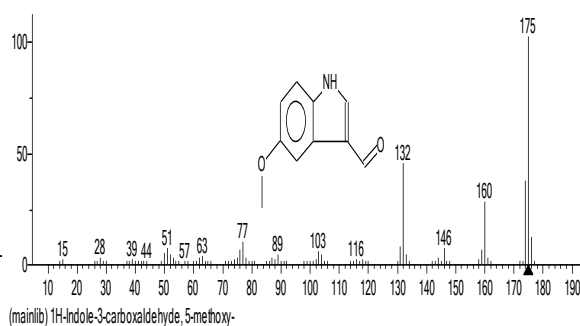
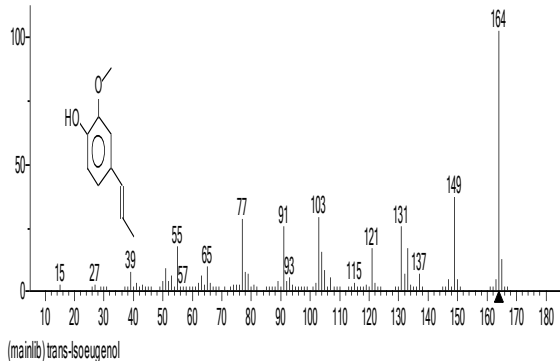
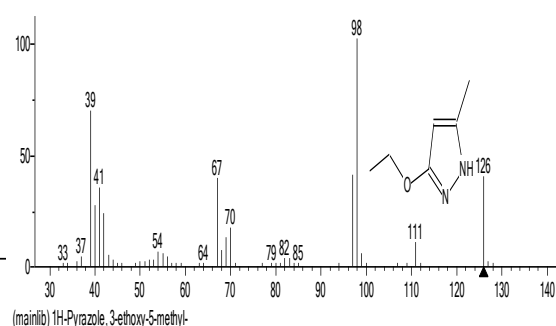
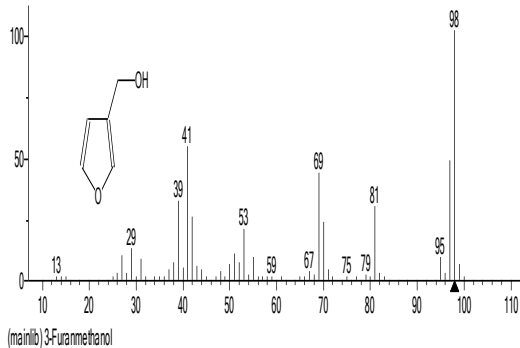
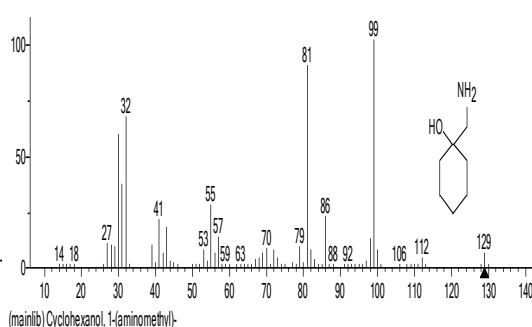
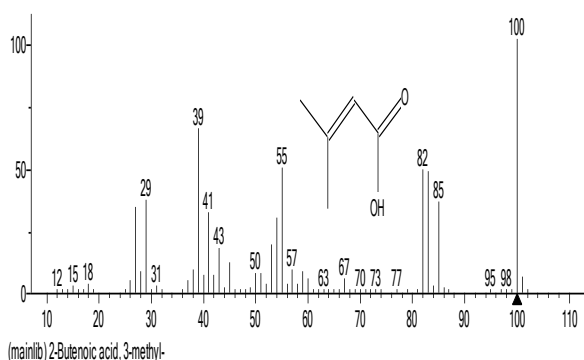
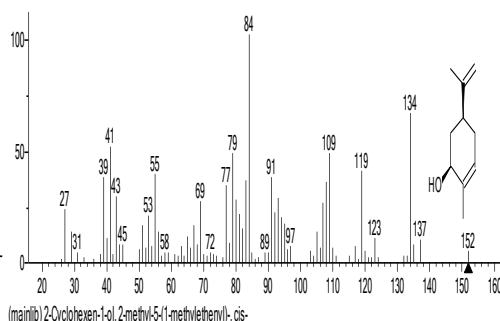
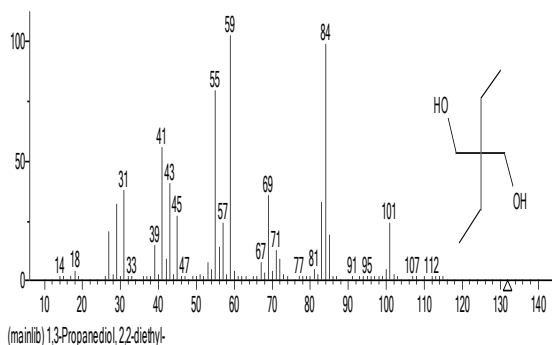
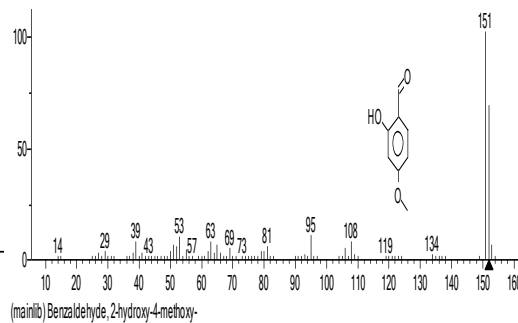
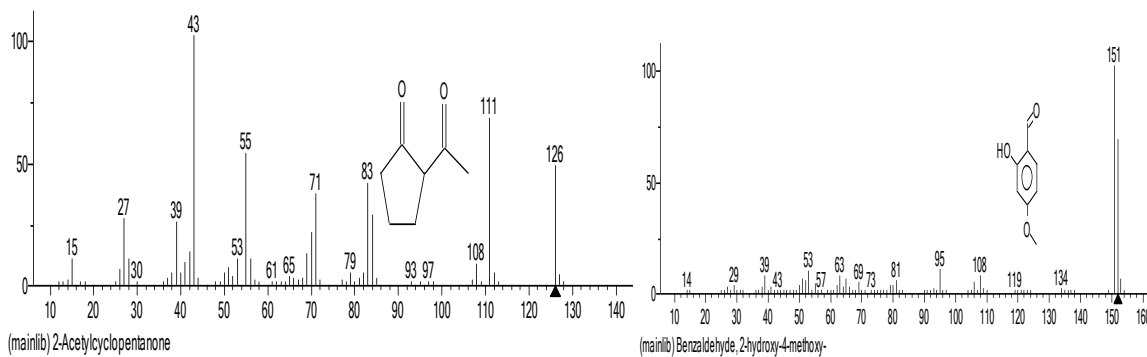
Figure1. GC-MS Chromatogram of *Ageratum conyzoides* whole plant chloroform extract.

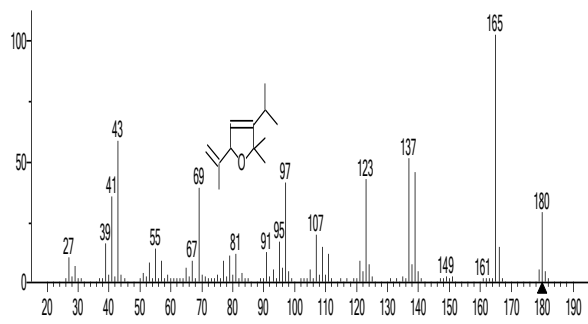
Table1. GC – MS analysis of *Ageratum conyzoides* showing molecular formula, molecular weight, percentage content, retention time

SN	RT	COMPONENT	FORMULA	MW	%
1	4.806	7-Oxabicyclo[4.1.0]heptanes	C ₆ H ₁₀ O	98	0.16
2	4.895	Octanoic Acid	C ₈ H ₁₆ O ₂	144	0.26
3	5.218	Azulene	C ₁₀ H ₈	128	0.25
4	5.259	2,3,4,7-Tetrahydro-1H-indene	C ₉ H ₁₂	120	0.18
5	5.409	Benzeneacetic acid	C ₈ H ₈ O ₂	136	0.23
6	5.469	n-Decanoic acid	C ₁₀ H ₂₀ O ₂	172	0.16
7	5.521	2-Decenal, (Z)-	C ₁₀ H ₁₈ O	154	0.28
8	5.686	Phenol, 2-methyl-5-(1-methylethyl)	C ₁₀ H ₁₄ O	150	0.36
9	5.754	Phenol, 2,3,5,6-tetramethyl-	C ₁₀ H ₁₄ O	150	0.27
10	5.866	2-Methoxy-4-vinylphenol	C ₉ H ₁₀ O ₂	150	0.32
11	5.956	2-Acetylcyclopentanone	C ₇ H ₁₀ O ₂	126	0.44
12	6.020	Benzaldehyde, 2-hydroxy-4-methoxy-	C ₈ H ₈ O ₃	152	0.22
13	6.279	1,3-Propanediol, 2,2-diethyl-	C ₇ H ₁₆ O ₂	132	0.36
14	6.301	2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, cis	C ₁₀ H ₁₆ O	152	0.27
15	6.357	2-Butenoic acid, 3-methyl-	C ₅ H ₈ O ₂	100	0.19
16	6.395	Cyclohexanol, 1-(aminomethyl)-	C ₇ H ₁₅ NO	129	0.19
17	6.481	3-Furanmethanol	C ₅ H ₆ O ₂	98	0.21
18	6.537	1H-Pyrazole, 3-ethoxy-5-methyl-	C ₆ H ₁₀ N ₂ O	126	0.33

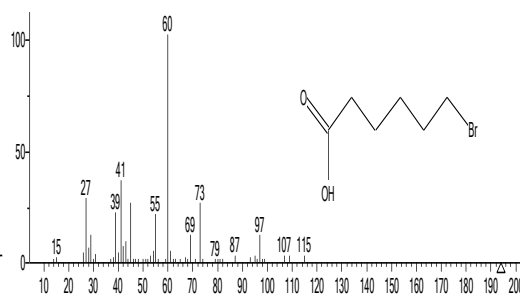
19	6.627	Phenol, 2-methoxy-4-(1-propenyl)-, (E)	C ₁₀ H ₁₂ O ₂	164	0.25
20	6.736	1H-Indole-3-carboxaldehyde, 5-methoxy	C ₁₀ H ₉ NO ₂	175	3.68
21	6.796	Furan, 2,5-dihydro-2,2-dimethyl-5-(1-methylethenyl)-3-(1-methylethyl)-	C ₁₂ H ₂₀ O	180	0.19
22	6.916	Hexanoic acid, 6-bromo-	C ₆ H ₁₁ BrO ₂	194	0.30
23	7.100	Dodecanoic acid	C ₁₂ H ₂₄ O ₂	200	0.42
24	7.178	α -Calacorene	C ₁₅ H ₂₀	200	0.28
25	7.231	2H-1-Benzopyran-2-one, 6-hydroxy-7-methoxy-4-methyl-	C ₁₁ H ₁₀ O ₄	206	1.07
26	7.295	Tetradecane	C ₁₄ H ₃₀	198	0.48
27	7.332	N,N-Diethyl-p-nitroaniline	C ₁₀ H ₁₄ N ₂ O ₂	194	0.56
28	7.396	(-)-Spathulenol	C ₁₅ H ₂₄ O	220	0.55
29	7.445	Caryophyllene oxide	C ₁₅ H ₂₄ O	220	0.79
30	7.520	3-Buten-2-ol, 2-methyl-	C ₅ H ₁₀ O	86	0.59
31	7.564	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1 α ,2 α ,5 β)-	C ₁₀ H ₂₀ O	156	0.59
32	7.617	Methyl 7-(2-furyl)heptanoate	C ₁₂ H ₁₈ O ₃	210	0.24
33	7.688	10,10-Dimethyl-2,6-dimethylenebicyclo[7.2.0]undecan-5 β -ol	C ₁₅ H ₂₄ O	220	0.50
34	7.711	Pyrimidine, 4-(2-hydroxy-5-methoxyphenyl)-	C ₁₁ H ₁₀ N ₂ O ₂	202	0.43
35	7.759	Methyl diphenylphosphinite	C ₁₃ H ₁₃ OP	216	0.24
36	7.797	Limonene oxide, cis-	C ₁₀ H ₁₆ O	152	0.32
37	7.902	2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	C ₁₅ H ₂₆ O	222	0.16
38	7.936	Longipinocarveol, trans-	C ₁₅ H ₂₄ O	220	0.16
39	8.052	Tetradecanoic acid	C ₁₄ H ₂₈ O ₂	228	1.35
40	8.097	6-Amino-2,4-dimethyl-5-methoxyquinoline	C ₁₂ H ₁₄ N ₂ O	202	0.51
41	8.187	Carbonic acid, octadecyl 2,2,2-trichloroethyl ester	C ₂₁ H ₃₉ Cl ₃ O ₃	444	0.36
42	8.220	Heptadecane	C ₁₇ H ₃₆	240	0.80
43	8.307	Norfenefrine	C ₈ H ₁₁ NO ₂	153	0.44
44	8.389	1,19-Eicosadiene	C ₂₀ H ₃₈	278	1.36
45	8.419	2-Undecanone, 6,10-dimethyl-	C ₁₃ H ₂₆ O	198	0.96
46	8.490	Pentadecanoic acid	C ₁₅ H ₃₀ O ₂	242	1.31
47	8.543	Benzenemethanol, 4-(1,1-dimethylethyl)-	C ₁₁ H ₁₆ O	164	0.28
48	8.577	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C ₂₀ H ₄₀ O	296	0.81
49	8.663	4-Allyl-5-pyridin-3-yl-2,4-dihydro-[1,2,4]triazole-3-thione	C ₁₀ H ₁₀ N ₄ S	218	0.54
50	8.753	Pentadecanoic acid, 14-methyl-, methyl ester	C ₁₇ H ₃₄ O ₂	270	0.43
51	8.783	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	C ₁₇ H ₂₄ O ₃	276	0.31
52	9.041	n-Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256	30.69
53	9.278	Methyl 2-hydroxy-pentadecanoate	C ₁₆ H ₃₂ O ₃	272	0.30
54	9.341	Heptadecanoic acid	C ₁₇ H ₃₄ O ₂	270	1.07
55	9.398	1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetrahydro-, stereoisomer	C ₁₁ H ₁₂ O	160	0.47
56	9.428	1-Hexadecene	C ₁₆ H ₃₂	224	1.32
57	9.619	Kaur-16-ene	C ₂₀ H ₃₂	272	0.44
58	9.720	9,12-Octadecadienoic acid (Z,Z)-	C ₁₈ H ₃₂ O ₂	280	12.48
59	9.806	Octadecanoic acid	C ₁₈ H ₃₆ O ₂	284	4.97
60	9.889	Tetratetracontane	C ₄₄ H ₉₀	618	1.19
61	10.050	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	C ₁₇ H ₃₂ O	252	0.43
62	10.099	Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-	C ₁₅ H ₂₄	204	0.39
63	10.312	Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-	C ₁₅ H ₂₄	204	0.60
64	10.590	Diazoacetic acid, 2-isopropyl-5-methylcyclohexyl ester	C ₁₂ H ₂₀ N ₂ O ₂	224	0.54
65	10.631	Kaur-16-ene	C ₂₀ H ₃₂	272	1.04
66	10.698	Bicyclo[11.3.0]hexadecane-2,14-dione	C ₁₆ H ₂₆ O ₂	250	0.45
67	10.740	3,3,6,6-Tetramethyl-1,2,3,4,5,6,7,8-octahydroacridine	C ₁₇ H ₂₅ N	243	1.61
68	11.283	19-Hydroxy-3 α ,5-cyclo-5 α -androstan-17-one	C ₁₉ H ₂₈ O ₂	288	1.44
69	16.063	cis-4,4-Dimethylbicyclo(6.3.0)undecane-2,6-dione	C ₁₃ H ₂₀ O ₂	208	1.89
70	16.647	2-Heptenoic acid, 4-cyclopropyl-5-methylene-, methyl ester, (E)-	C ₁₂ H ₁₈ O ₂	194	1.23
71	18.882	cis-4-Acetoxy-trans-1-(m-methoxyphenyl)cyclohexanecarbonitrile	C ₁₆ H ₁₉ NO ₃	273	11.52



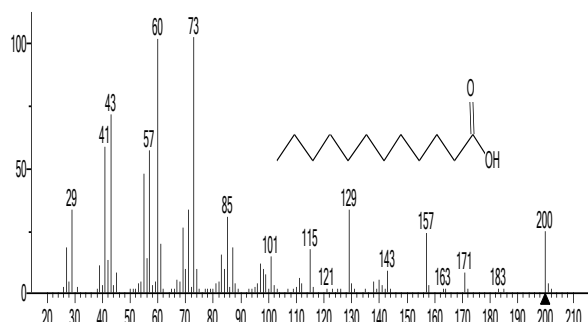




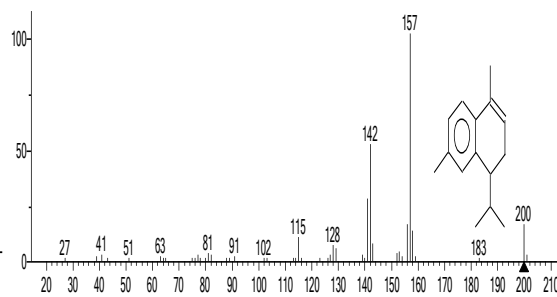
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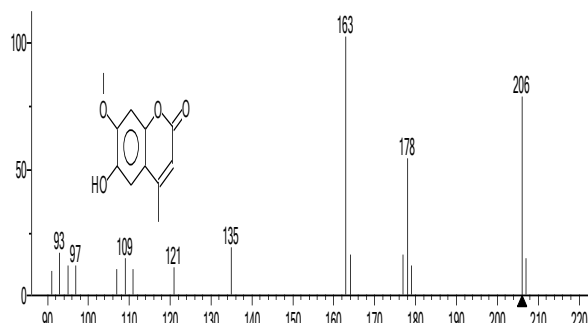
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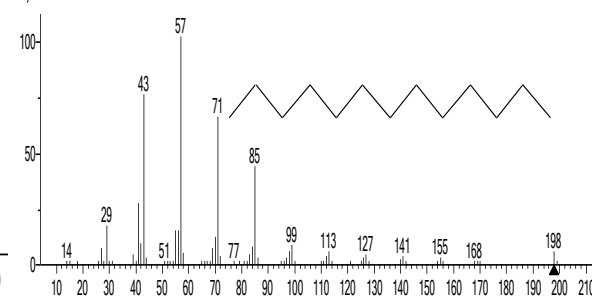
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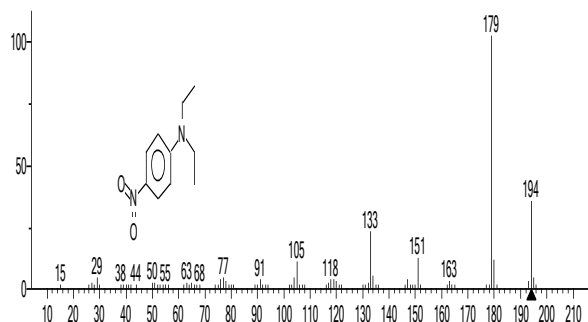
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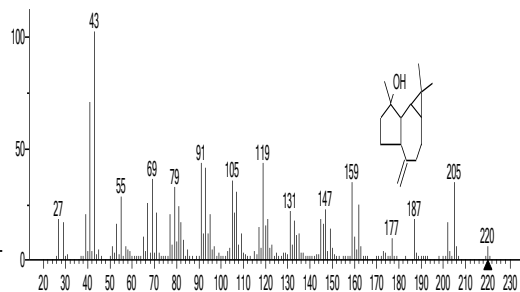
(mainlib) 2H-1-Benzopyran-2-one, 6-hydroxy-7-methoxy-4-methyl-



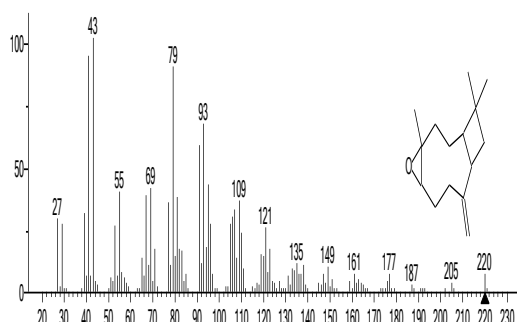
(mainlib) Tetradecane



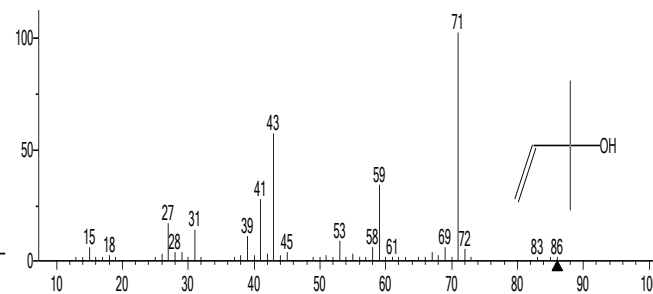
(mainlib) N,N-Diethyl-p-nitroaniline



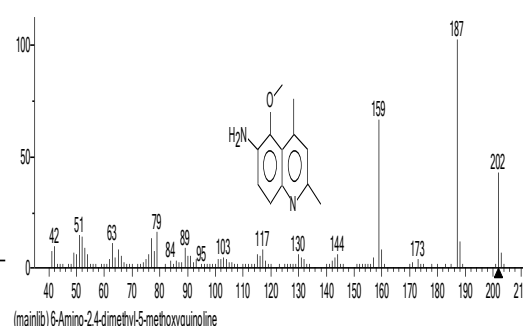
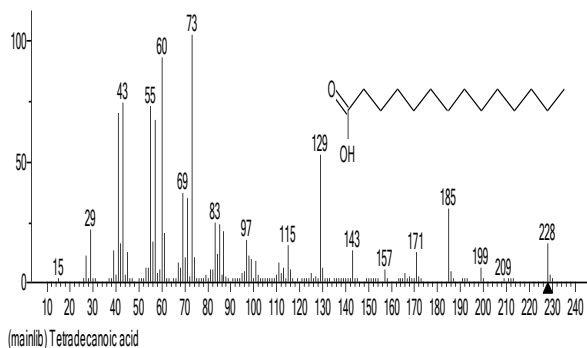
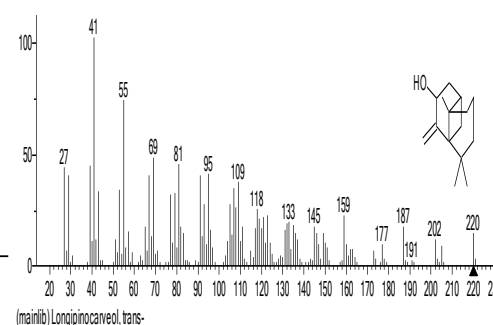
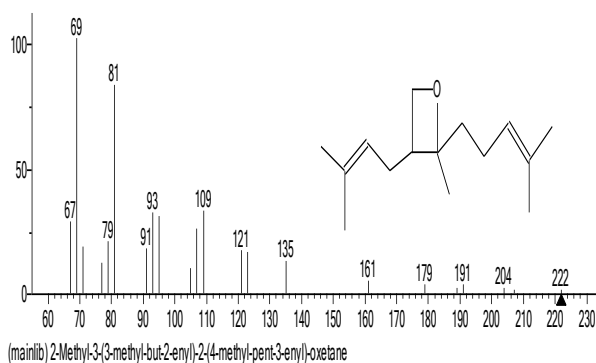
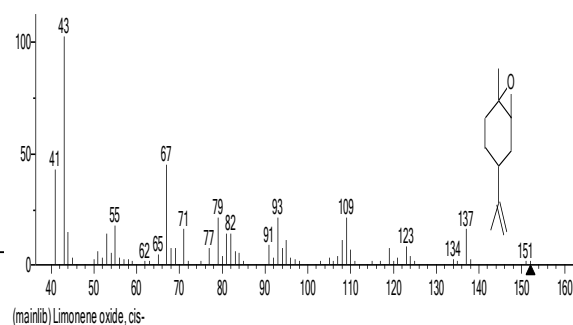
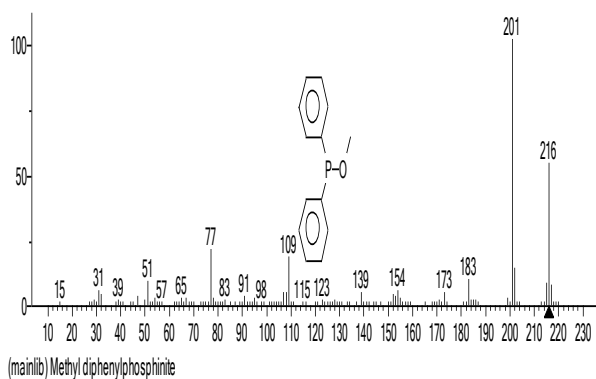
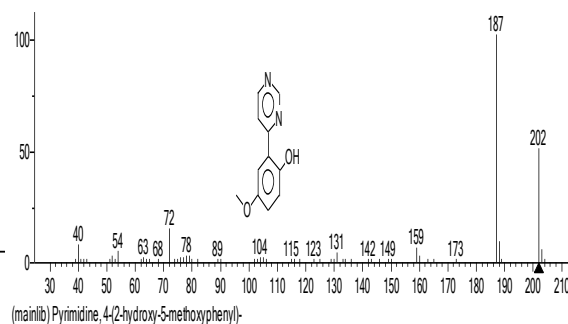
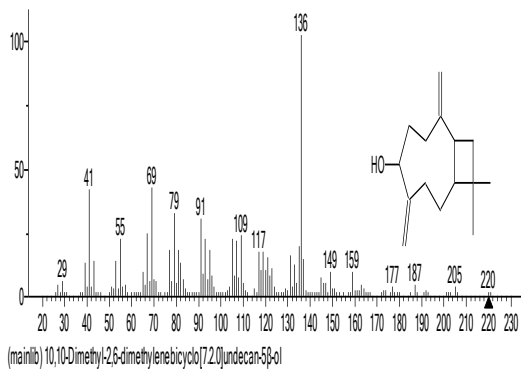
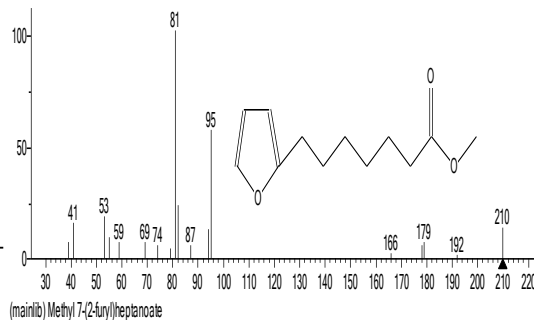
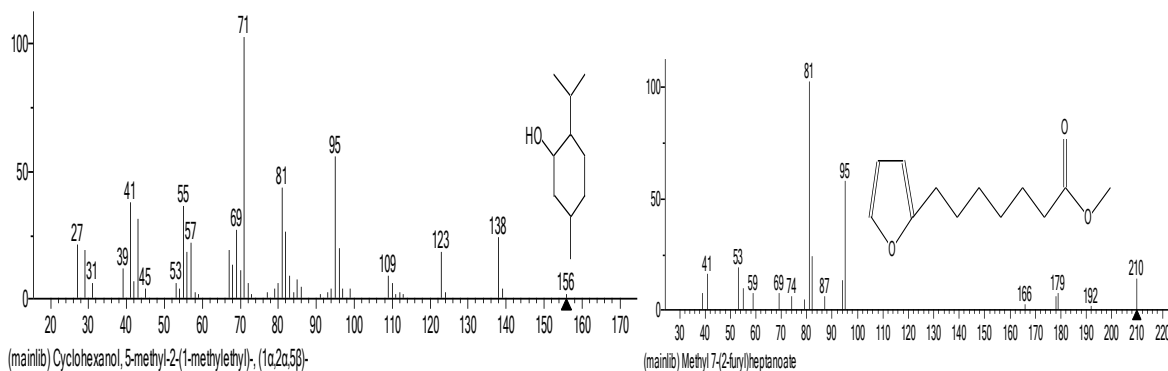
(mainlib) (-)-Spathulenol

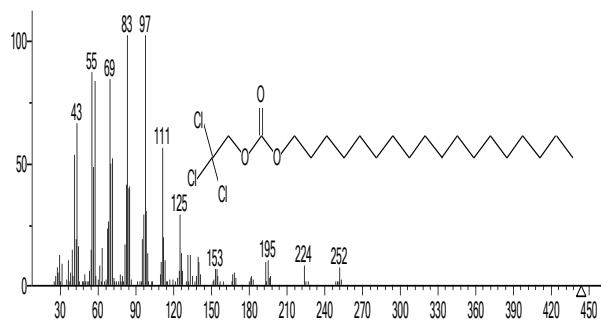


(mainlib) Caryophyllene oxide

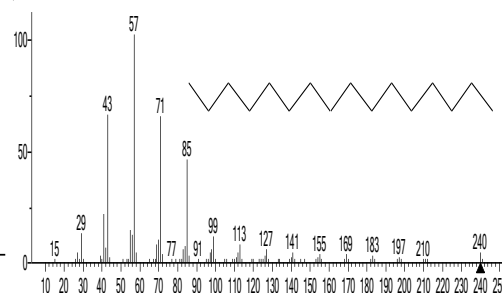


(mainlib) 3-Buten-2-ol, 2-methyl-

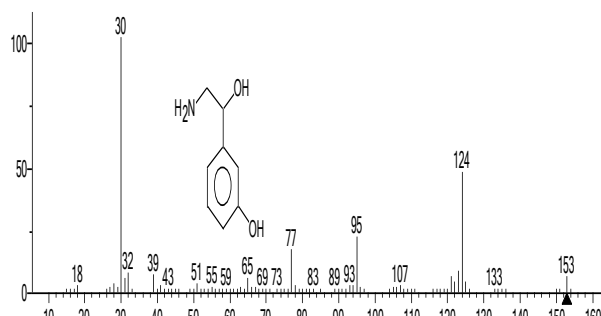




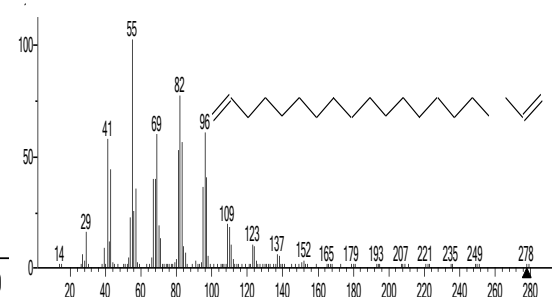
(mainlib) Carbonic acid, octadecyl 2,2,2-trichloroethyl ester



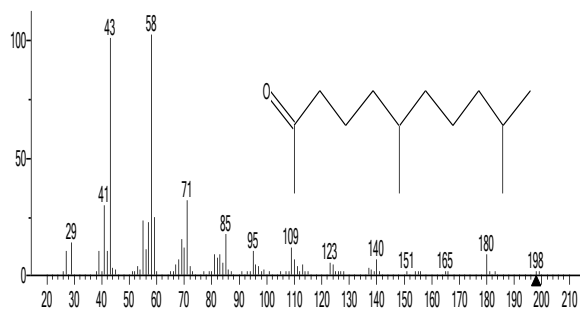
(mainlib) Heptadecane



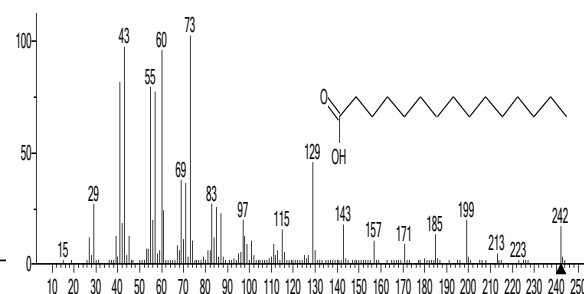
(mainlib) Norfenefine



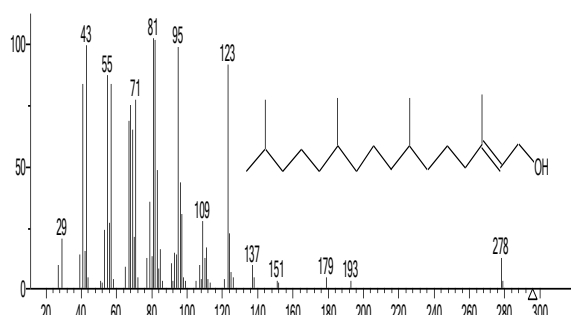
(mainlib) 1,19-Eicosadiene



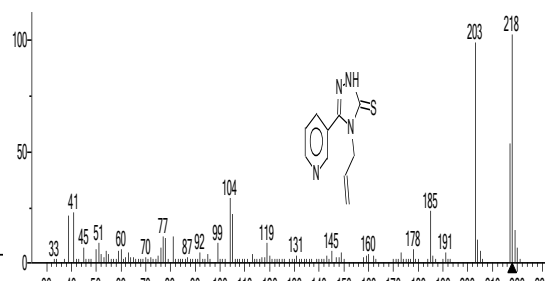
(mainlib) 2-Undecanone, 6,10-dimethyl-



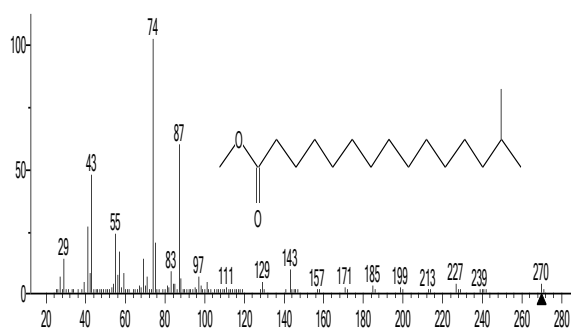
(mainlib) Pentadecanoic acid



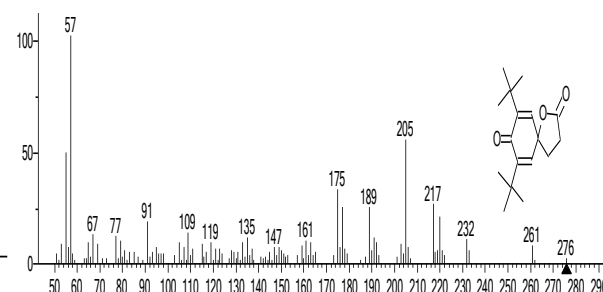
(mainlib) 3,7,11,15-Tetramethyl-2-hexadecen-1-ol



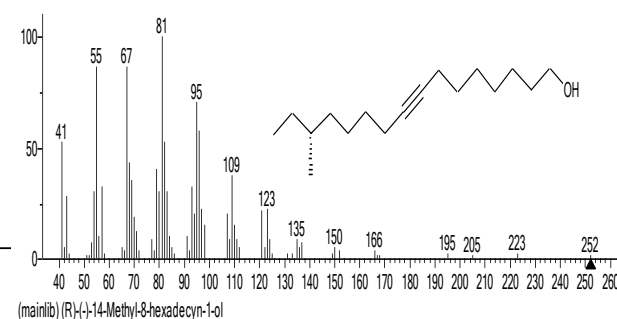
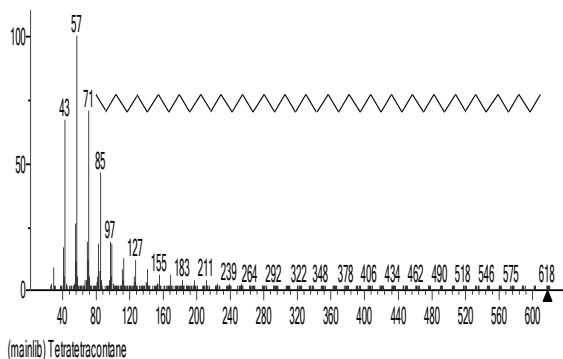
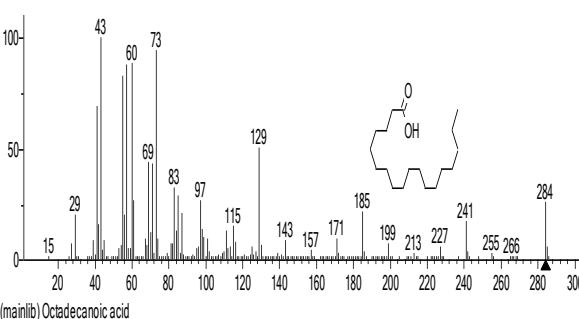
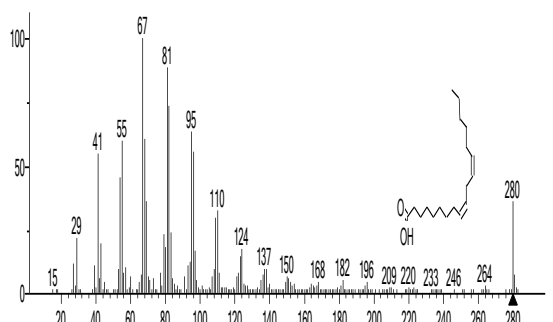
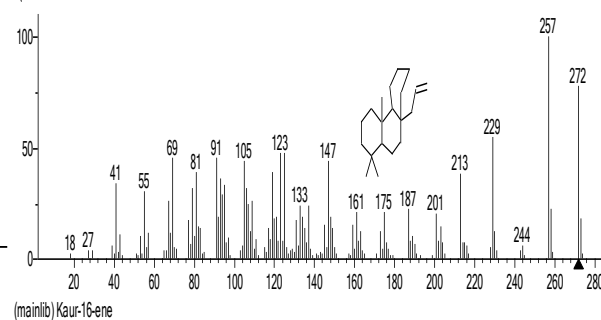
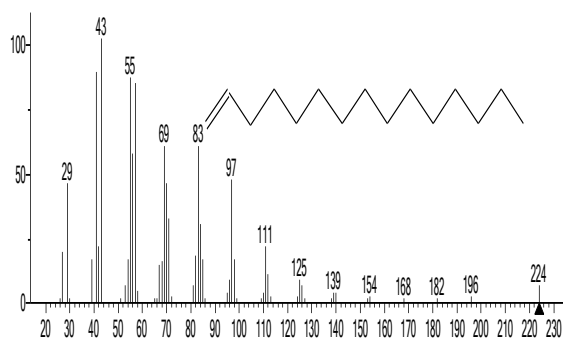
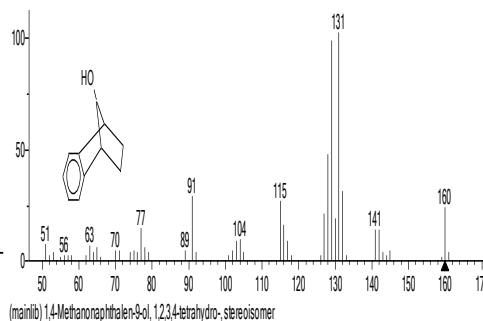
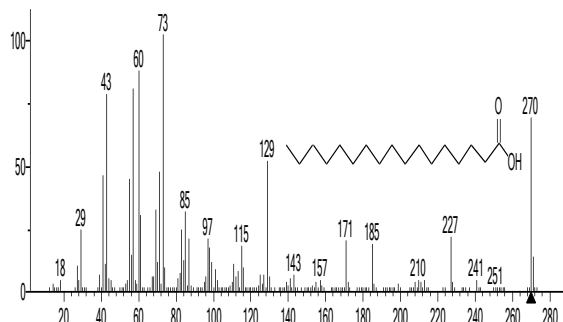
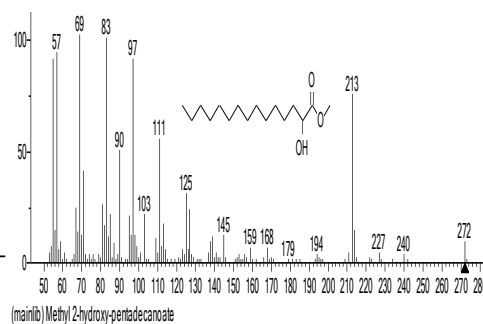
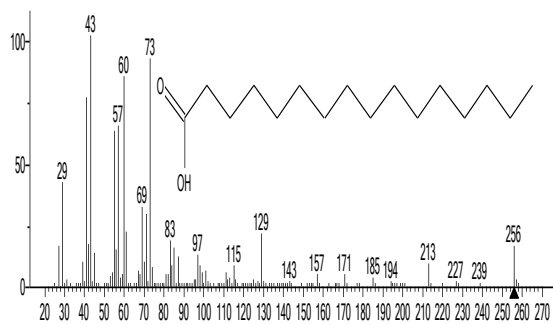
(mainlib) 4-Allyl-5-pyridin-3-yl-2,4-dihydro-1,2,4-triazole-3-thione



(mainlib) Pentadecanoic acid, 14-methyl-, methyl ester



(mainlib) 7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione



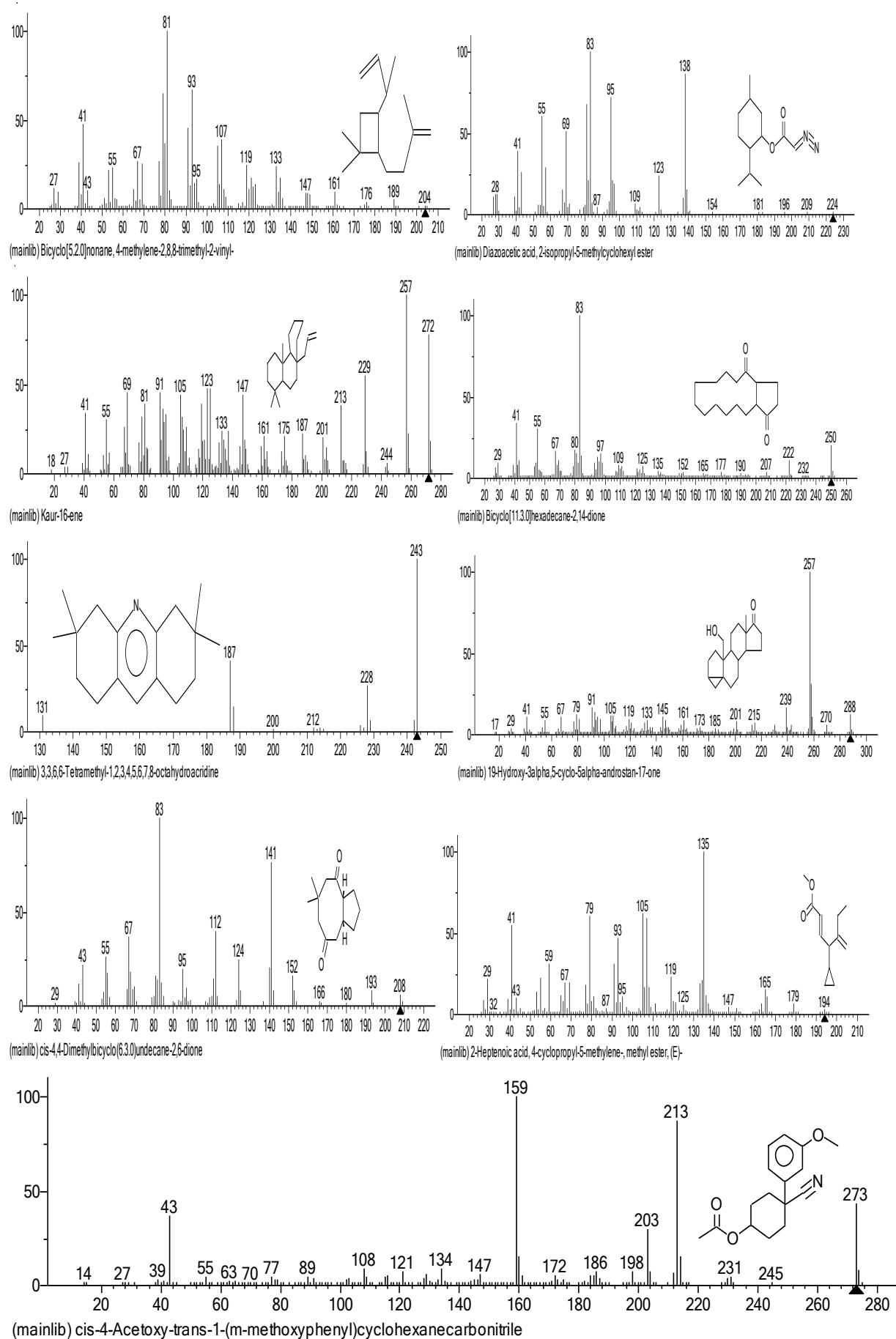


Figure 2. GC-MS of Mass Spectra *Ageratum conyzoides* whole plant chloroform extract

4. CONCLUSION

This present study revealed the presence of seventy one components in *Ageratum conyzoides* through GC-MS analysis. The plant specie used in this study has been discovered to possess promising medicinal potentials. This study has suggests that chloroform extract contain more of the phytochemicals. The presence of bioactive components justifies the use of the plant for various ailments by traditional practioners. In view of the medicinal importance associated with the phytocompounds found in this plant, further investigation should be carried out in order to purify, characterize the structure of these bioactive compounds and enhance their potentials as drugs.

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