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GC–MS Analysis of Ethanol Root Extract of *Datura stramonium*

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ABSTRACT: Identification of the phyto constituents present in the ethanolic root extract of *D. stramonium.* The structural formula of the phytochemicals of *D. stramonium* root extract were determined by analysing of the spectra of GC-MS using the reference standard of National Institute of Standard and Technology (NIST). GC-MS analysis of D. stramonium root showed the presence of nineteen bioactive compounds. The compounds are Eburnamenin-14-ol, 14,15-dihydro-,(14);2,3-dihydro-1H-cyclopenta[4,5]pyrimido[1,2-a]benzimidazol-11-ol; bis[4-[m-hydroxyanilino]-3-nitrophenyl]sulfone; acetamide, 2,2,2-trifluoro; 3,3-dimethoxycarbonyl-cis-(2,2')(5,5')pyridinophane; butylphosphonic acid, 2,6-dimethoxyphenyl nonyl ester; iso-Valeraldehyde propyleneglycol acetal; iso-Valeraldehyde propyleneglycol acetal; 11-oxatetracyclo[6.2.1.0(2,7).0(3,6)]undec-9-ene, 2,3,4,4,5,5,6,7-octafluoro; (E)-1-methylsulfinyl-2-phenylethene; isovaline, 3-hydroxy; valeric acid, 2-diethylaminoethyl ester; N-(2-nitro)benzylidene-2-(4-methylphenylthio)aniline; mitragynine; methyl 3',27-dihydroxyolean-12-en-28-oate; 4H-naphtho[2,3-b]pyran-4-one, 5,10-bis(acetyloxy)-2,3-dihydro-3-hydroxy-2-methyl-, trans; trans-2,3-Bis(2,4,5-trimethyl-3-thienyl)-2,3-dihydrofuro[2,3-f][4,7]phenanthroline;3,8-dioxa-11-azatetracyclo[4.4.1.0 (2,4).0(7,9)] undecane, 11-(phenylsulfonyl)-, (1',2',4',6',7(,9β); phenol, 2,2'-[(hydroxyimino)bis(4,5-dihydro-5,3-isoxazolediyl)]bis. It was concluded that the bioactive compounds support the use of *D. stramonium* root for the management of breast cancer, cancer of the esophagus, anaphylaxis and Parkinson's disease.

KEYWORDS: Bioactivity, *D. stramonium,* ethanol, gas chromatography, mass spectra, plant,

I. INTRODUCTION

D. stramonium is an annual, erect, branching herb with a foul-smell. It forms a bush up to 60 to 150 cm (2 to 5 ft) height [1]. It has a white fibrous long thick root while the stem is leafy with a yellow-green to reddish purple color [2]. The leaves of *D. stramonium* are long, smooth, toothed, soft and irregularly undulated with a length of about 8 to 20 cm (3–8 in) [2] .The upper surface of the leaves are dark green, while the bottom is light green in colour [1].The leaves taste bitter and nauseating. The bitter and nauseating taste remains even after drying and extraction [2].

The active agent in *D. stramonium* is atropine. Atropine has been used in herbal medicine and recreational activities over the years [3]. Generally, the leaves are smoked either in a cigarette or in a pipe [4,5]. *D. stramonium* are used as analgesic to render patients unconscious while broken bones were healed [6]. The Asians used it as a form of anesthesia during surgical operations [7]. *D. stromonium* is culturally used in management of inflammation. Gupta and Co-workers [8] subjects ethanol extract of *D. stromonium* leaves to preliminary anti-inflammatory activity screening in albino rats. They reported that ethanol extracts of *D. stromonium* leaves exhibited significant anti-inflammatory activity against carrageenan induced rat paw edema when compared to diclofenac [8]

Many authors have reported the GC-MS analysis of plant extract [9-11]. In our previous publication we reported the GC-MS analysis *of D. stromonium* ethanol leave extract [12]. To the best of our knowledge, the GC-MS analysis of *D. stromonium* ethanol root extract has not been reported in literature. Biological active phytocomponents present in the leaves *of D. stromonium* root is hereby studied for future

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reference studies. This study is aimed at the determination of compounds present in *D. stromonium* ethanol root extract by GC–MS analysis.

II. EXPERIMENTATION

a) Plant sample

Fresh *D. stromonium* root were harvested from Ohafia, Abia State Nigeria on 25th June, 2020. The leaves were identified by a Botanist at the Department of Plant Science and Biotechnology, MOUAU, Nigeria.

b) Extraction of crude extracts

The *D. stromonium* root were air dried at room temperature for 3 days. The dried roots were grounded using electric grinder. The powdered *D. stromonium root* were subjected to extraction using ethanol. The extract was then subjected to evaporation by using rotary evaporator.

c) GC-MS Analysis

The GC–MS spectra of bioactive compounds of *D. stromonium* root extracts were analysed using agilent 6890N gas chromatography equipped with an auto sampler connected to an agilent Mass Spectrophotometric Detector . A micro-litre of sample was injected in the pulsed spitless mode onto a 30m x 0.25 mm ID DB 5MS coated fused silica column with a film thickness of 0.15 micrometer. Helium gas was used as a carrier gas and the pressure of the column head was maintained at 20 psi to give a constant of 1ml/min. The temperature of the column was held initially at 55 ^{o}C for 0.4 min and then raised to 200 ^{o}C at a rate of 25 ^{o}C/mins,. It was increased to 280 ^{o}C at a rate of 8 ^{o}C/mins and to a final temperature of 300 ^{o}C at a rate of 25 ^{o}C/mins for 2 mins . The identification time was based on retention time. Components with lower retention time eluted first before the ones of higher retention time.

d) Identification of chemical constituents

The structural formula of the compounds present in ethanol extract of *D. stromonium* root were ascertained by the interpretation of mass spectrum of GC-MS using the reference standard of NIST library. The mass spectra of the unknown compounds were cross-marched with the spectra of the known compounds stored in the NIST library.

III. RESULTS AND DISCUSSION

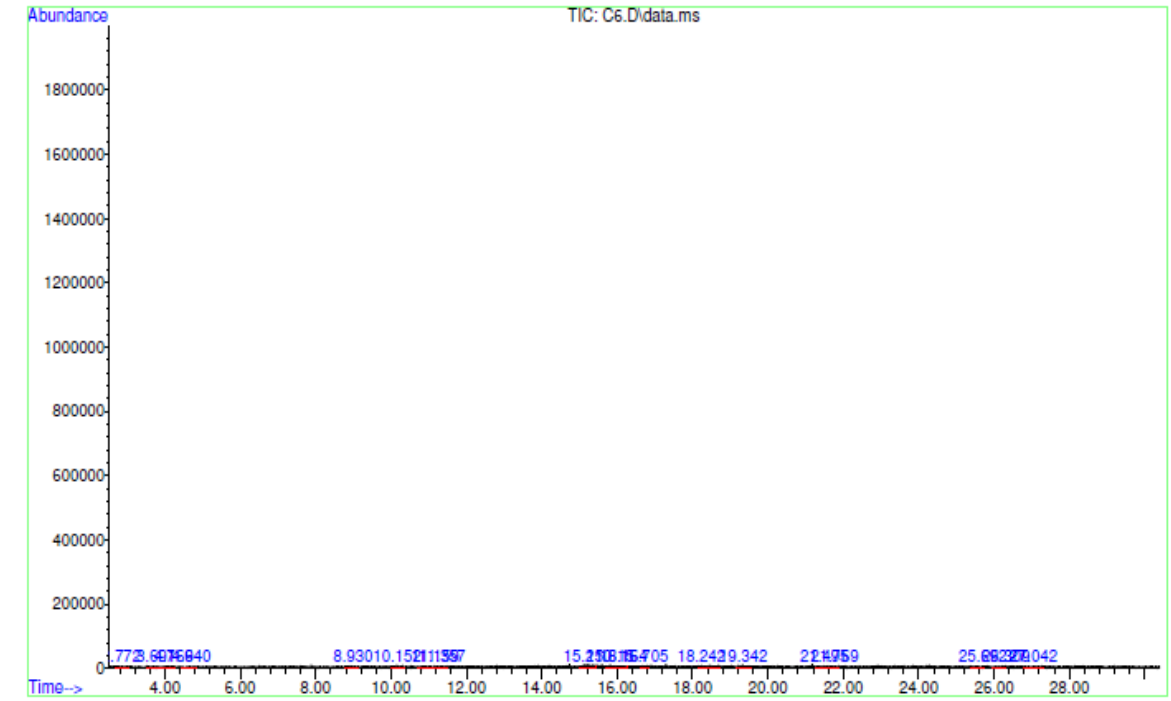

Figure 1: Gas chromatogram of *D. stromonium* ethanol root extract

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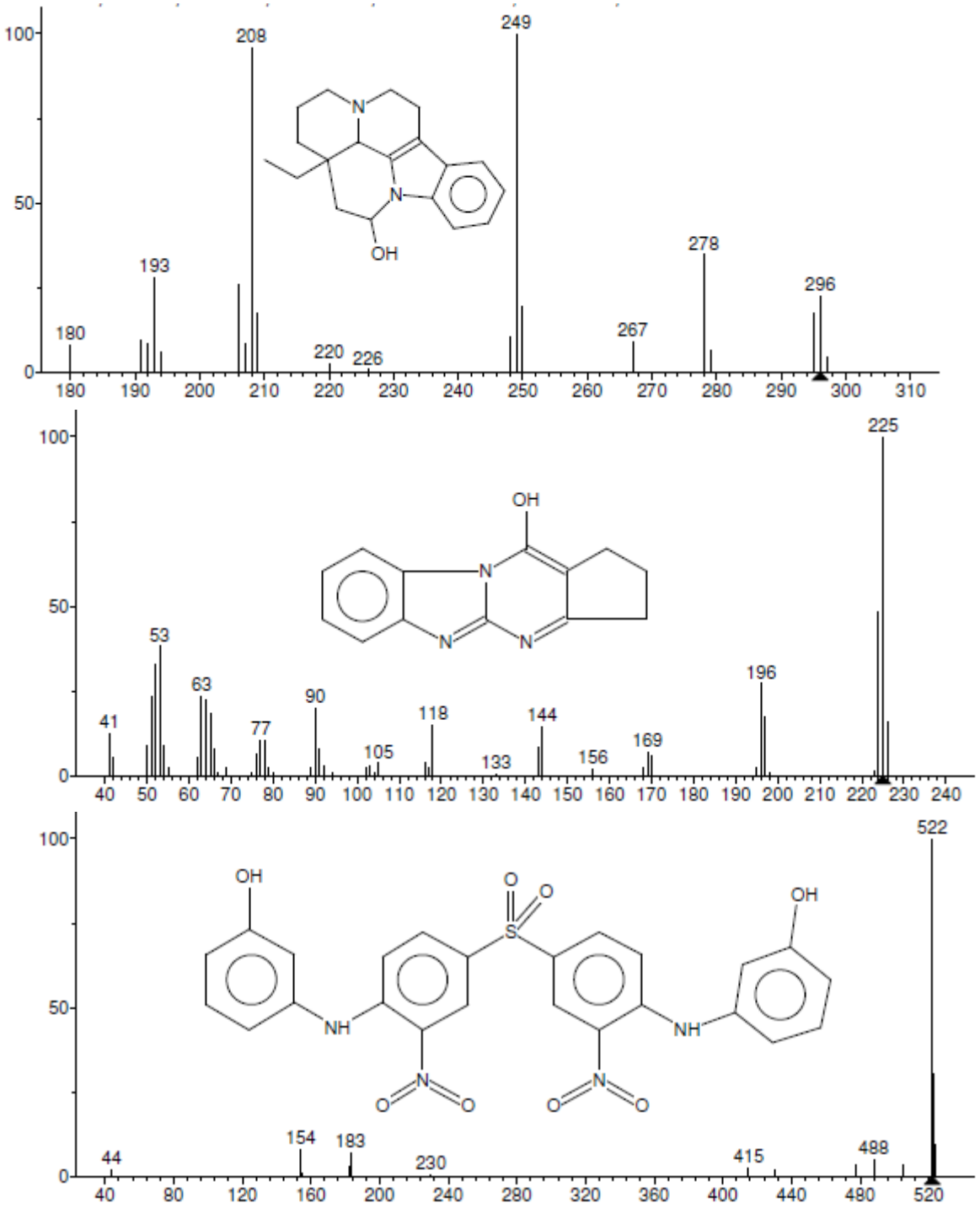

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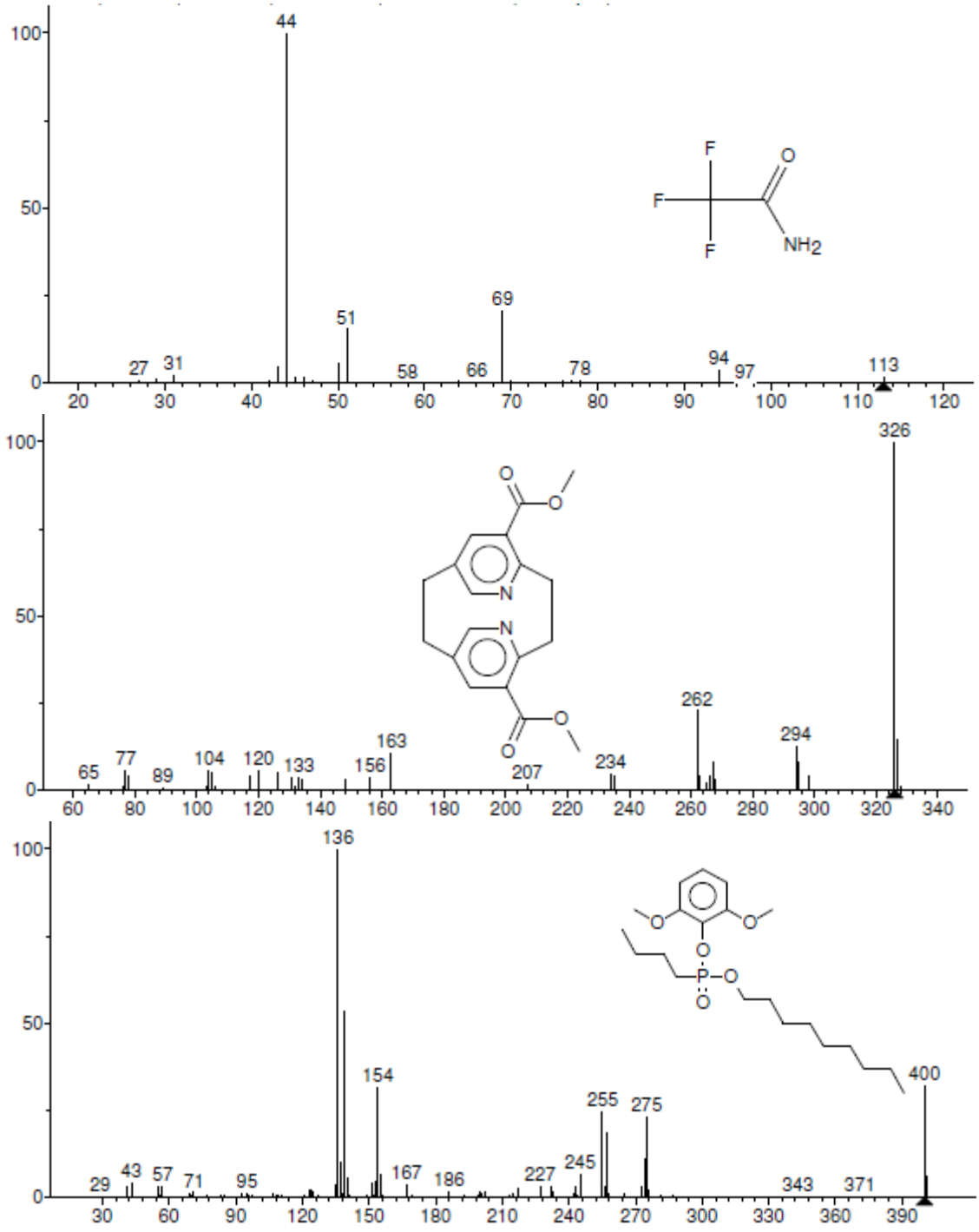

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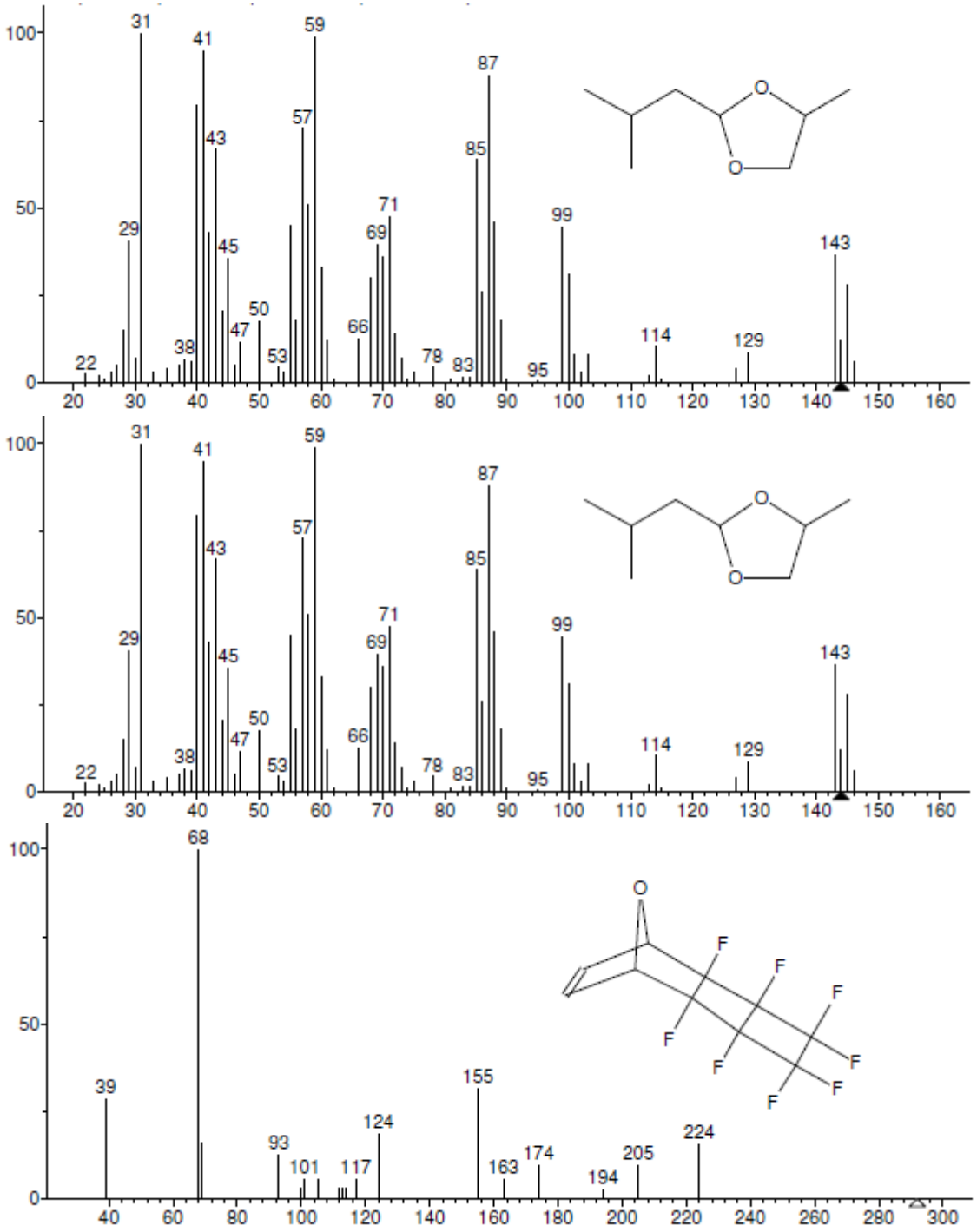

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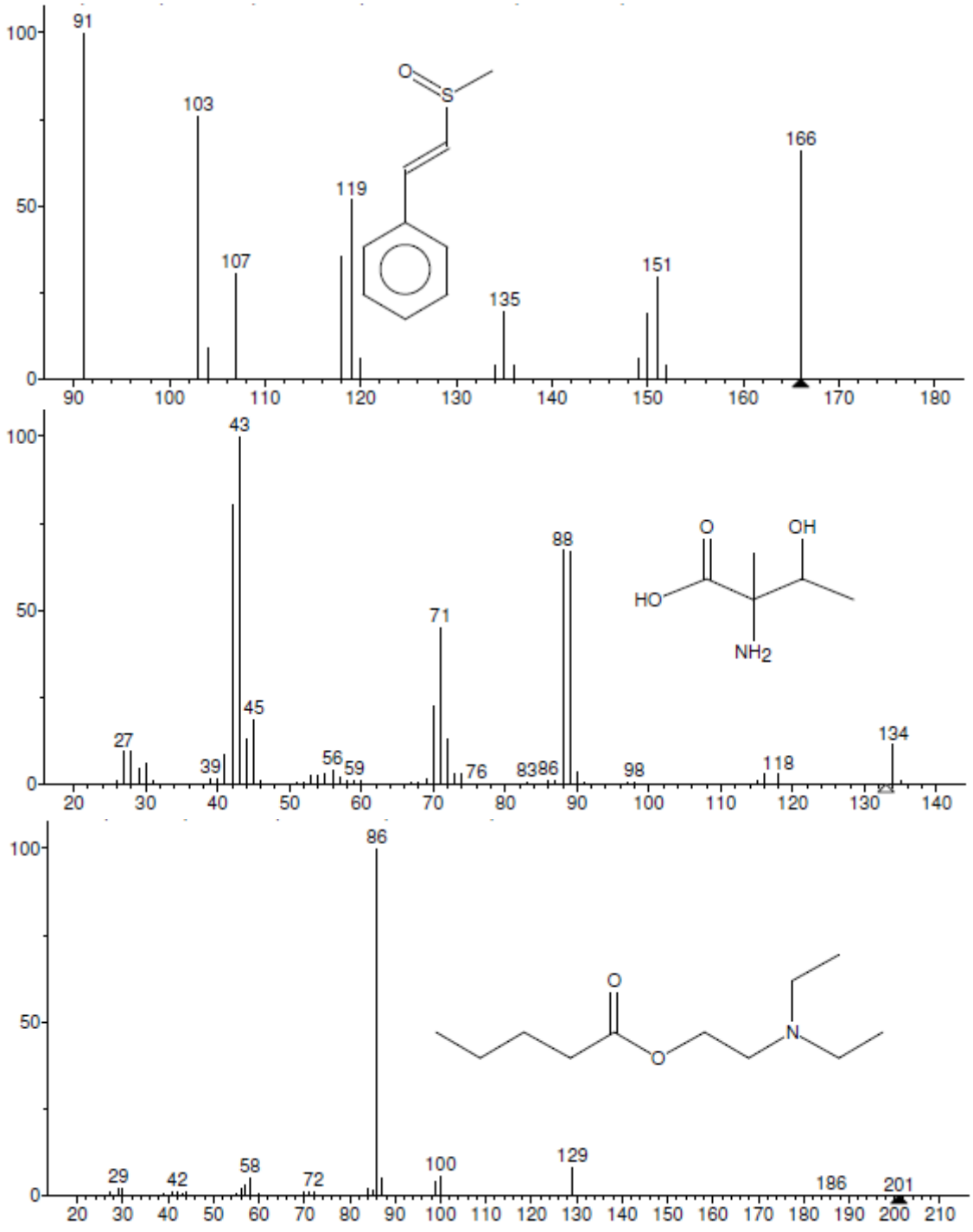

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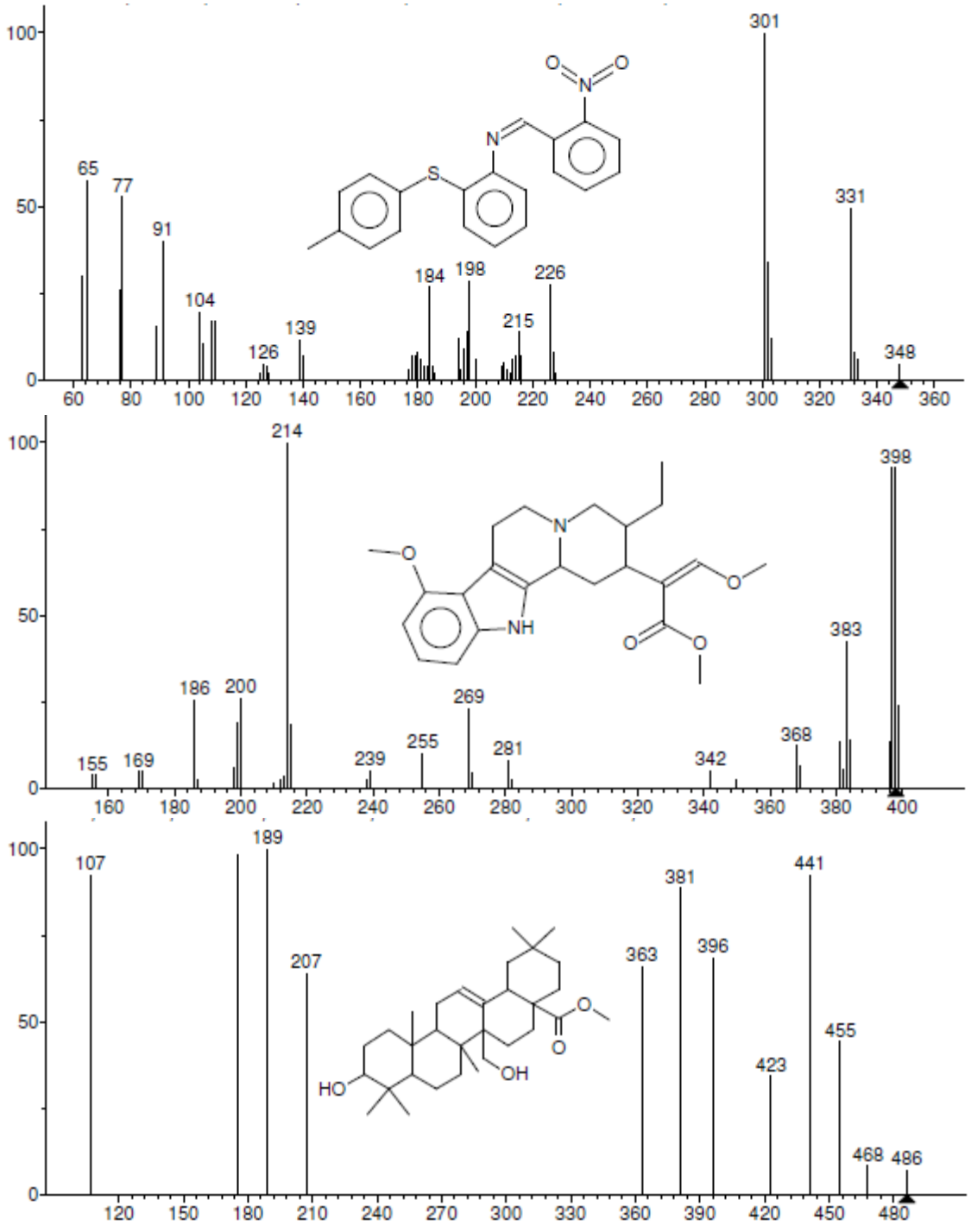

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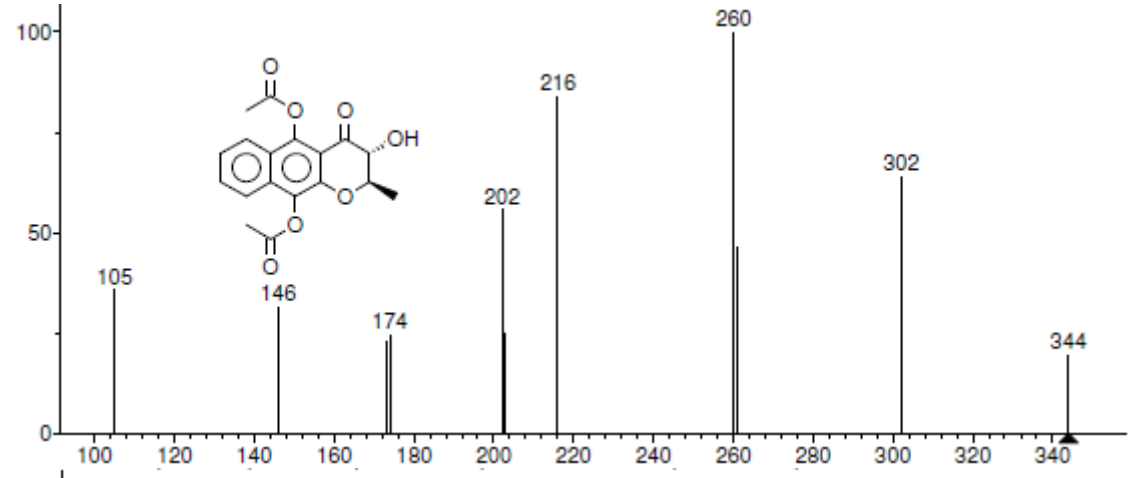

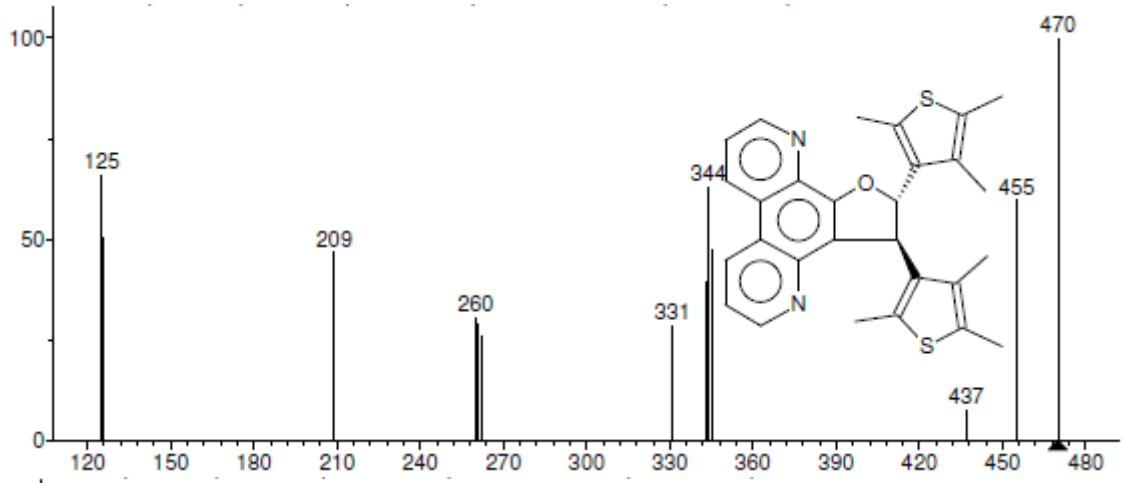

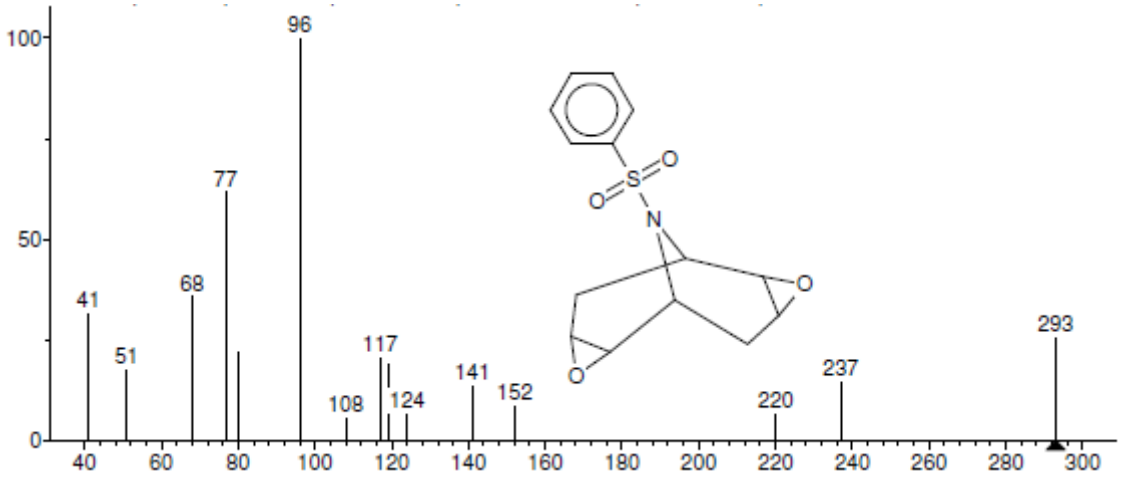

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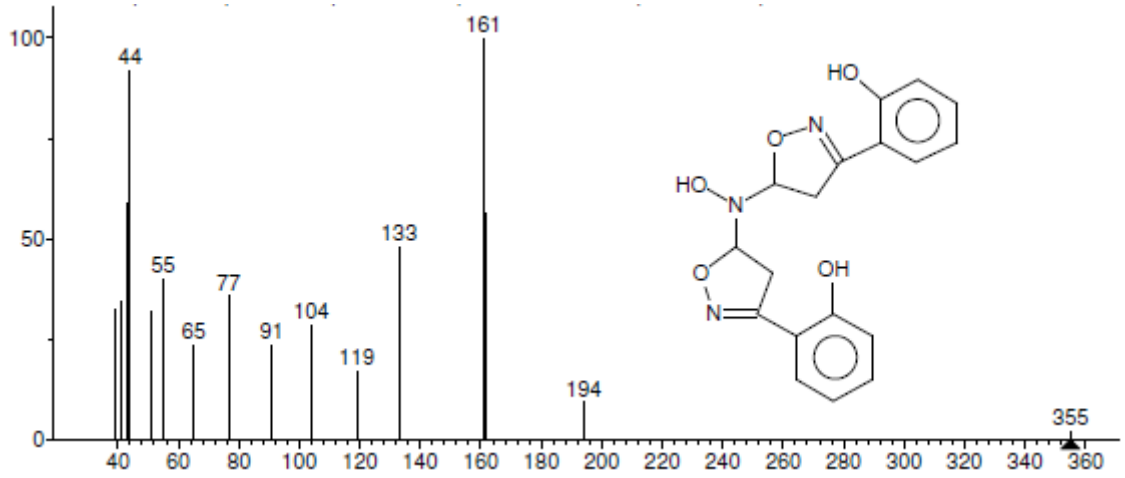

Figure 2: Mass spectra bioactive compounds present in ethanol extract of *D. stranonium* root

Table 1: Bioactive compounds present in ethanol extract of *D. stranonium* root

S/No	Compound	Bioactivity
1	Eburnamenin-14-ol, 14,15-dihydro-, (14)	Oligosaccharide Provider
2	2,3-Dihydro-1H-cyclopenta[4,5]pyrimido[1,2-a]benzimidazol-11-ol	Not found
3	Bis[4-[m-hydroxyanilino]-3-nitrophenyl]sulfone	Not found
4	Acetamide, 2,2,2-trifluoro	Not found
5	3,3-Dimethoxycarbonyl-cis-(2,2')(5,5')pyridinophane	Not found
6	Butylphosphonic acid, 2,6-dimethoxyphenyl nonyl ester	Increase Aromatic Amino Acid Decarboxylase Activity, Arachidonic acid-Inhibitor
7	Iso-Valeraldehyde propyleneglycol acetal	Not found
8	Iso-Valeraldehyde propyleneglycol acetal	Not found
9	11-Oxatetracyclo[6.2.1.0(2,7).0(3,6)]undec-9-ene, 2,3,4,4,5,5,6,7-octafluoro	Not found
10	(E)-1-Methylsulfinyl-2-phenylethene	Anticancer (Esophagus)
11	Isovaline, 3-hydroxy	17-beta-hydroxysteroid dehydrogenase-Inhibitor
12	Valeric acid, 2-diethylaminoethyl ester	Increase Aromatic Amino Acid Decarboxylase Activity, Arachidonic acid-Inhibitor
13	N-(2-Nitro)benzylidene-2-(4-methylphenylthio)aniline	Anaphylactic (antidote)
14	Mitragynine	Not found
15	Methyl 3',27-dihydroxyolean-12-en-28-oate	Catechol-O-Methyltransferase-Inhibitor, Methyl-Guanidine-Inhibitor
16	4H-Naphtho[2,3-b]pyran-4-one, 5,10-bis(acetyloxy)-2,3-dihydro-3-hydroxy-2-methyl-, trans	Not found
17	trans-2,3-Bis(2,4,5-trimethyl-3-thienyl)-2,3-dihydrofuro[2,3-f][4,7]phenanthroline	Not found
18	3,8-Dioxa-11-azatetracyclo[4.4.1.0(2,4).0(7,9)]undecane, 11-(phenylsulfonyl)-, (1',2',4',6',7(,9β)	Not found
19	Phenol, 2,2'-[(hydroxyimino)bis(4,5-dihydro-5,3-isoxazolediyl)]bis	Not found

Bioactive compounds present in ethanol extract of *D. stranonium* root have been presented in Table 1. *D. stranonium* root have been reported as oligosaccharide provider, aromatic amino acid decarboxylase activity inducer, arachidonic acid-inhibitor, anticancer (esophagus), 17-beta-hydroxysteroiddehydrogenaseinhibitor,anaphylactic(antidote), catechol-O-methyltransferase-inhibitor, methyl-guanidine-inhibitor [13].

An oligosaccharide is a saccharide polymer that consist of three to ten monosaccharides. Oligosaccharides have numerous functions such as cell recognition and cell binding [14]. A typical example of oligosaccharide cell recognition is the role of glycolipids in determining blood types. Glycolipids also play vital role in the immune response [15].

Among all endocrine therapies for the treatment of breast cancer, inhibition of estrogen biosynthesis is becoming an interesting complementary approach to the use of antiestrogens. The enzyme 17-beta-hydroxysteroid dehydrogenase-Inhibitor (17beta-HSD) plays a critical role in the biosynthesis of estradiol catalyzing preferentially the reduction of estrone into estradiol, the most active estrogen. Consequently, this enzyme is an interesting biological target for designing drugs for the treatment of estrogen-sensitive diseases such as breast cancer [16].

Aromatic L-amino acid decarboxylase (AAAD) was discovered 70 years ago in mammalian tissue [17]. Its specific importance in pharmacology was established when it was demonstrated that its substrate L- DOPA relieved the clinical symptoms of Parkinson's disease (PD) [18-20] by supplementing lost dopamine from nigrostriatal neurons.

Catechol-O-methyltransferase inhibitors are category of medicines that are used along side carbidopa-levodopa therapy in the management of symptoms of Parkinson's disease. Catechol-O-methyltransferase inhibitors can extend the effectiveness of carbidopa-levodopa therapy, and permit for lower doses of carbidopa-levodopa [22].

Arachidonic acid and its metabolites have recently generated a heightened interest because of growing evidence of their significant role in cancer biology. Thus, inhibitors of arachidonic acid have originally been of interest in the management of inflammatory disorders and certain types of heart disease. They are now receiving increased attention as an arsenal against cancer [23].

Methylguanidine is a suspected uraemic toxin that accumulates in kidney failure; however it also exhibits anti-inflammatory effects. Recent evidence suggests that methylguanidine significantly inhibits nitric oxide synthase activity and tumor-necrosis factor (TNF) release [24]. This suggests that methylguandine can attenuate the degree of inflammation and tissue damage related to endotoxic shock.

IV. CONCLUSION

Nineteen compounds have been identified from the GC-MS analysis of ethanol extracts of *D. stranonium* root. The bioactive compounds support its use in the management of diseases like breast cancer, cancer of the esophagus, anaphylaxis and Parkinson's disease.

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