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GC–MS ANALYSIS OF PHYTOCHEMICALS PRESENT IN ETHANOL EXTRACT OF *Datura stramonium* LEAVES

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ABSTRACT

GC-MS analysis was carried out in order to investigate the phytoconstituents present in the ethanolic extract of *Datura stramonium* leaves. The structural formula of the phytochemicals of *D. stramonium* leaves 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* leaves showed the presence of eighteen bioactive compounds. The compounds are glycine N-methyl-n-propoxycarbonyl dodecyl ester, picolinyl 16-methyl-heptadec-9-enoate, isosilychristin hexaacetate, benzenetridecanoic acid, 4-methoxy-, 2-decyl-3-methoxy-5-pentylphenyl ester,1,3,3-Trimethyl-1-(2'-trimethylsilyloxyphenyl)-4-trimethylsilyloxyindane,naproxen, 2-Phenanthrenol, 1,2,3,4,4a,9,10,10a-octahydro-7-methoxy-1,1,4a-trimethyl, N,N'-bis(salicylidene)-3, 3'-bis(aminopropyl)aminocobalt(II), 2-methoxycarbony l-3-amino-6,7-dimethyl-quinoxaline, 1,3,4-thiadiazol-2-amine, 5-(ethylthio), cyclobutanone, 2,3,3,4-tetramethyl, phenol, 2,4,6-triiodo, butaperazine, 4-Iodohistidine, methyl ester, 5,12-naphthacenedione, 6,8,11-tris(acetyloxy)-8-[(acetyloxy)acetyl]-7,8,9,10-tetrahydro-1-methoxy,1,2,3,4-Tetrahydro-1-(4-methoxyphenyl)-2-phenylisoquinoline, 7-Isoquinolinol, 1,2,3,4-tetrahydro-6-methoxy-1-[(4-methoxyphenyl)methyl]-2,8-dimethyl, 2-(2-hydroxybenzylidene-amino)-3-pyrrolidin-1-yl-benzofuran. It was concluded that the phytocompounds support the use of *D. stramonium* leaves for the management of heavy metal overload, cancer, Parkinson's and cardiovascular diseases.

Keywords: Ethanol, *Datura stramonium* gas chromatography, mass spectra, plant

I. INTRODUCTION

Natural products have always played an important role in the management of human infections and diseases worldwide. The demand for medicinal natural product is increasing in both developed and developing countries due to recognition of their bioactivity. The use of herbal extract is a vital part of both cultural and modern system of medicines [1]. *Datura stramonium* is a fast growing annual plant from the Solanaceae family. It is a well recognized folklore medicinal herb. It is a widespread flowering plant and has been reported as a local source for tropane alkaloids, containing a methylated nitrogen group (N-CH_3) [2]. It also consist of anti-cholinergic drugs atropine, and scopolamine [2]. An extract made from the leaves of *D. stramonium* can be administered orally for the management of asthma and sinus infections. Stripped barks of the plant are rubbed externally to curb swellings, burns and ulcers [2]. The incidence of poisoning caused by *D. stramonium* has been associated with death and severe illness. The plant has anti-inflammatory property and can be use in stimulation of the central nervous system, alopecia, management of toothache, lungs decongestion, and management of dental and skin infections [2].

GC-MS characterization has been applied by many authors to identify compounds in natural products [3-5]. Analysis of biological active phytocomponents present in the leaves of *D. stramonium* has been studied for future reference studies on a common plant in Nigeria. There are few publications that demonstrate the compounds present in the ethanol extracts of *D. stramonium* leaves by GC-MS analysis. This study is aimed at the determination of compounds present in the *D. stramonium* leaves by GC–MS analysis.

II. METHODOLOGY

a) Plant sample

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

c) GC-MS Analysis

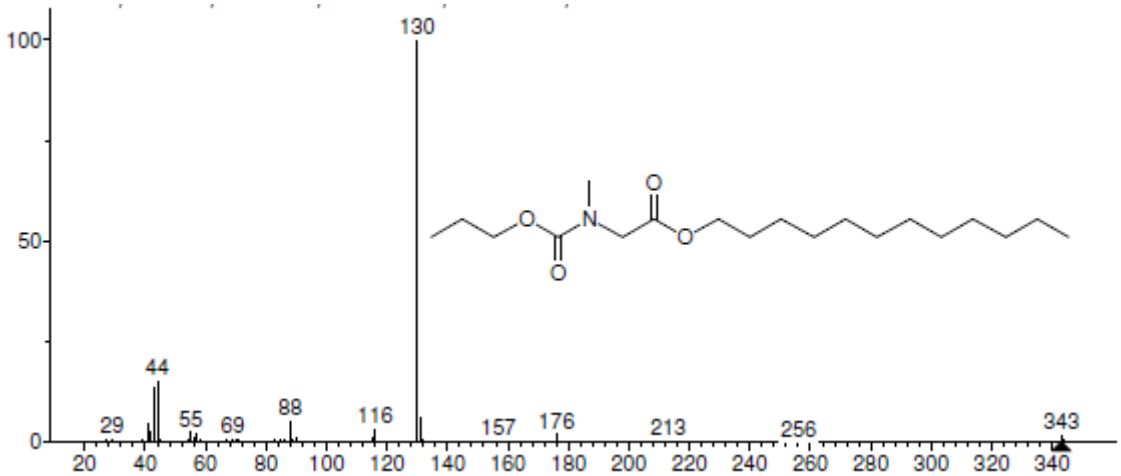
The GC–MS spectra of bioactive compounds of *D. stranonium* leaves extracts were analysed using agilent 6890N gas chromatography equipped with an auto sampler connected to an agilent Mass Spectrophotometric Detector . A micro-litre of sample was injected in the pulsed spitless mode onto a 30m x 0.25 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 ºC for 0.4 min and then raised to 200 ºC at a rate of 25 ºC/mins,. It was increased to 280 ºC at a rate of 8 ºC/mins and to a final temperature of 300 ºC at a rate of 25 ºC/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.

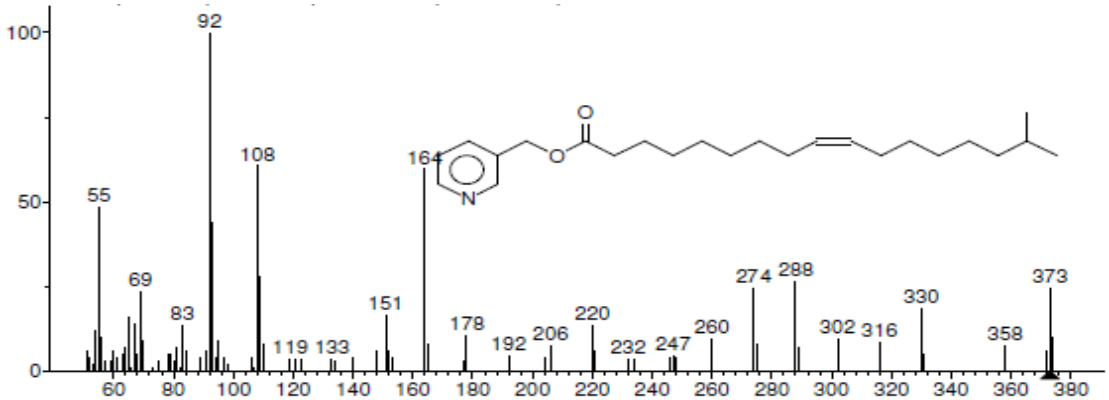
d) Identification of chemical constituents

The structural formula of the compounds present in ethanol extract of *D. stranonium* leaves 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 ethanol leaves extract of *Datura stranonium*

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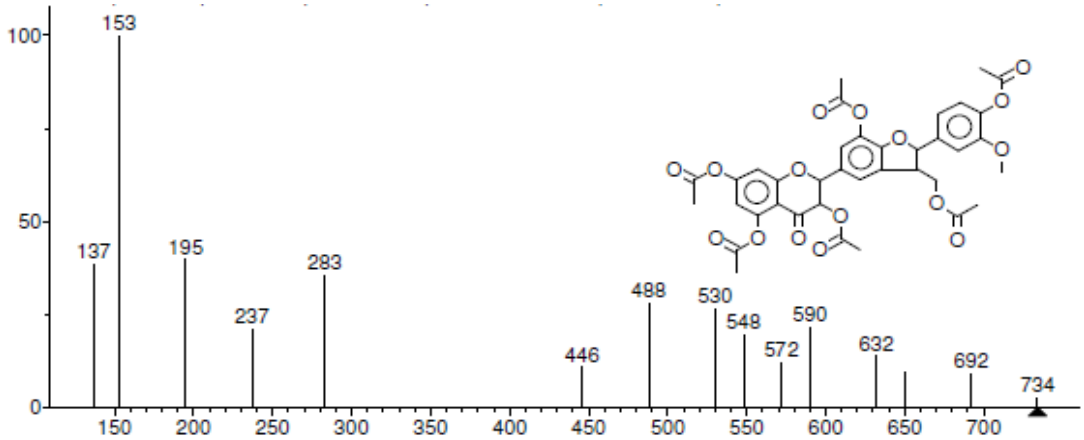
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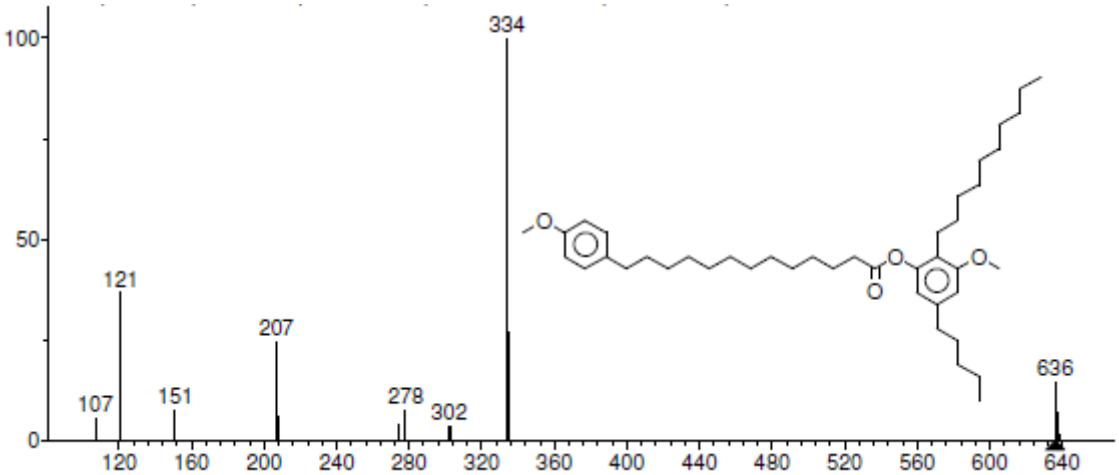
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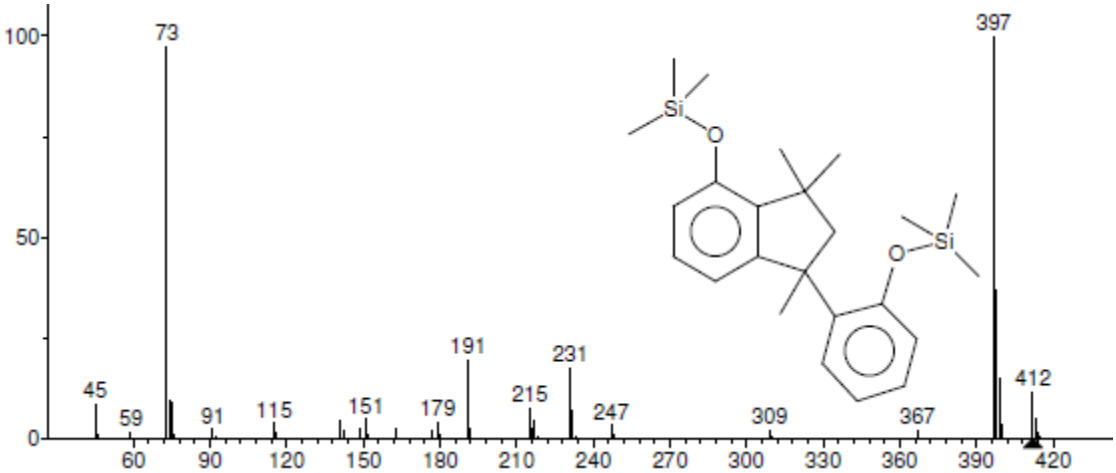
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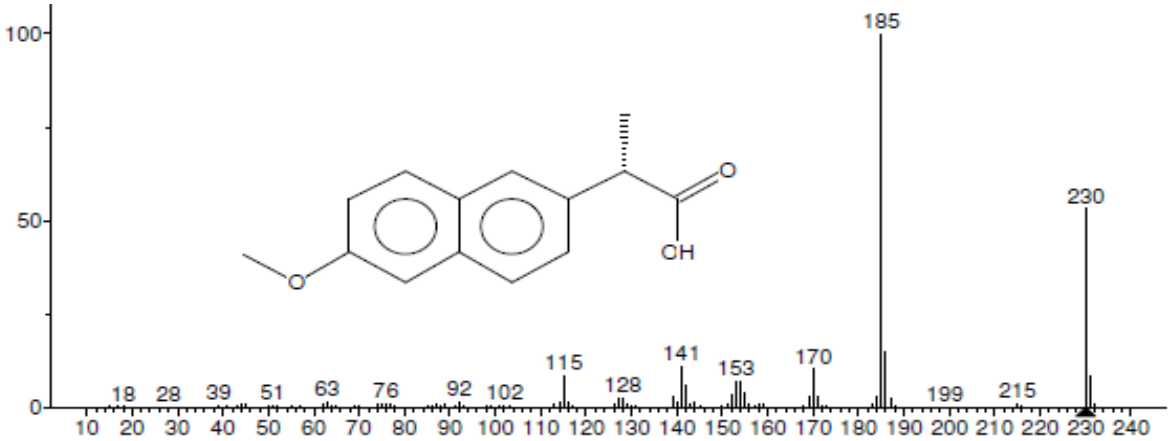
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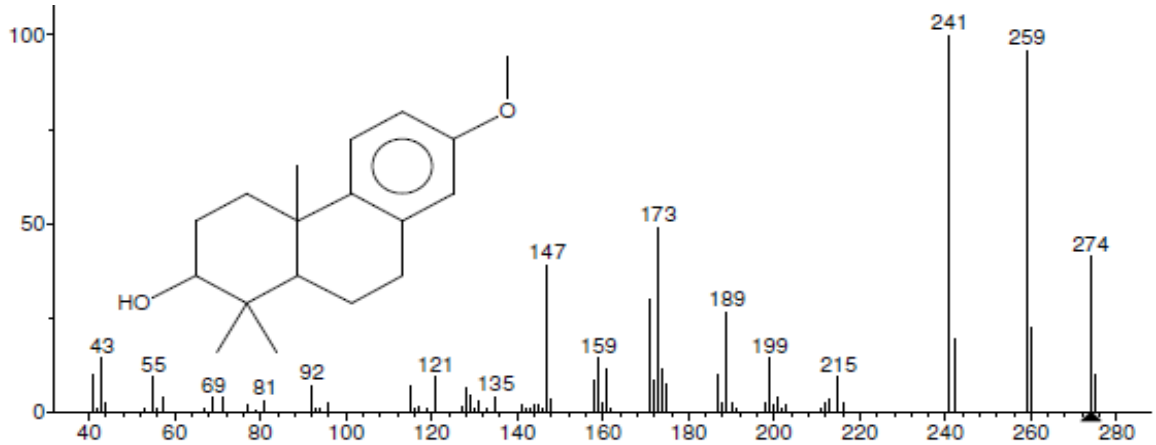
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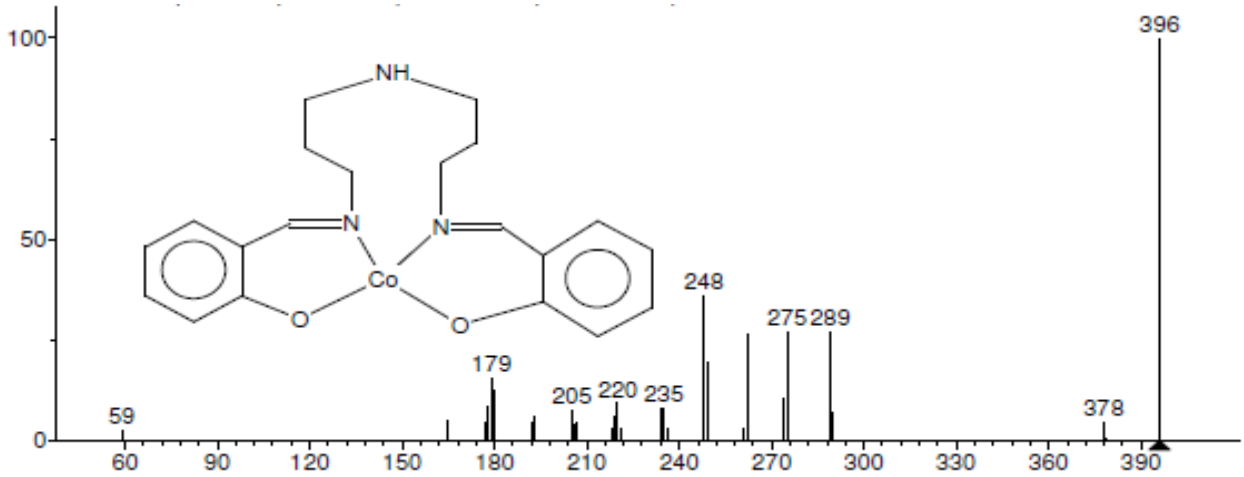
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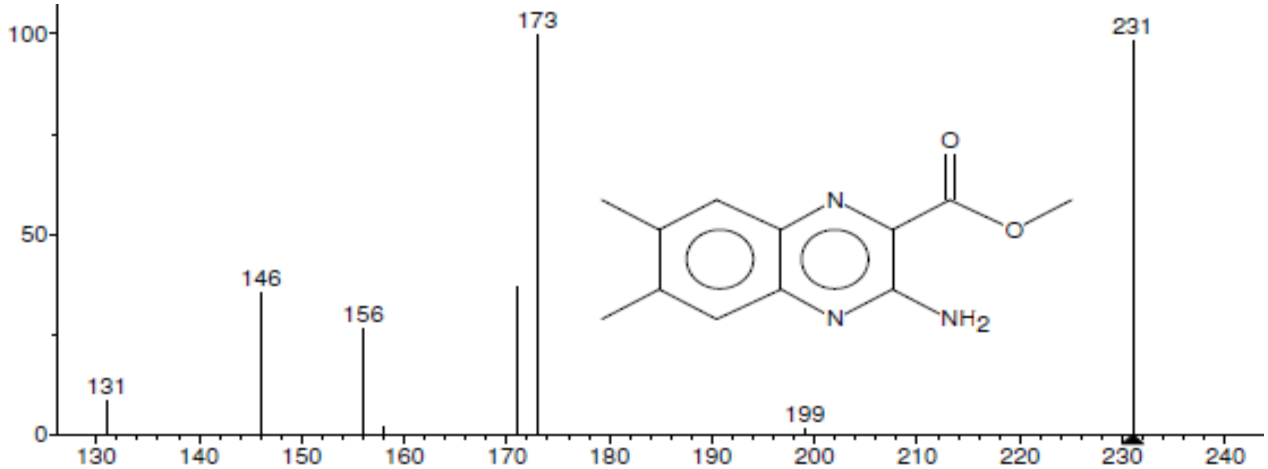
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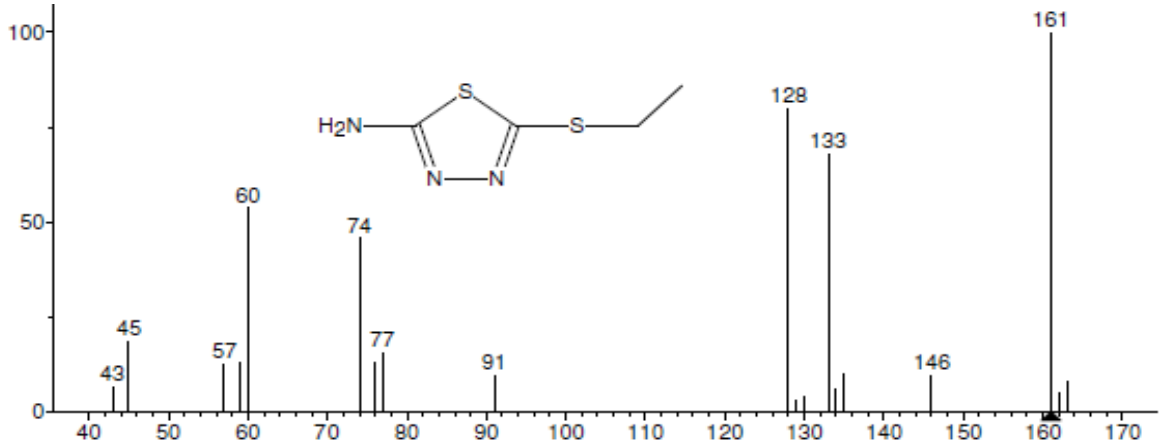
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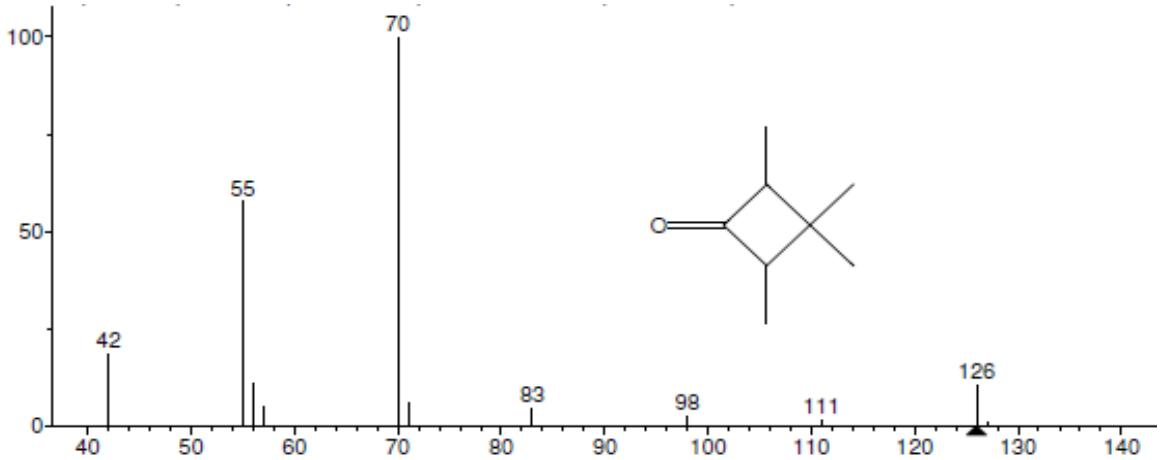
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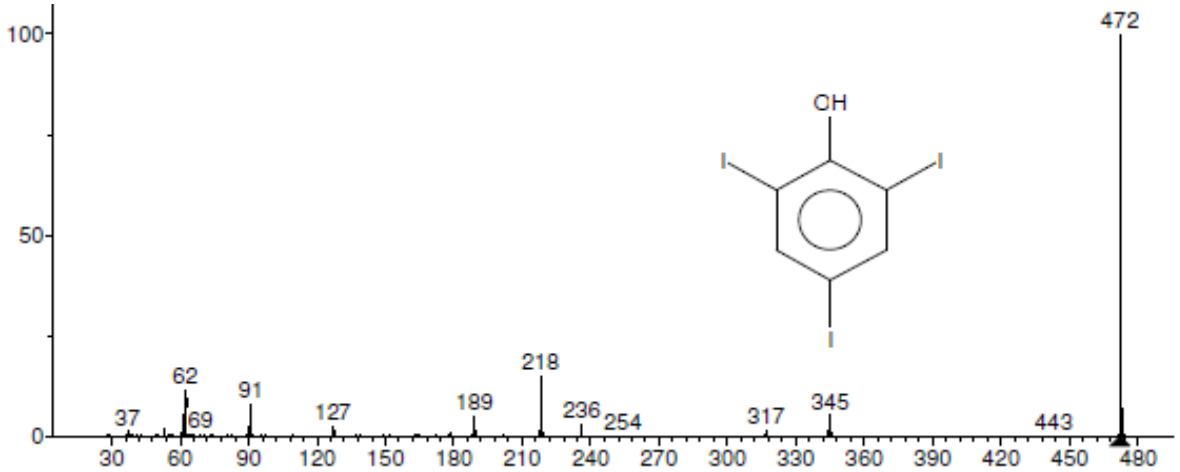
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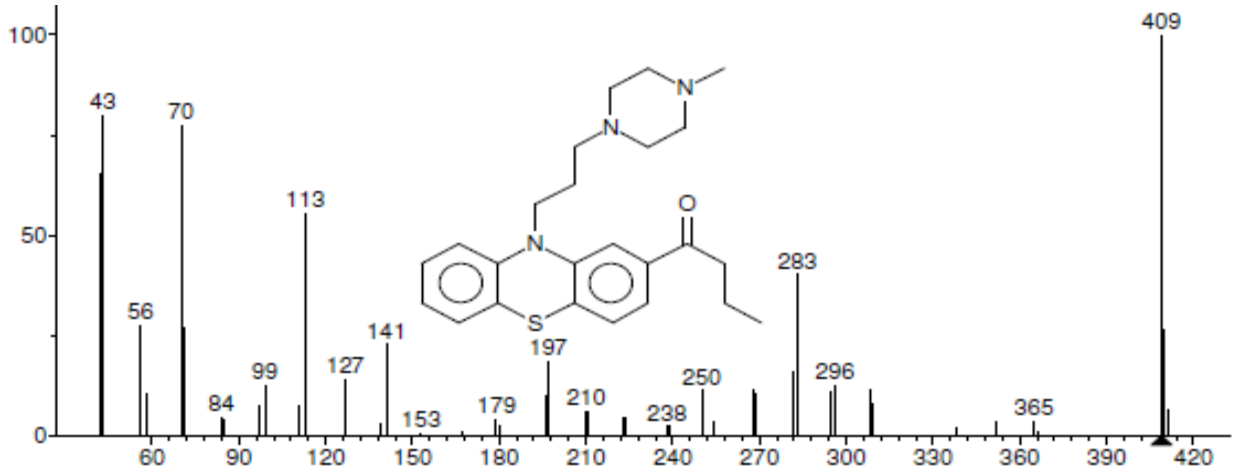
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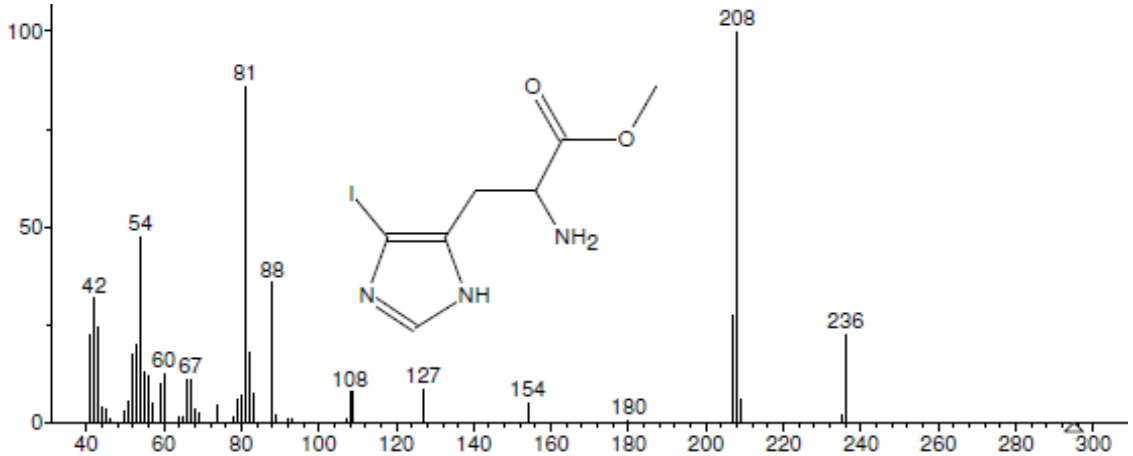
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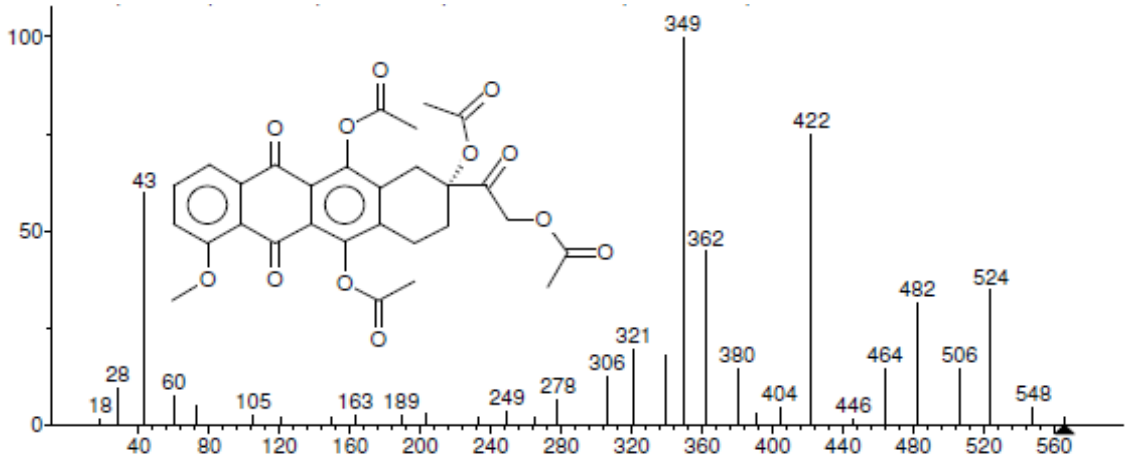
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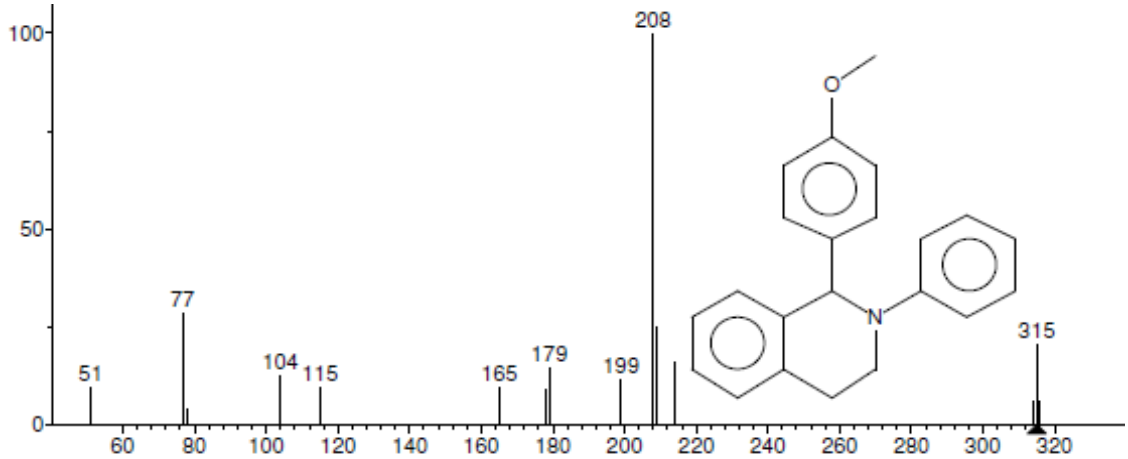
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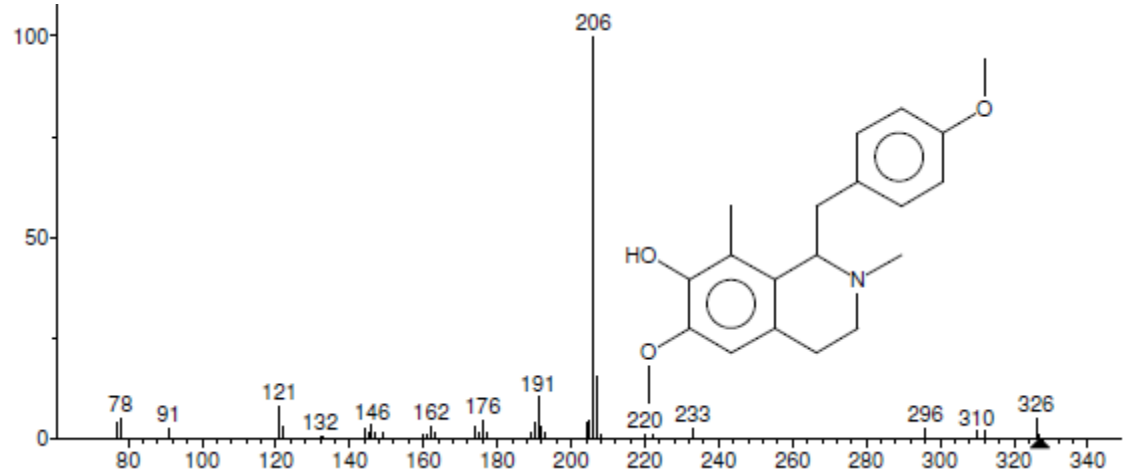
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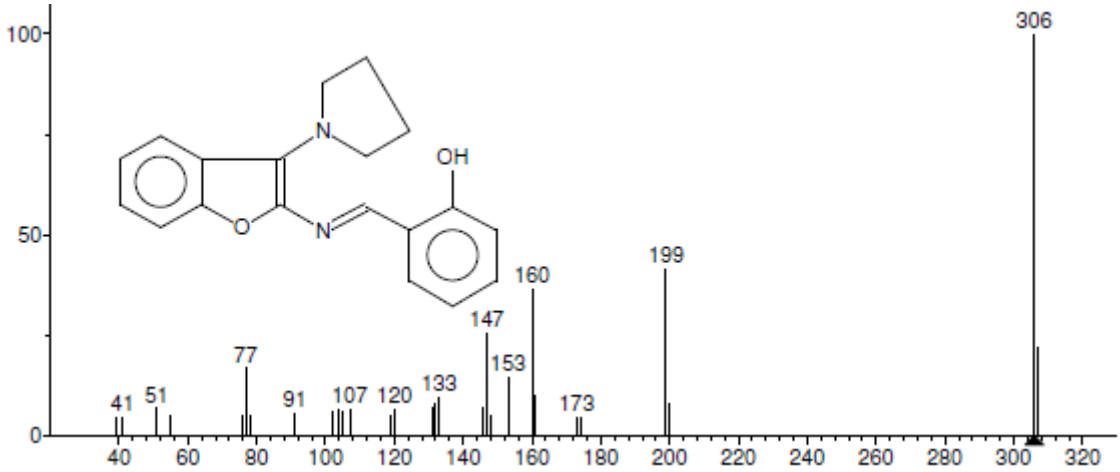

Figure 2: Mass spectra of ethanol extract of *Datura stranonium* leaves

Table 1: Bioactive compounds present in ethanol extract of *Datura stranonium* leaves

S/No	Compound	Bioactivity
1	Glycine, N-methyl-n-propoxycarbonyl-, dodecyl ester	Methyl-guanidine-inhibitor
2	Picolinyl 16-methyl-heptadec-9-enoate	Methyl-guanidine-inhibitor, catechol-O-methyltransferase-inhibitor
3	Isosilychristin hexaacetate	Not found
4	Benzenetridecanoic acid, 4-methoxy-, 2-decyl-3-methoxy-5-pentylphenyl ester	Arachidonic acid-inhibitor, increase aromatic amino acid decarboxylase activity, inhibit production of uric acid
5	1,3,3-Trimethyl-1-(2'-trimethylsilyloxyphenyl)-4-trimethylsilyloxyindane	Not found
6	Naproxen	Not found
7	2-Phenanthrenol, 1,2,3,4,4a,9,10,10a-octahydro-7-methoxy-1,1,4a-trimethyl-	5-alpha-reductase-inhibitor, acetyl-CoA-carboxylase-inhibitor,
8	N,N'-Bis(salicylidene)-3,3'-bis(aminopropyl)aminocobalt(II)	Antitopoisomerase-II, Casein-Kinase-II-Inhibitor, Topoisomerase-II-Inhibitor
9	2-Methoxycarbonyl-3-amino-6,7-dimethyl-quinoxaline	Increase Aromatic Amino Acid Decarboxylase Activit
10	1,3,4-Thiadiazol-2-amine, 5-(ethylthio)	Not found
11	Cyclobutanone, 2,3,3,4-tetramethyl	Not found
12	Phenol, 2,4,6-triiodo	Not found
13	Butaperazine	Not found
14	4-Iodohistidine, methyl ester	Catechol-O-Methyl-Transferase-Inhibitor, Methyl-Guanidine-Inhibitor
15	5,12-Naphthacenedione, 6,8,11-tris(acetyloxy)-8-[(acetyloxy)acetyl]-7,8,9,10-tetrahydro-1-methoxy	Not found
16	1,2,3,4-Tetrahydro-1-(4-methoxyphenyl)-2-phenylisoquinoline	Not found
17	7-Isoquinolinol, 1,2,3,4-tetrahydro-6-methoxy-1-[(4-methoxyphenyl)methyl]-2,8-dimethyl	Not found
18	2-(2-Hydroxybenzylidene-amino)-3-pyrrolidin-1-yl-benzofuran	Increase aromatic amino acid decarboxylase activity

Aromatic L-amino acid decarboxylase (AAAD) was discovered 70 years ago in mammalian tissue [6]. 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) [7-9] by supplementing lost dopamine from nigrostriatal neurons. 2-(2-Hydroxybenzylidene-amino)-3-pyrrolidin-1-yl-benzofuran have been reported to Increase aromatic amino acid decarboxylase activity [10]. Table 1 shows that *D. stranonium* ethanol leaves extract has been reported as catechol-O-methyl-transferase inhibitor [10]. 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 [11]. Benzenetridecanoic acid, 4-methoxy-, 2-decyl-3-methoxy-5-pentylphenyl ester has been reported as arachidonic acid inhibitor [10]. 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 [12]. Glycine, N-methyl-n-propoxycarbonyl-, dodecyl ester is a methylguanidine inhibitors [10]. 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 [13]. This suggests that methylguandine can attenuate the degree of inflammation and tissue damage arelated to endotoxic shock.

IV. CONCLUSION

The GC-MS analysis clearly revealed the presence of biological important compounds in the ethanol extracts of *D. stranonium* leaves. The bioactive compounds support the use of *D. stranonium* leaves in the management of diseases like heavy metal overload, Parkinson's and cardiovascular diseases.

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