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PHYTOCHEMICAL EVALUATION AND FUNCTIONAL GROUP DETECTION OF ETHANOLIC LEAF AND ROOT EXTRACTS OF *Datura metel*

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ABSTRACT: *Datura metel is a plant with various medicinal parts. This work gears towards the phytochemical evaluation, identification and functional group detection of ethanolic leaf and roots extracts of Datura metel. Gas Chromatography-Mass spectrometry (GC-MS) and Fourier –Transform Infrared Spectroscopy (FTIR) analytical instruments were used for studies. The preliminary phytochemical evaluation of plant parts revealed presence of alkaloids, flavonoids, saponins, tanins and terpenes. The chromatogram result for the Gas Chromatography-Mass Spectroscopy (GC-MS), detected 30 bioactive compounds with high percentage composition and molecular weights. Thiophene, 2,3-dehydro, an isomer of dehydrothiophene (C_4H_6HS) had the least retention time and highest percentage composition of 38.914% for the root extracts while 2-methyl-3-thiosemicarbazide ($C_2H_7N_3S$) and Benzene hexanenitirle, dimethyl-Ɛ-oxo ($C_{14}H_{17}HNO$) both had the highest percentage composition for the leaf extracts. The chromatogram result for Fourier –transform infrared spectroscopy (FTIR) revealed that alkenes (=C-H) and carbon tetrachloride (C-CL_4) had the highest and least wavelengths for both extracts respectively. The presence of bioactives detected and identified in this study, showed that plants may serve as reservoir for biologically active compounds and hence in addition to its medicinal values can also be used for diverse purposes in the industry.*

KEYWORDS: Datura metel, Phytochemicals, FTIR, GC-MS, Functional group, Bioactives.

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INTRODUCTION

Nature has endowed us with so many botanical wealth which provides us with medicinal plants that has some potential and valuable effect in health care. Medicinal plants has been used for health purposes for several thousands of years (Chavhan etal.,2018), due to the presence of phytochemicals synthesized as secondary metabolites that helps to protect them from environmental damage and also contribute to their colour, aroma and flavor (Mattai,2010).

Datura metel is one of the most commonly used medicinal plant. It was first described by the scientist Linneaus in the year 1753 (Dixon and Jeena,2017). The plant is said to have originated from North America (Alabiri etal., 2013) and widely cultivated in all tropical and subtropical regions of the globe for its beautiful flowers (Monira and Munan,2012). It has numerous common names such as Jimson weed, Thorn apple, Devil apple, Angel trumpet (Jmdhade etal.,2010). *Datura metel* is about 1.5m tall, its leaves are simply broad and dark green in colour. The fruits are like capsule covered with short spines or thorns (Monira and Munan,2012). According to several reports on preliminary phytochemical investigations, *Datura metel,* is found to be rich in some bioactive compounds like alkaloids, flavonoids, tanins, saponins. Scopolamines is its major bioactive components under category of alkaloids (Dixon and Jeena, 2017) and are responsible for its medicinal properties. *Datura metel* is used in treatment of some diseases like epilepsy, heart disease, asthma (Alabiri etal.,2013),in Nigeria. it also has a wide application in pharmacology as it is used in producing some medications used for wound healing, treatment of hairfall, dandruff, skin disorder, diarrhea, fever, pain etc. (Yang etal.,2014). Despite all these application, *Datura metel* also have intoxicating and hallucinogenic properties.

Gas Chromatography and Mass Spectometry (GC-MS) is mainly used in the separation and analysis of multi component mixtures such as essential oils, hydrocarbons and solvents (Kadhim etal. 2010). It is also used for quantitative and qualitative analysis of mixtures, purification of compounds and determination of thermochemical constants in solution and vapor pressure and activity coefficient. GC-MS analysis can identify nature of compounds even less than 1mg present in crude plant extract (Muthulaskshmi etal. 2012). Fourier transform Infrared Spectroscopy (FTIR) has been the most powerful tool for identifying the type of chemical bond or functional group present in analytes. It interprets its infrared absorption spectrum by varying observation in wavelength of the light absorbed which is the salient feature of the chemical bonds as seen in the annoted spectrum. (Coates, 2000)

It is important to isolate, identify and characterize, the bioactive present in these traditionally grown medicinal plants as well as attention given to harness other components beneficial for man such as industrially and agriculturally, hence the objective of this research work.

MATERIALS AND METHODS

Collection and authentication of plant materials.

The leaves and roots of *datura metel* were harvested in Federal University of Technology Owerri, Imo State. It was identified by a plant taxonomist, Dr D.I. Edet from department of Forestry and Wildlife, School of Agricultural and Agricultural Technology, Federal University

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of Technology Owerri. The plant was pressed by Dr, F.A. Faruwa, and deposited at the university herbarium with voucher number FUTO/FW/HERB/2019/052 for reference purpose.

Preparation of plant extracts

The plant leaf and root were detached, washed free of sand and debris, air-dried for about five weeks at room temperature, and pulverized using an electric blender. Solvent extracts of *datura metel* was prepared by weighing 50g of powdered sample into 1000ml capacity beaker, then 500ml of ethanol added to each beaker containing the samples, the sample was thoroughly mixed and allowed to stand for 24 hours, then filtered, using muslin bag and whatmann filter paper . The sample was further concentrated using a water bath at a temperature of 35ºC, covered firm and refrigerated at temperature of 4ºC.

Preliminary phytochemical screening

Wagner reagent test was used in testing for alkaloids. From each of the extracts, 3ml filtrate was acidified in 1ml hydrochloric acid and few drops of wagner'sreagent added. A reddish brown precipitate indicated the presences of alkaloids. Lead Acetate was used to test for presence of flavonid. 1ml of each extracts was taken and lead acetate solution added, a yellow precipitate confirmed the presence of Flavonids. To 1ml of extracts, 20ml of distilled water was added and agitated in a graduated cylinder for 15 minutes. The formation of 1cm layer of foam indicated presence of saponins, using the foam test. Terpenoids present was tested using salkwoski test, hence 5ml of each extract was added to 2ml of chloroform and 3ml of Con H_2SO_4 to form a layer of reddish brown coloration, its interface was said to form a positive result. Presence of tannins was determined using iron (iii) chloride solution ($FeCl_3$). Hence 5% $FeCl_3$ solution was added to extract and a blue black colouration was formed.

Structural elucidation of samples

This was carried out using GC-MS procedure. Exact 2g of extracted powder was weighed into an amber glass bottle and added 3ml ethanol. The sample was then shaken vigorously for 2 hours filtered and concentrated, 2ml of the extracted samples were then analyzed in GC column. This operation was carried out using GC (Agilent 6890N) and MS (5975B MSD). It was equipped with DB-5ms capillary columns (30m by 0.25m) film thickness (0.25µm) and temperature was set at 40ºC, then to 15ºC and 230ºC at the rate of 10ºC/mins which held for 5 minutes. Heluim served as gas carrier having a flu rate of 1ml/mins. Split rate and ionization voltage were 110ev and 70ev respectively. Phytochemicals were identified by mass spectra peak value which was compared with the database of National Institute of Science and ¹Technology.

Determination of functional bonds and chemical groups

This was carried out using Fourier transform spectrometer (vectex 80, Bruker optics) equipped with an attenuated total reflectance (ATR) accessory (MIRracle, Pike technologies). The spectrum was recorded in the spectral range of 600cm⁻¹ to 4000cm⁻¹ at a resolution of 2cm⁻ with a mercury cadmium tellun dedectector (MCT Dectector) (Coates, 2000).

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RESULT

The preliminary phytochemical screening for active compounds of ethanolic leaf and root extracts of *Datura metel* was qualitatively analyzed and the results listed in table 3.1. Then Table 3.2.and 3.3.Showed results from Fourier Transform Infrared Spectroscopy (FTIR) analysis revealing presence of alkenes, alkane, amine, alkyl halides and isothiocynate groups for both ethanolic extracts.

The Gas Chromatography Mass spectrometry (GC-MS) chromatogram for both extracts of *Datura metel* showed various peaks and indicated presence of 30 compounds as shown in tables 3.4 and 3.5. These compounds were identified and confirmed by interpretation of mass spectrum of GC-MS using the database of National Institute of Standards and Technology (NIST).

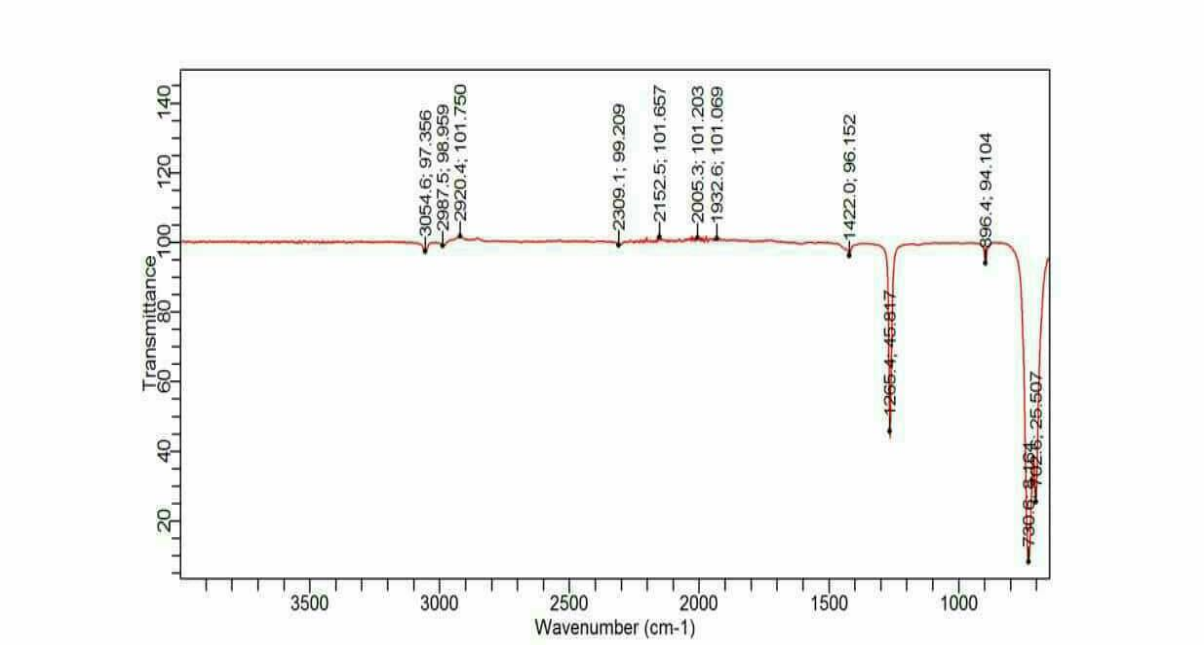

Fig 1.0. The chromatogram of the FTIR analyses of the ethanolic leaf extract of *Datura metel*

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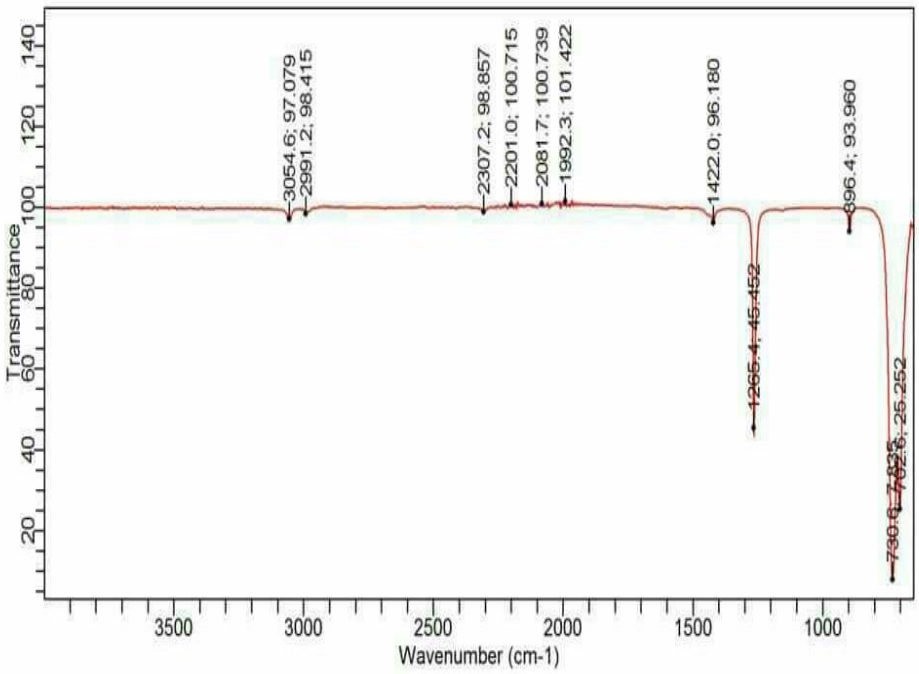

Fig 2.0. The chromatogram of the FTIR analyses of the ethanolic root extract of *Datura metel*

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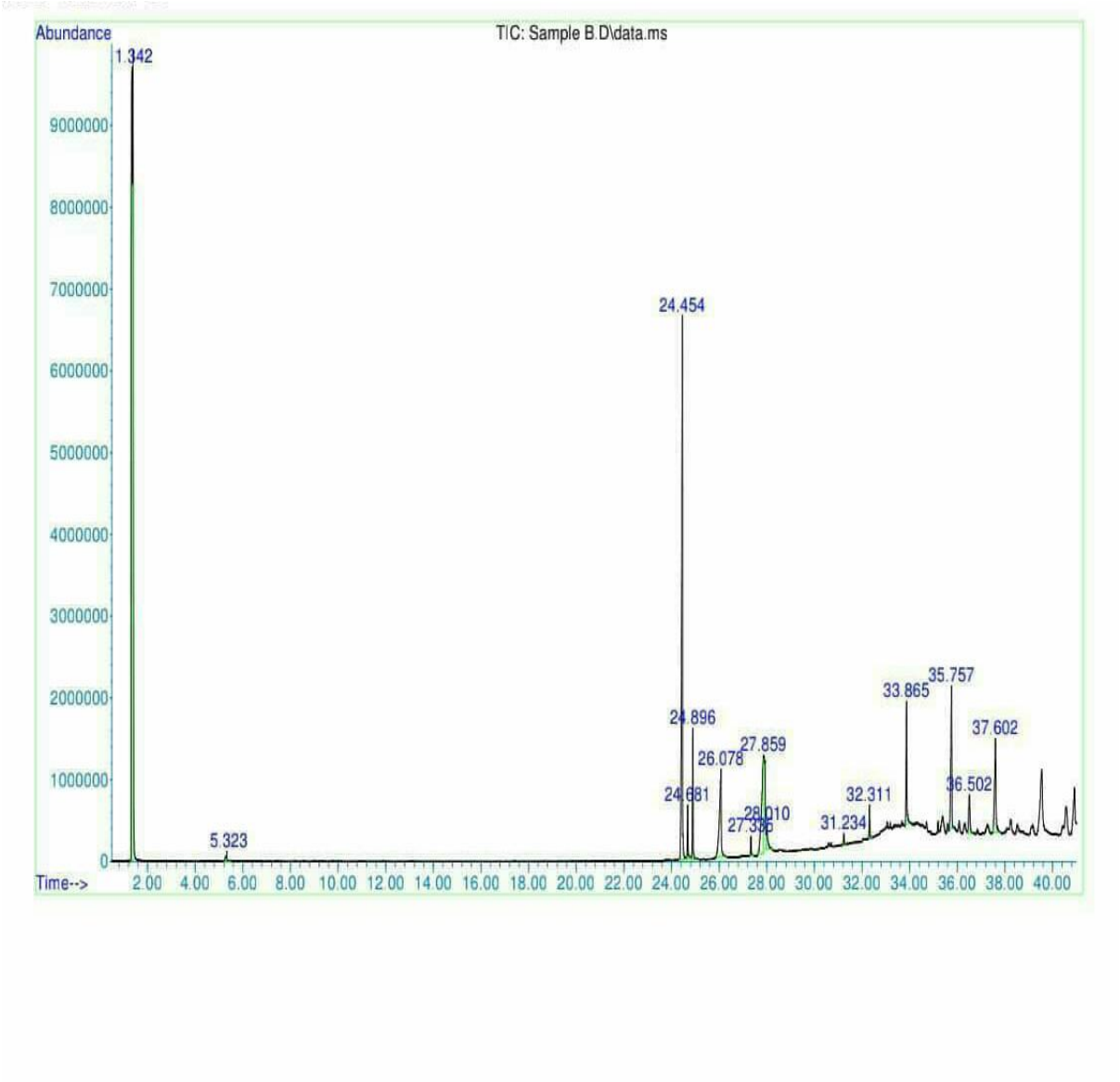

Fig 3.0. The chromatogram of the GC-MS analyses of the ethanolic Root extract of *Datura metel*

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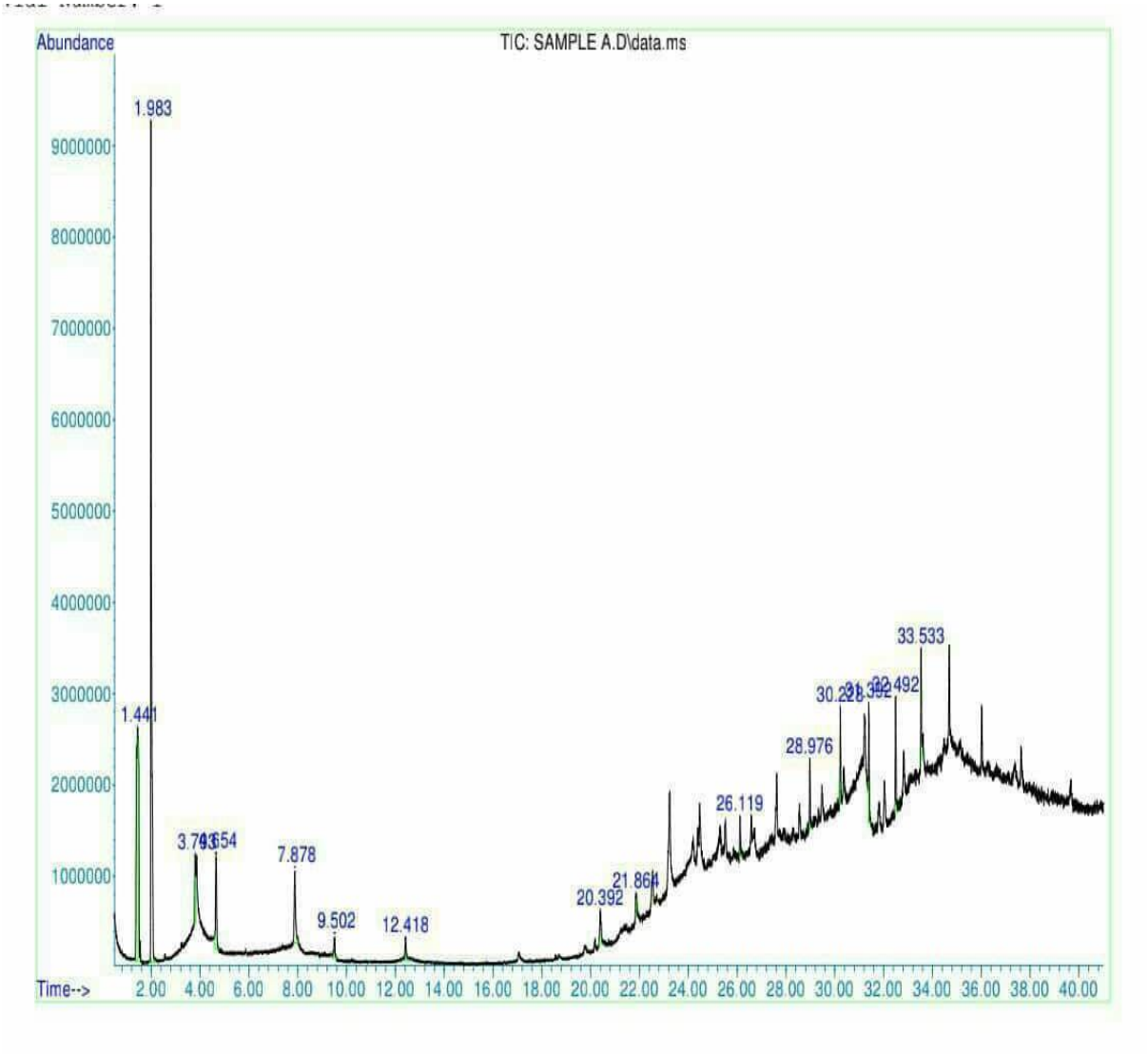

Fig 4.0. The chromatogram of the GC-MS analyses of the ethanolic leaf extract of *Datura metel*

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Table 3.1. Results on the preliminary phytochemical screening of ethanolic leaf and root extract of *Datura metel.*

PHYTOCHEMICAL	RESULTS/INFERENCE
ALKALOID	+
SAPONINS	+
TANINS	+
FLAVONOIDS	+
TERPENES	+

KEY + = PRESENT

Table 3.2. Results for FT-IR analysis of ethanolic Leaf extract of *Datura metel*

S/N	Wavelenght	Functional Group
1	3054.6	=C-H
2	2987.6	C-H
3	2920	C-H
4	2309.1	Isothiocyanate (-NCS)
5	2152.5	Isothiocyanate (-NCS)
6	2005.3	Isothiocyanate (-NCS)
7	1932.6	Amines
8	1442	Methyl (C-H)
9	1265.4	C-N
10	896.4	C-H
11	730	$-(CH_2)_n$
12	702.6	C-Cl

Table 3.3.Results for FT-IR analysis of ethanolicRoot extract of *Datura metel*

S/N	Wavelenght	Functional Group
1	3054.6	=C-H
2	2997.2	-C-H
3	2201	-C=C-
4	2081.7	Transition metal carbonyls
5	1992.3	Transition metal carbonyls
6	1422	C=C
7	1265.4	C-O
8	896.4	C-H
9	730.6	C-Cl
10	702.6	-OH

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Table 3.4 Result for GC-MS Analysis of the ethanolic Leaf extract of *Datura metel*

S/NO	Retention time(R.T) (Mins)	Name of compound	Molecular weight	Molecular formular	% composition
1	1.441	Adenosine,4'de (hydroxymethyl)-4'-(N-ethylaminoformyl	442	$C_{20}H_{22}N_6O_6$	20.804
2	1.441	Chlorozotocin	313	$C_9H_{16}ClN_3O$	20.804
3	1.983	2-methyl-3-thiosemicarbazide	105	$C_2H_7N_3S$	38.621
4	1.983	Benzenehexanenitrile,β,β-dimethyl-ε-oxo	215	$C_{14}H_{17}NO$	38.621
5	3.793	Hexestrol,pentafluoropropionyl-	416	$C_{21}H_{21}F_5O_3$	3.065
6	3.793	(1,2-Diethylethylene)bis(phenylene) diacetate	354	$C_{22}H_{26}O_4$	3.065
7	4.654	3-Methylbenzylalcohol,trifluoroacetate	218	$C_{10}H_9F_3O_2$	5.575
8	4.654	4-Methylbenzyl alcohol, trifluoroacetate	218	$C_{10}H_9F_3O_2$	5.575
9	7.878	Trisiloxane ,1,1,1,5,5,5-hexamethyl-3-〔(trimethylsily)oxy〕	296	$C_9H_{28}O_3Si_4$	5.282
10	7.878	Cyclotetrasiloxane,octamethyl-	296	$C_8H_{24}O_4Si_4$	5.282
11	9.502	Estragole	148	$C_{10}H_{12}O$	1.521
12	9.502	Anethole	148	$C_{10}H_{12}O$	1.521
13	12.418	(-)-Epigallocatechin	290	$C_{15}H_{14}0_6$	1.580
14	12.418	Catechin	290	$C_{15}H_{14}O_6$	1.580
15	20.392	Ellagic acid	302	$C_{14}H_6O_8$	2.632
16	20.392	1,1'-Biphenyl〕-3,3'-dicarboxaldehyde,6,6'-dihydroxy-5,5'-dimethoxyl	302	$C_{16}H_{14}O_6$	2.632
17	21.864	Vitamin E	430	$C_{29}H_{50}O_2$	0.797
18	21.864	(+)-γ-Tocopherol,o-methyl-	430	$C_{29}H_{50}O_2$	0.797
19	26.119	3-Pyridinecarboxylicacid,2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta〔a〕cyclopropa〔f〕cycloundecen-11-yl ester,〔1Ar-1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11As*)	597	$C_{32}H_{39}N0_1$	1.551

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20	26.119	Hexadecanoic 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta〔a〕cyclopropa〔e〕cyclodecen-6-yl ester, 〔1aR-(1a,9a,10a)〕	586	$C_{36}H_{58}O_6$	1.551
21	28.976	Lorazepam	320	$C_{15}H_{10}Cl_2N_2O_2$	2.630
22	28.976	Quinazoline-2-carboxaldehyde,6-chloro-4-(2-chlorophenyl)-	320	$C_{15}H_8Cl_2N_2$	2.630
23	30.228	2,4-Imidazolidinedione,5-[3,4-bis[(trimethylsily)oxy]phenyl]-3-methyl-5-phenyl-1-(trimethylsilyl	516	$C_{25}H_{40}N_2O_4Si_3$	3.006
24	30.228	(+)-Prostaglandin F2$^{\delta}$,4TMS Derivatives	642	$C_{32}H_{66}O_5Si_4$	3.006
25	31.392	Benzofuran-2-Carboxylic acid	162	$C_9H_6O_3$	4.396
26	31.392	Benzofuran-5-carboxylic acid	162	$C_9H_6O_3$	4.396
27	32.492	PGF2ǎ	354	$C_{20}H_{34}O_5$	4.485
28	32.492	Aceticacid,1-acetoxyl-10a,12a-dimethyl-5-oxo-hexadecahydro-6-oxabenzo[3,4]ctclohepta[1,2-E]inden-8-yl ester	406	$C_{23}H_{34}O_6$	4.485
29	33.533	ǎ-Tocopheryl acetate	472	$C_{31}H_{52}O_3$	4.054
30	33.533	(±)-ǎ-Tocopherol acetate	472	$C_{31}H_{52}O_3$	4.054

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Table 3.5 Result for GC-MS Analysis of the ethanolic root extract of *Datura metel*

S/N	Retention time (R.T)(Mins)	Name of compound	Molecular weight	Molecular formular	% composition
1	1.342	*Thiophene,2,3 − dihydro*	86	C_4H_6S	38.914
2	1.342	*Thiophene,2,5 − dihydro*	86	C_4H_6	38.914
3	5.323	*Bis(2 − ethylhexyl)phytalate*	390	$C_{24}H_{38}O_4$	0.542
4	5.323	*Diisooctylphythalate*	390	$C_{24}H_{38}O_4$	0,542
5	24.45	*Iron (1,2 − ethanediyl{bis(1 − − ethyl − 2,4 − cyc*	426	$C_{22}H_{44}FeP_2$	19.744
6	24.45	*Hydrido − iron, {n − 5(1 − ethlcuc − bis(diisopropylph*	426	$C_{22}H_{44}FeP$	19.744
7	24.68	3,7,11,15-Tetramethyl-2-hexadecen-1 -ol	296	$C_{20}H_{40}O$	1.497
8	24.68	*Phytolacetate*	338	$C_{20}H_{42}O_2$	1.497
9	24.89	*Phytylhexadecanoate*	534	$C_{36}H_{70}O_2$	3.664
10	24.89	hexadecanoicacid,3,7,11,15-tetramethyl-2-hexadecenylester, 〔R-〔R,R-E〕	534	$C_{36}H_{70}O_2$	3.664
11	26.07	I-(+)-Ascorbicacid 2,6-dihexadecanote	652	$C_{38}H_{68}O_8$	6.501
12	26.07	n-Hexadecanoic acid	256	$C_{16}H_{32}O_2$	6.501
13	27.335	Ethyl iso-alocholate	436	$C_{26}H_{44}0_5$	0.568
14	27.335	1-Heptatriacotanol	536	$C_{37}H_{76}O$	0.568
15	27.85	Linoelaidic acid	280	$C_{18}H_{32}O_2$	8.403
16	27.85	(Z)-18-Octadec-9-enolide	280	$C_{18}H_{32}O_2$	8.403
17	28.010	4-Androstene-3,17-dione17-mono(O-methyloxime	315	$C_{20}H_{29}NO_2$	1.188
18	28.010	5,19-cyclo-5ß-androst-6-ene-3,17-dione	284	$C_{20}H_{29}NO_2$	1.188

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19	31.234	3',8,8'-Teimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone	487	$C_{28}H_{25}NO_7$	0.277
20	31.234	6,19-Cycloandrostane-3,7-diol,3ß-methoxyl	320	$C_{20}H_{32}0_3$	0.277
21	32.311	(S)-(+)-Epichlorohydrin	92	C_3H_5CIO	0.859
22	32.311	Oxirane(chloromethyl)	92	C_3H_5CIO	0.859
23	33.865	9,10-Anthracenedione	208	$C_{14}H_8O_2$	4.339
24	33.865	9,10-Phenanthrenedione	208	$C_{14}H_8O_2$	4.339
25	35.757	Amodiaquine	355	$C_{20}H_{22}CLN_3O$	6.118
26	35.757	Amopyroquine	355	$C_{20}H_{22}CLN_3O$	6.118
27	36.502	ß-Tocopherol,o-methl	430	$C_{29}H_{50}O_2$	2.003
28	36.502	(+)-$_\gamma$-Tocopherol,o-methyl	430	$C_{29}H_{50}O_2$	2.003
29	37.602	7H-Pyranol〔2,3-c〕acridin-7-one, 3,12-dihydro-6,11-dihydroxy-3,3,12-Trimethyl-5-(3-methyl-2-butenyl)	391	$C_{24}H_{25}NO_4$	5.382
30	37.602	1-Azaspiro〔4.5〕dec-3-ene,2-(diphenylmethylene)-4-methyl-1-phenyl	391	$C_{29}H_{29}N$	5.382

DISCUSSION

The phytochemical Evaluation of leaf and root ethanolic extract of *Datura metel* showed presence of alkaloid, saponins, tannins, flavonoid and terpenes. Studies are in line with results from Datura *metel Linn* by sundaramoorthy, 2014. Phytochemical are known for their biological activities such as antimicrobial, antioxidant, antifungal, anticancer and antidiabetic strength (Hossain, 2011). Tannins, Saponins, Flavonoids have anti-hypoglycaemic and anti-inflammatory properties, terpenes have analgesic properties and as well as central nervous system (CNS) activity (Ayoola etal, 2008). Alkaloids have antioxidant, antifungal, protective properties.

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Fourier Transform Infrared Spectroscopy (FTIR) of both leaf and root ethanolic extracts of plant, showed presence of functional groups such as alkanes, alkenes, amines, isothicyanates and alkyl halides The wavelength study was in line with observation from *Cleome gynandra* leaf (Deepashree etal, 2013) were the band range between 20005.3m-2997.2m were transition metals and isothiocynate (-NCS). Wavelength of 2987m and 2920m indicates presence of compounds such as methyl (-C-H). Wavelength of 3054m showed presence of alkene (C=C). Wavelength of 1990m -2150m showed presence of nitrogen multiple and cumulative double bound compounds isothiocyanate (–NCS). Wavelength of 1932m indicates primary amines. Wavelength of 1150m -1210m, aliphatic chloro compound (C-CL). Wavelength within 1200m-1800m, showed transition metals and Wavelength of 590m-720m indicated Alcohol (-OH) and Hydroxyl compounds. (Coates 2000).

The results from GC-MS analysis showed that roots and leaves extracts of *datura metel* contained so many bioactive compounds belonging to various classes of phytochemicals which plays some biological roles in the body system as discussed in tables 4.1 and 4.2.

Table 4.1 Biological Activity of Identified Compound in Ethanolic Leaf extract of Datura *metel*.

S/No	**Compound Biological Activity**	**Uses**	**Reference**
1	$Adenosine, 4'\ de(hydroxymethyl)$-4'-(N-ethylaminoformyl)	Binds readily with adenosine than to other endogenous purines with two pharmacologically distinguishable type (a_1 and$_2$) to exert biological effect.	NCBI, 2021.
2	$Chlorozotocin$	A nitroso urea used for cancer therapy and analogue of streptozotocin	Cooke, 2006.
3	$2-methyl-3-thiosemicarbazide$	Exhibit an anti-arrangement between thione S atom and hydrazine N atom	Jesus Valdes-Martinez, 2007.
4	$Benzenehexanenitrile, _{\beta,\beta}-dimethyl-\varepsilon-oxo$	Is an Aromatic ketone	TSCA,2006
5	$Hexestrol, pentafluoropropionyl-$	Non-steriodal estrogen previously used for estrogen-replacement therapy and treatment of certain hormone dependent cancers.	J.elks (2014).
6	$(1,2-Diethylethylene)bis(phenylene)diacetate$	No activity reported	Nil
7	$3-Methylbenzylalcohol, trifluoroacetate$	No activity reported	Nil

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8	*4 – Methylbenzyl alchol, trifluoroacetate*	No activity reported	Nil
9	*Trisiloxane ,1,1,1,5,5,5 –hexamethyl – 3 – {(trimethylsily)oxy}*	No activity reported	Nil
10	*Cyclotetrasiloxane, octamethyl –*	Used in manufacture of polymeric materials widely used in cosmetics	EPA.2016
11	*Estragole*	Used as flavouring agent in pharmaceutical industry, cosmetic and food industry, antioxidant, antimicrobial properties.	Friedman,2002
12	*Anethole*	Is the main fragrance and bioactive compound in some plant species. It has antimicrobial, antifungal, antihelmetic and insecticidal activity	Astani,2011
13	(-)-Epigallocatechin	It reduces inflammation, aid weight loss, helps prevent heat and brain disease.	Ansley2019
14	Catechin	It is a phenolic compound, mostly found in tea, cocoa and berries and have antioxidant actitvity.	Tania,2006
15	Ellagic acid	Natural phenol, antioxidant found in fruits and vegetables	Ryszand,2012
16	1,1'-Biphenyl〕-3,3'-dicarboxaldehyde,6,6'-dihydroxy-5,5'-dimethoxyl	No activity reported	Nil
17	*Vitamin E*	Antiageing, Analgesic, Antidiabatic, Antiinflammatory, Antioxidant,	Juliana Kubala, 2021.
18	*(+)-γ-Tocopherol,o-methyl-*	Fat soluble antioxidant	Gamze Guelu, 2021.

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19	*3-Pyridinecarboxylicacid,2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta〔a〕cyclopropa〔f〕cycloundecen-11-yl ester,〔1Ar-1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11As*)*	No activity reported	Nil
20	*Hexadecanoic 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta〔a〕cyclopropa〔e〕cyclodecen-6-yl ester,〔1aR-(1a,9a,10a)〕*	No activity reported	Nil
21	*Lorazepam*	Used in healing anxiety disorder, active seizure, alcohol withdrawal, chemotherapy, induced nausea and vomiting	Julie Maves (2021).
22	*Quinazoline-2-carboxaldehyde,6-chloro-4-(2-chlorophenyl)-*	No activity reported	Nil
23	2,4-Imidazolidinedione,5-[3,4-bis[(trimethylsily)oxy]phenyl]-3-methyl-5-phenyl-1-(trimethylsilyl	No activity reported	Nil
24	(+)-Prostaglandin F2$^{\delta}$,4TMS Derivatives	Notable for promotion of uterine contraction	Emmanuel etal, 2011
25	Benzofuran-2-Carboxylic acid	Anti-inflammatory, local anaesthetics, cytotoxicity against human cancer cell line.	Saku etal, 2010.
26	Benzofuran-5-carboxylic acid	Antiviral, antioxidant, anti-inflammatory, antioxidant, Antimicrobial, antitumor activity	Hayakwa etal, 2004
27	PGF2ă	Is a stable prostaglandin that stimulates the contraction of uterine and bronchial smooth muscle and tightening in some blood vessels	Jian Zhang etal, 2010.

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28	Aceticacid,1-acetoxyl-10a,12a-dimethyl-5-oxo-hexadecahydro-6-oxabenzo[3,4]ctclohepta[1,2-E]inden-8-yl ester	No activity reported	Nil
29	ă-Tocopheryl acetate	Also known as vitamin E acetate and safe for use in cosmetics and skincare products	SAS 2016
30	(±)-ă-Tocopherol acetate	Also known as vitamin E acetate and safe for use in cosmetics and skincare products	SAS 2016

Table 4.2: Biological Activity of Identified Compound in Ethanolic Root extract of Datura *metel*.

S/no	Compounds biological activity	Uses	Reference
1	$Thiophene,2,3-dihydro$	Antimicrobial, analgesic, anti-inflammatory, antihypertensive and antitumor	Pillai etal, 2005
2	$Thiophene,2,5-dihydro$	Inhibitors of corrosion of metals and fabrication of light-emitting diode in material science	Benabdlellh etal,2006
3	$Bis(2-ethylhexyl)phytalate$	DEHP is used as plasticizers in many products, especially in medicinal device such as intravenous bags and tubing, blood bags, infusion tubing, peritoneal dialysis bags.	Hung P.C etal, 2008.
4	$Diisooctyl\,phythalate$	DIOP is used in rubber compounds for manufacture of automobile hoses and parts	Kent Carlson, 2010

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5	*Iron (1,2 − ethanediyl{bis(1 − methylethyl)i − ethyl − 2,4 − cyclohexadien -*	No activity reported yet	Nil
6	*Hydrido − iron, {n − 5(1 − ethlcuclohexadienyl) − bis(diisopropylphosphino)ethan*	No activity reported yet	Nil
7	3,7,11,15-Tetramethyl-2-hexadecen-1 -ol	No activity reported yet	Nil
8	*Phytolacetate*	Used as a food addictive and flavouring agent	EU, 2012.
9	*Phytylhexadecanoate*	No activity reported yet	Nil
10	hexadecanoicacid,3,7,11,15-tetramethyl-2-hexadecenylester,〔R-〔R,R-E〕	No activity reported yet	Nil
11	I-(+)-Ascorbicacid 2,6-dihexadecanote	It is a vitamin C compound, used for treating cold, gum disease acne and infections. It is also an antioxidant in the skin by scavenging and quenching free radicals generated by ultraviolent radiation	Okenwa, 2014
12	n-Hexadecanoic acid	Also called palmitic acid, has anti-inflammatory property and can be seen in food addictives, or as surfactants in cosmetics	Vasudevan., 2012.
13	Ethyl iso-alocholate	Also called Ethyl Cholate, is more stable than other ligands, and serve as inhibition for dehydropteroate synthase, and can also be used as antimicrobial agent	Malathi etal,2016
14	1-Heptatriacotanol	Has anti-cholesterol effect	Love junwei, 2018
15	Linoelaidic acid	It can modulate cancer, atherosclerosis, obesity, tumour and diabetics	David A, Z. 2013

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16	(Z)-18-Octadec-9-enolide	Has antibacterial, anti-parasitic properties	Lalthanpuii etal, 2019
17	4-Androstene-3,17-dione17-mono(O-methyloxime)	Is a drug or nutritional supplement, which increases testosterone-estrogen ratio.	Van thuyne etal, 2005.
18	5,19-cyclo-5ß-androst-6-ene-3,17-dione	Has androgenic activity	Charles. 2012
19	3',8,8'-Teimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone	No activity reported yet	Nil
20	6,19-Cycloandrostane-3,7-diol, 3ß-methoxyl	No activity reported yet	Nil
21	(S)-(+)-Epichlorohydrin	Used to produce glycerol, plastics, epoxy glues and resins	ECN,2003
22	Oxirane(chloromethyl)	Also known as ethylene oxide, used to make detergents, thickeners, solvents.	Boogaard P.J.2014
23	9,10-Anthracenedione	Also called Antraquine, serves as building blocks for dyes, bleaches, pulp for paper making	IUPAC 2014
24	9,10-Phenanthrenedione	Serves as initial mediator for electron acceptor/donor containing formate dehydrogenase, reduction of carbon dioxide to formate.	Robert,2013
25	Amodiaquine	Medication used in treating malaria,	Nair etal, 2012
26	Amopyroquine	Medication against chloroquin resisitant strain of *Plasmodium falciparuim*	Lewis Noble,2012
27	ß-Tocopherol,o-methl	Has antioxidant properties	Zing etal, 2013
28	(+)-$_{\gamma}$-Tocopherol,o-methyl	Scavenge ROS during lipid oxidation	Zing etal, 2013
29	7H-Pyranol〔2,3-c〕acridin-7-one, 3,12-dihydro-6,11-dihydroxy-3,3,12-Trimethyl-5-(3-methyl-2-butenyl)	No activity reported yet	Nil

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30	1-Azaspiro〔4.5〕dec-3-ene,2-(diphenylmethylene)-4-methyl-1-phenyl	No activity reported yet	Nil

CONCLUSION

Presence of various bioactive compounds in both plant extracts reveals the biological, pharmacological and industrial strength of the *Datura metel*. Antioxidants, anticancer, hypocholesterolemic, hypoglycemic, antibacterial activities, as seen in compounds got from phytochemical screening, proves that plant has many medicinal properties. Root extracts effect of plant as seen in epichlorohydrin shows plants importance in industrial use as they can exert harmless or harmful effects. In the industy. Results from this study has justified that *datura metel* leaf and roots may be very useful in pharmaceutical, health, medicinal and industrial applications for the welfare of human

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