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Identification and Characterization of Bioactive Components in *Datura stramonium* Leaves: an insight into Drugs Discovery

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ABSTRACT: Medicines from plants help in treating ailments, but to utilize them effectively in the management of diseases requires the identification of potent phytochemicals relative to conventional drugs. These phytochemicals are compared with synthetics drugs in line with their treatment regimen. An investigation was designed to identify, and characterized the different phytochemicals in *Datura stramonium* (Jimson weed) leaves and compared them with conventional or standard drugs. The identified phytochemicals were blasted on the drugs bank website to find their correlation and relativity. GC/MS technique was used to analyze the phytochemicals. The results showed 80 different phytochemicals belonging to several categories of phytochemicals - alkaloids, flavonoids, terpenoids, saponins, amine, and steroids. The flavonoid class had - 1.24% of 5H-Dibenzo[c, f][1, 2] diazepine, 3, 8 dichloro-6,11-dihydro, at 3.702 RT, Alkaloid class has – 2.98% 2,6-Dibromobenzoquinone was detected at 4.403 RT, steroid – 2.98% Acetanilide, 2-chloro-4'-nitro- at 4.403 RT was obtained and Terpene – 2.05% of Methyl-beta.-[N-methylanilino]acrylate was detected at 4.719 RT, respectively. Most of the identified phytochemicals matched with synthetic drugs and confirmed the purpose of their applicability in traditional medicine. Considering the presence of numerous components and their correlation with conventional drugs, one can infer that this plant species has a good therapeutic application and can be utilized for health benefits.

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There are several reports about the health benefits of herbal medicines. A lot has been tested on animal models as randomized trials in managing and controlling different ailments such as diabetes mellitus, arthritis, ulcer, cancers, and cases of flu, dysentery, and diarrhea. At most, the researcher may implicate the curative effect of the plant extract to the existence of several bioactive including alkaloids, flavonoids, terpenes, steroids, saponins, amines, and alcohols. Considering that each of the listed phytochemicals has sub-compound or classes of compounds, one may wonder which particular type or classes of these phytochemicals could ameliorate the effects of a disease on the test organism. To bridge the gap of generalizing the implication of the plant's extract, this work investigated the phytochemicals in *Datura stramonium* (Linn) leaves (Okpashi *et al.*, 2020). The phytochemicals were identified, quantified, and characterized. The identified phytochemicals were blasted on the conventional or synthetic drug bank website to match their correlations and relativity. Meanwhile, synthetic drugs have descriptions of formulation, synthesis, and indication for application. This plant was chosen or selected because of its applications in various fields. The plant itself is very toxic with leaves, seeds, and fruits, which limit its utilization as herbal therapy. This also caused the therapist to assume or perceived that only a small therapeutic dose can be utilized, compared to a toxic dose. Curiously, it's been used as an esoteric cannabinoid in some parts of Nigeria due to its intoxication. The learning of natural products in the expansion of curative interaction includes aspects of stereo-chemistry, biochemistry, biosynthesis, bioinformatics, and biological accomplishment to providing pathologically useful compounds. Primary metabolites are plant compounds that are expressed continuously (Jamal *et al*., 2016 cited in Babiker *et al.*, 2017). *Datura stramonium* is known as Jimson weed (Lee, 2007). It is usually grown in recently disturbed areas and is often invasive especially in waste-dumped sites, which explain the abundance of many phytochemicals. Solanaceae that is rich in primary metabolites is a weed belonging to the Apiaceae. It has been described by the World Health Organization (WHO) as one whose many of its parts contain substances that can be used for the synthesis of useful drugs. The demand for medicinal plants is aggregating because of the rising recognition of regular products (Tatini and Raja, 2017). Plants chemicals are non-

nutrient bioactive mixtures in plant parts. Phytochemicals are a defensive and blocking mediator against many deteriorating infections including aging, and inflammation (Debasis *et al.,* 2015). People have been exploring plants products in pursuit of novel medicines. This has led to the use of a wide quantity of curative plants to treat various ailments. The leaves of D. stramonium are used in asthma treatment (Pretorius and Marx, 2006; Savithramma *et al.,* 2007). The vital naturally active constituents in *Datura stramonium* comprised of alkaloids, atropine, and scopolamine. Atropine has been utilized in treating Parkinson's disease, peptic ulcers, diarrhea, and bronchial asthma (Ivancheva *et al.,* 2006). Its vegetation mucilages and PolyVinyl Pyrrolidone mixture has been used as matrix-forming substances for the continual production of matrix remedies (Ahad *et al.,* 2012). *D. stramonium* is a normal source of antioxidants and phytochemicals with antimicrobial activities (Akharaiyi, 2011). Its juice usually expresses considerable antimicrobial activity against several microorganisms including *Staphylococcus aureus*, *Proteus Vulgaris*, *Pseudomonas aeruginosa, Escherichia coli*, *Aspergillus niger,* and Fusarium species (Reddy, 2009). The secondary metabolites of *D. stramonium* are vastly active against dissimilar ailments such as antidiabetic, antiviral, etc. (Nain *et al.,* 2013). Water extract also shows insecticidal activities (Fan and Kriton, 2005). *Datura stramonium* is applied in Ayurvedic drugs (Gaire and Subedi, 2013). The ethanol juice shows potent antimicrobial activities than water extracts. The leaves extracts suggest better efficacy than stem and root extract (Gachande and Khillare, 2013). In India, about 75 % of the prescriptions are plants based (Solomon, 2015). The investigation on plant's natural products continues for the realizing several original energetic secondary metabolites (Ramendra and Vishnu, 2014), which have antifungal, antibacterial, and anticancer activities. The basic extracts and uncontaminated compounds isolated from plant species are applied in herbal and traditional medications. Currently, it is necessary to isolate, identify and characterize novel secondary metabolites for the treatment of diverse maladies (Jalal 2016). The unidentified organic compounds in a complex mixture can be determined through the interpretation and matching of their spectra with reference spectra (Rahim *et al.,* 2018). The present work was carried out to identify some of the bioactive components in the leaves extract of *Datura stramonium* and matched with the reference spectra for nascent drug discovery, production of drugs, and proper therapeutic regiment.

MATERIALS AND METHODS

Collection of plant sample: Fresh and mature *Datura stramoniu*m leave (fruit stage), were obtained from Boki Local Government Area (LGA) of Cross River State, Nigeria. The fresh leaves were identified by Dr. Ekpene Solomon in the Department of Biological Sciences, Cross River University of Technology, Calabar. The leaves were washed with running water and rinsed with distilled water. It was chopped into pieces and air-dried for 21 days at room temperature. The dried samples were coarse using a blender. The coarse samples were stored at room temperature for two days before extraction.

Preparation of Plant Extract: Twenty-five grams (25g) of the coarse leaves were weighed and transferred into the thimbles of the soxhlet extractor, One hundred and fifty (150 ml) normal-hexane) was measured and transferred into the round bottom flask of the soxhlet extractor. The solvent was heated to reflux through the heating mantle. After the extraction, the extracts were concentrated using a rotor for five days.

Screening of the Extract with GC/MS: A Gas Chromatography (Agilent 6890) was armed with a straight a deactivated 2 mm injector and 15 m All-tech EC-5 column (250 µ I.D., 0.25 µ film thickness). A split injection was used to inject the sample. The split ratio was set - 10:1. The oven temperature starts at 35 °C, holds for 2 to 5 minutes, and ramped from 20 °C to 30 °C. The helium gas carrier was at a 2 ml/minute flow rate. A GC mate II bench-top double-focusing magnetic sector was operated in electron ionization (EI) mode. TSS-20001 software was used for the analyses. Low-resolution mass spectra were attained at a determining power of 1000 (20 % height definition), while scanning starts from m/z 25 to m/z 700 at 0.3 seconds per scan with a 0.2-second inter-scan delay. High-resolution mass spectra were achieved at a resolving power of 5000 (20 % height definition) with a scanning of the magnet from m/z 65 to m/z 750 at 1 second per scan. The identification of the bioactive components of the pure compounds was matching their logged spectra with the data bank mass spectra of NIST library V 11 provided by the software of the instrument. During the analysis, the following conditions apply to the use of GC/MS techniques: GC/MS-QP2010 Agilent 6890 Plus; Ion source temperature: 200.00°C; Interface temperature: 250.00°C; Solvent cut time: 2.50 min; Detector gain mode: MS; Detector gain: 0.00 kV; Threshold: 2000; Column oven initial temperature: 70.0°C; Injection final temperature: 250.00°C; Injection Mode: Split; Flow control mode: linear velocity; Pressure: 116.9 kPa, total Flow: 40.8 ml min−1; Column flow: 1.80 ml min−1; Linear velocity: 49.2 cm sec−1; Trap and purge flow: 3.0 ml min−1; Split Ratio: 20.0; High-pressure injection: OFF; Carrier Gas: Helium; Splitter hold: OFF.; While oven rating was as follows: Oven Temp. Program Rate Temperature (°C) Hold Time (min) Initial: 0.00 70.0 0.00 Final: 10.0 280 5.00.

RESULTS AND DISCUSSION

Bioactive components detected in D. stramonium leaves extract: Results of bioactive analysis of *Datura*

Stramonium leaves are presented in Tables designated as Table 1a, b, c, d, e, f, g, and h, separately.

Table 1a. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Min. Q
1	3.702	1.24	5H-Dibenzo[c,f][1,2]diazepine, 3,8	Flavonoid	124275	000955-66-8	74
			dichloro-6,11-dihydro-	-	100763	000774-74-3	64
			Acetyl chloride, (2,4-dichlorophenoxy)-	Flavonoid	142388	1000387-64-2	48
			[5-(5-Bromopyridin-3-yl)-2H-1,2,4-triazol-3-yl]acetic acid				
2	3.834	1.29	1,5-Hexadiene, 1,1,2,5,6,6-hexachl oro-	Terpenoid	146542	098141-62-9	62
			5-Bromo-2,3-dimethoxy-6-nitrobenzene	Flavonoid	149053	1000253-65-8	43
			aldehyde	Flavonoid	131828	023595-42-8	35
			2,2',4',5'-Tetrachloroacetanilide				
3	4.236	0.96	2-Oxo-3-[4-bromophenyl]propanoic acid	Flavonoid	104693	038712-59-3	40
			s-Triazole-3-carboxaldehyde, 5-(p-	-	71809	026899-27-4	35
			chlorophenyl)	Flavonoid	144540	1000305-64-9	35
			3-Bromo-4-chloro-5-methylbenzene sulfonic acid				
4	4.329	1.50	1H-Tetrazole, 1-ethyl-5-phenyl-	Flavonoid	43503	024433-71-4	53
			Acetamide, 2-[4-(4-bromophenyl-	Alkaloid	154793	017969-16-3	51
			thiazolyl]-	Alkaloid	122371	1000401-58-8	51
			1,3,5-triazine-2-amine, 4-chloro-N-(4-ethenylphenyl)-6-methoxy-				
5	4.403	2.98	2,6-Dibromobenzoquinone	Alkaloid	125049	019643-45-9	47
			Ethyl 5-[2-pyridyl]-4-	Pyrazole	154049	1000211-49-9	38
			bromopyrazolcarboxylate	alkaloids	78571	017329-87-2	35
			Acetanilide, 2-chloro-4'-nitro-	Steroid			
6	4.719	2.05	Methyl .beta.-[N-methylanilino]acrylate	Terpene	56745	084591-20-8	25
			Methyl 2,4-tridecadiynoate	Flavonoid	83274	1000336-39-6	18
			Tetryl	Alkaloid	147304	000479-45-8	15
7	4.818	1.38	Benzenesulfinic acid,4-chloro-Oxazolidine,	Alkaloid	44721	000100-03-8	35
			2-isopropyl-4-[2-allyli]phenoxy]methyl]-	-	135472	070687-97-7	30
			Boron, difluoro(1,3-diphenyl-1,3-propanediol to)-	Alkaloid	132302	014947-61-6	25

Table 1 b. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Min. Qual.
8	4.892	7.68	4-benzoxazole, 2-(trifluoromethyl	Alcohol	67709	1000396-05-4	47
			)-	Amide	9818	000644-98-4	41
			Pyridine, 2-(1-methyl ethyl)-	Alkaloid	5132	004177-16-6	35
			Pyrazine, ethenyl-	Pyrazine			
9	5.008	1.08	Ethyl 5-[4-pyridyl]-4-	Alkaloid	154050	1000211-51-2	25
			bromopyrazol- carboxylate	Alkaloid	150489	347331-84-4	25
			Pyrrole-3-carboxaldehyde, 1-(4-bro	Alkaloid	49053	001521-39-7	25
			mo-3-methyl phenyl)-2,5-dimethyl- Veratramide				
10	5.178	0.95	8-(2,3-Dimethylanilino)naphtho-	Alkaloid	137361	1000058-06-7	50
			1,2-quinone	Alkaloid	135285	351073-49-9	48
			Acetamide, 2-chloro-N-(2,3-dihydro -1-methyl-pyrrolo[2,3-b]quinolin-4-yl)-	Alkaloid	122365	1000147-02-5	30
			Dimethyl trans,trans-3-(4-cyano-buta-1,3-dienyl)isoxazole-4,5-dicarboxylate				
11	5.210	0.94	Terephthalonitrile N, N'-dioxide	Alkaloid	32504	003729-34-8	92
			5-Bromo-6-methoxy-2-methyl-8-nitroquinoline	Alkaloid	154789	1000214-70-0	38
			4,5,6-Trichloro-2-benzoxazolinone	Alkaloid	99549	050995-94-3	35
12	5.320	2.66	Benzene, 1-azido-4-nitro-Methyl	Alkaloid	35302	001516-60-5	30
			.beta.-[N-methylanilino]acrylate	Alkaloid	56745	084591-20-8	25
			Tetryl	Alkaloid	147304	000479-45-8	12
13	5.609	1.09	1,3,4-Oxadiazol-2-amine, 5-(4-	Amine	101482	033621-62-4	55
			bromophenyl)-	Flavonoid	32504	003729-34-8	53
			Terephthalonitrile N, N'-dioxide	Flavonoid	44125	041536-79-2	53
			3(2H)-Isoquinolinone, 1-amino-, oxime				
14	5.641	1.41	s-Triazole-3-carboxaldehyde, 5-	Flavonoid	71809	026899-27-4	50
			chlorophenyl)-	Alkaloid	54382	015448-59-6	46
			2-Methyl-2,3-epoxy-2,3-dihydro-naphthoquinone	Alkaloid	77220	944030-47-1	44
			4-Phenyl-2-(pyrrolidine-2-yl)-1H-imidazole				

The Tables are indicated with peaks numbers (peak height), retention time (chromatogram peak number), area percentage (analyte concentration), library identified analytes (detected chemicals), bioactive

classes (secondary metabolites), reference number, CAS numbers, and minimum quality. About 80 variable bioactive were qualitatively and quantitatively detected in *D. stramonium* leaves with different concentrations. In most instances, three bioactive of the same or different metabolites will have the same peak height and area concentration, but different retention time, reference number, and CAS number. For example, Table 1a has 5H-Dibenz,f][1,2]diazepine, 3, 8, dichloro-6, 11-dihydro whose metabolite is flavonoid had 1.24% area concentration at 3.702 retention time (minutes) on peak 1. A similar arrangement follows with other bioactive presented in Table 1b to 1h.

Table 1 c. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Min. Qual.
15	5.670	0.94	Ethane, 1-[(2-chloroethyl)thio]-2-	Alkane	51593	092569-22-7	90
			(ethylthio)-	Flavonoid	71809	5026899-27-4	47
			s-Triazole-3-	Alkaloid	69825	056055-54-0	45
			carboxaldehyde,chlorophenyl)-				
			Methyl 5,6-dichloropyridine-3-carb				
16	5.696	0.92	s-Triazole-3-carboxaldehyde, 5-	Flavonoid	71809	026899-27-4	92
			chlorophenyl)-	Steroid	71753	049558-03-4	56
			Furazan, nitrophenyl-, 5-oxide	isoquinoline al	154789	1000214-70-0	53
			5-Bromo-6-methoxy-2-methyl-8-	kaloid			
			nitroquinoline				
17	5.837	1.67	Benzenesulfinic acid, 4-chloro-1H-	Flavonoid	44721	000100-03-8	53
			Tetrazole, 1-ethyl-5-phenyl-	Alkaloid	43503	024433-71-4	53
			5-Methyl-4-[4-(1,2,4-triazole-1-ylm	Alkaloid	131973	1000410-40-8	49
			ethyl)phenyl]-1,2,4-triazole-3-thiol				
18	6.027	1.73	9,10-Di[chloromethyl]-S-	Terpenoid	141786	018256-06-9	53
			octahydroanthracene	Quinoline alka	154789	1000214-70-0	38
			5-Bromo-6-methoxy-2-methyl-8-	loid	29487	058679-08-6	35
			nitroquinoline	Terpene			
			1,2-Butadiene, 1,1,4-trichloro-				
19	6.052	1.09	N-(2-Phenylethyl)undeca-(2Z,4E)-diene-	Amide	137413	099615-80-2	38
			8,10-diynamide	Amide	75605	040707-01-5	35
			5-Chloro-N-methylisatoic anhydrazide	Terpene	29487	058679-08-6	35
			1,2-Butadiene, 1,1,4-trichloro-				
20	6.558	1.12	s-Triazole-3-	Flavonoid	71809	5-026899-27-4	68
			carboxaldehyde,chlorophenyl)-	Quinoline alka	54382	015448-59-6	55
			2-Methyl-2,3-epoxy-2,3-dihydro-1,4-	loid	111878	035839-71-5	53
			naphthoquinone	Cyclic Alkane			
			1,2-Digermacyclopentane, 1,1,2,2-				
			tetramethyl-				
21	6.587	1.22	5-Bromo-6-methoxy-2-methyl-8-	Quinoline alka	154789	1000214-70-0	62
			nitroquinoline	loid	113828	000115-09-3	59
			Mercury, chloromethyl-	Alkane	137413	099615-80-2	38
			N-(2-Phenylethyl)undeca-(2Z,4E)-di	Amide			
			ene-8,10-diynamide				

Table 1 d. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Min. Quality
22	6.648	1.20	9,10-Di[chloromethyl]-S-octahydroanthracene	Alkaloid	141786	018256-06-9	43
			4,6-Dibromo-2-benzoxazolinone 3,5,6,7,7,8-				
			Hexachloro-5,6,7,8-tetrahydro-S-triazolo[4,3-	Alkaloid	150985	1000260-92-6	38
			a]pyridine	Alkaloid	185439	022841-85-6	38
23	6.947	1.14	Terephthalonitrile N, N'-dioxide	Steroidal Alkaloid	32504	003729-34-8	50
			Androstan-4,16-dien-3-one, 17-formyl-	Steroid	157994	114724-34-4	38
			Acetanilide, 2-chloro-4'-nitro-	Steroidal Alkaloid	78571	017329-87-2	35
24	6.989	0.95	1,4-Dioxaspiro[4.5]deca-6,9-diene-2,8-dione	Terpene	37021	004385-47-1	50
			6-Bromo-4,7-dimethoxy-2H-1,3-benzo dioxole-5-	Aldehyde			
			carbaldehyde		147355	109548-10-9	38
			2-Thiophenecarbonitrile, 4-Bromo-	Steroidal Alkaloid	53820	1000362-65-0	35
25	7.053	1.30	Methyl 2-bromo-3-cyano-6-methylpyr idine-4-	Alkaloid	115716	1000410-58-8	55
			carboxylate	Alkaloid	141694	1000111-66-8	47
			7,8-Methylenedioxy-5-oxo-1-fluorenecarboxylic	Alkaloid	145855	1000260-14-0	45
			acid, methyl ester				
			2,3-Diazabicyclo[3.3.0]octa-3,7-diene-4-				
			carboxylic acid, 2-(4-methoxyphenyl)-, ethyl ester				
26	7.069	1.72	Acetanilide, 2-chloro-4'-nitro-	Alkaloid	78571	017329-87-2	35
			7-[2-Chloroethyl]guanine	Steroid Nucleotide	77363	022247-87-6	35
			5-Bromo-6-methoxy-2-methyl-8-nitroquinoline	Isoquinoline	154789	1000214-70-0	35
27	7.120	1.70	(3-Nitro-benzyl)-O-tolyl-amine	Amine Alkaloid	103988	1000296-75-0	56
			4-Amino-6-morpholino-5-nitropyrimidine	Saponin Saponin	88749	024957-88-8	45
			Phenol, 2-cyclohexyl-4,6-dinitro-		125969	000131-89-5	44
28	7.644	1.06	(3-Nitro-benzyl)-O-tolyl-amine	Amine	103988	1000296-75-0	90
			[(2-Oxochromen-4-yl)sulfanyl]acetic acid	Flavonoid	97970	1000410-90-7	40
			5-Chloro-3-[(2-chloro-acetylamino)	Amine alkaloid	136837	1000294-79-5	40
			-methyl]-2-hydroxy-benzoic acid				

Table 1 e. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Min. Quality
29	7.773	0.98	5-Bromo-6-methoxy-2-methyl-8-nitro quinoline	Quinoline Alkaloid	154789	1000214-70-0	83
			Ethyl 4-([(E)-(2-nitrophenyl)methyl lidene]amino)benzoate	Alkaloid	157260	057707-09-2	45
			1H-1,2,3-benzotriazole, 5,6-dibromo-	Alkaloid	135658	1000401-84-4	42
30	7.924	0.93	5-Bromo-6-methoxy-2-methyl-8-nitro quinoline	Quinoline Alkaloid	154789	1000214-70-0	55
			N-(2-Cyclopropylphenyl)-N'-(2,5-di methylphenyl)thiourea	Flavonoid	155625	1000305-33-1	45
			2H-3,5a-Epoxynaphth[2,1-b]oxepin, dodecahydro-3,8,8,11a-tetramethyl-[3R-(3.alpha.,5a.alpha.,7a.beta.,11a.alpha.,11b.beta.)]-	Flavonoid	138442	038419-74-8	44
31	8.191	0.95	4-Bromo-.alpha.-toluenesulfonic acid	Alkaloid	111885	110874-72-1	43
			Lycoramine	Alkaloid	148854	021133-52-8	40
			2,5-Cyclohexadiene-1,4-dione, 2,5-dichloro-3,6-dimethoxy-	Terpene	98877	007210-71-1	35
32	8.287	0.99	1,4-Dioxaspiro[4.5]deca-6,9-diene-2,8-dione	Terpene	37021	004385-47-1	90
			Hydrazine, 1-(bromo)nitromethylide ne-2-(4-nitrophenyl)-	Alkaloid	148348	064817-09-0	55
			7-Nitro-2,1,3,4,5-[1,2,5]oxadiazol o[4,3-c]cinnoline-1,5-dione	Indole alka loid	110737	1000387-20-7	45
33	8.525	1.59	Terephthalonitrile N, N'-dioxide	Alkaloid	32504	003729-34-8	43
			N-[4-Chloro-2-chloroacetamidopheny l]piperidine o-Veratramide	Alkaloid Amide	145469 49053	1000254-96-6 001521-39-7	38 35
34	8.564	0.94	Benzene, pentachloronitro-	Alkaloid	152888	000082-68-8	42
			Terephthalonitrile N, N'-dioxide	Alkaloid	32504	003729-34-8	35
			5-Chloro-N-methylisatoic anhydrazide	Alkaloid	75605	040707-01-5	35
35	8.590	1.78	5H-Dibenzo[c,f][1,2]diazepine,3,8 -dichloro-6,11-dihydro-	Flavonoid	124275	000955-66-8	70
			1,2,5,6-Tetrahydropyridine, 1-meth yl-6-[2-pyridyl]-Benzofurazan, 4-Bromo-	Alkaloid Alkaloid	42951 63746	1000132-27-6 035036-93-2	56 48

Table 1 f. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Minimum Quality
36	9.352	1.61	2-Phenyl-6-nitrochromen-3-one, oxime	Flavonoid	143624	111421-24-0	56
			1(2H)-naphthalene, 3,4-dihydro-5 -methoxy-2-methyl-, oxime	Steroid	69606	1000396-08-3	46
			Ethane, 1-[(2-chloroethyl)thio]-2-(ethylthio)-	-	51593	092569-22-7	46
37	9.435	2.20	5-Bromo-2-amino benzophenone	Flavone	148494	039573-18-7	64
			hydrazones	Flavone	149053	1000253-65-8	50
			5-Bromo-2,3-dimethoxy-6-nitrobenzaldehyde	Flavone	157868	014058-65-2	44
			1H-Indolizino[8,7-b]indole-2-propanol, .beta.-ethyl-2,3,5,6,11,11b-hexahydro-				
38	9.546	0.96	s-Triazole-3-carboxaldehyde,5 chlorophenyls)-	Flavonoid	71809	026899-27-4	62
			2-Phenyl-6-nitrochroman-3-one, oxime	Flavonoid	143624	111421-24-0	56
			6-(2-Imino-3-oxazolidinyl)-N,N,N', N'-tetramethyl-1,3,5-triazine-2,4-diamine	Flavonoid	111988	087166-33-4	55
39	9.644	1.34	6-(2-Imino-3-oxazolidinyl)-N,N,N', N'-tetramethyl-1,3,5-triazine-2,4-diamine	Alkaloid	111988	087166-33-4	72
			Ethanone, 1-[4-(3-indolylmethylen) amino]phenyl-	Amine Flavonoid	123000 134384	088701-57-9 1000251-54-3	48 48
			2-[2-Methyl-4-chlorobenzoyl]benzoic acid				
40	9.738	1.05	Ethane, 1-[(2-chloroethyl)thio]-2-(ethylthio)-	Terpene	51593	092569-22-7	48
			1,2-Cyclopentanedicarboxylic acid, 4-[(trimethylsilyl)methylene]-, d	Terpene	130059	109613-12-9	45
			imethyl ester, trans-2-Methyl-2,3-epoxy-2,3-dihydro-1,4 -naphthoquinone	Quinone Alkaloid	54382	015448-59-6	44
41	9.760	1.77	6,8,9-Trimethoxy-2-methyl-2,3-dihy-	Alkaloid	149757	1000195-16-7	44
			dronaphtho[1,2-b]furan-2-ol	Alkaloid	148183	000481-30-1	44
			Androst-4-en-3-one, 17-hydroxy-, (17.alpha.)-	Steroid	147975	1000251-43-8	44
			5,10-Methano-2,7-dichloro-5-methyl dibenzo[a,d]cycloheptane				
42	9.931	0.99	5-Bromo-6-methoxy-2-methyl-8-nitroquinoline	Isoquinoli ne	154789 153126	1000214-70-0 023469-59-2	74 60
			11H-Dibenzo[c,f][1,2]diazepin-11-ol, 3,8-dichloro-,5-xidediethylselanadiselenide	Flavonoid Alkaloid	158086	1000374-05-3	55

Table 1 g. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Minimum Quality
43	9.988	1.21	4-(1-Benzofuran-2-yl)-7-	Flavon	151822	108154-51-4	44
			methoxychromen-2-one	Flavonoid	147355	109548-10-9	25
			6-Bromo-4,7-dimethoxy-2H-1,3-	Alkaloid	151993	054833-65-7	25
			benzodioxole-5-carbaldehyde				
			Pyrrolo[2,3-b]indole, 1-benzoyl-1,				
			2,3,3a,8,8a-hexahydro-3a,8-dimethy				
			l-, (3aS-cis)-				
44	10.001	1.25	2,3,5-Trichlorophenol, O-	Alkaloid	152147	1000374-26-9	30
			trifluoroacetyl-	Flavonol	152146	1000365-26-5	30
			2,4,6-Trichlorophenol, trifluoroacetate	Amide	151235	131022-82-7	25
			2-Chloro-5-methyl-4,6-bis(2-thienyl)				
			pyrimidine				
45	10.310	1.38	Ethyl 4-([(E)-(2-	Flavonoid	157260	057707-09-2	25
			nitrophenyl)methylidene]	Flavonoid	157867	055670-04-7	25
			amino)benzoate	Flavonoid	139558	1000124-95-9	15
			1H-Indolizino[8,7-b]indole-1-propanol,				
			.beta.-ethyl-2,3,5,6,11,11b-hexahydro-				
			Chromone, 5-hydroxy-6,7,8-				
			trimethoxy-2,3-dimethyl-				
46	11.039	1.43	1H-Benzotriazole, 4,5,6,7-tetrachloro-	Flavonoid	116404	002338-10-5	47
			3-(3,4-Methylenedioxy)phenyl-4-	Flavone	123534	1000111-64-4	46
			nitrocyclohexanone	Alkaloid	82127	022936-87-4	45
			4-Methyl-6-phenyl-3-thioxo-3,4-				
			dihydro-1,2,4-triazine-5(2H)-one				
47	11.037	2.06	Carbazol-1-ol, 1,2,3,4-tetrahydro-6-	Flavonoid	152409	1000263-26-5	90
			Bromo-9-ethyl-	Terpenoid	152287	020992-89-6	58
			Ethyl 4-Bromo-alpha-cyano-beta-	Terpenoid	152889	000082-68-8	56
			methyl-cis-cinnamate				
			Benzene, pentachloronitro-				
48	11.069	1.06	Pyrazole, 1-methyl-3-(4-nitrophenyl)-	Alkaloid	67254	073387-59-4	58
			1,3,4-Oxadiazol-2-amine, 5-(4-	Alkaloid	101482	033621-62-4	55
			bromophenyl)-	Alkaloid	43503	024433-71-4	53
			1H-Tetrazole, 1-ethyl-5-phenyl-				
49	11.339	1.45	4-(4-Chlorophenyl)-3-	Flavonoid	149595	142405-54-7	46
			morpholinopyrrol-2-carbaldehyde	Flavonoid	137963	027188-36-9	46
			Dibenzo[b,f][1,4]diazocine, 5,6,11,12-	Flavonoid	136769	014401-73-1	45
			tetrahydro-2-(trifluoromethyl)				
			Ethanone, 1-(3,5-bromophenol)-				

Table 1 h. Bioactive Profile of *Datura stramonium* leaves Screened with GC-MS

Peak H.	RT	Area %	Library/ID	Metabolites	Ref no	CAS	Minimum Quality
50	11.664	1.33	Mercury, chloromethyl-	Alkaloid	113828	000115-09-3	80
			5-Bromo-6-methoxy-2-methyl-8-nitroquinoline	Isoquinolin	154789	1000214-70-0	62
			4,5,6-Trichloro-2-benzoxazolinone	e	99549	050995-94-3	62
				Isoquinolin			
				e			
51	11.850	1.03	3-Bromo-2,5-dichlorothiophene 5-Bromo-6-	Flavonoid	93483	060404-18-4	40
			methoxy-2-methyl-8-nitroquinoline	Quinoline	154789	1000214-70-0	38
			3,5-Dichloro-2-hydrazinopyridine	Alkaloid	45439	104408-23-3	30
52	13.229	1.01	Pyrazole, 1-methyl-3-(4-nitrophenyl)-	Alkaloid	67254	073387-59-4	59
			1H-Tetrazole, 1-ethyl-5-phenyl- 1,3,4-	Alkaloid	43503	024433-71-4	53
			Oxadiazol-2-amine, 5-(4-bromophenyl)-		101482	033621-62-4	46
53	13.911	1.25	1,3,4-Oxadiazol-2-amine,5-(4-bromophenyl)-	Flavonoid	101482	033621-62-4	55
			1H-Tetrazole, 1-ethyl-5-phenyl-	Alkaloid	43503	024433-71-4	53
			s-Triazole-3-carboxaldehyde, 5 chlorophenyls)-	Alkaloid	71809	026899-27-4	50
54	14.126	21.66	Phytol, 4-Chloro-6,7-dimethyl-3-N-(oxolan-	Alkaloid	155850	000150-86-7	53
			2-ylmethyl)-2H-pyrrolo[3,4-c]pyridine-1,3-				
			diimine	Alkaloid	151308	1000388-01-6	41
			2,2,6-Trimethyl-1-(3-methyl beta-1, 3-dienyl)-7-	Flavonol	85557	1000191-85-4	41
			oxabicyclo[4.1.0]heptan-3-ol				

Key: Peak H = Peak height; RT = Retention time

An investigation to identify, quantifies, and characterized the different bioactive compounds in *Datura stramonium* (Jimson weed) leaves was carried out. The results showed 80 different bioactive constituents belonging to different metabolites including alkaloids, flavonoids, terpenoids, saponins, amine, and steroids. Several phytochemicals were detected and quantified - flavonoid had - 5H-Dibenzo[c,f][1,2]diazepine – 1.24% concentration at 3.702 retention time see Table 1a. This compound is also called 3-amino-5,12,12a-trihydro-4-oxo-1Hpyrazolo[4,3-e] thiochromeno [4,3-c] [1,2] diazepines (Ramendra and Vishnu, 2014). 5H-Dibenzodiazepines are used in treating an array of health problems. They act by activating a sedative substance in the brain and central nervous system (CNS). Negative outcomes may include dizziness, poor coordination, and depression (Salzman, 1990).

5H-Dibenzodiazepines are usually used for the temporary management of severe insomnia. 5H-Dibenzodiazepines remain a potent anticonvulsant and vastly effective at averting protracted epileptic seizures. The dangerous part of this leave extract is when used in combination with alcohol or opioids (American Psychiatric Association, 1998). 5H-Dibenzodiazepines bind stereo-specifically to an exclusive portion of GABA receptors with large protein complexes, located at some neurons in the CNS. GABA is the main inhibitory neurotransmitter in the brain (Stahl, 2002). 5H-Dibenzodiazepines potentiate GABA-mediated transmission and are indirect GABA agonists (Buffett-Jerrott and Stewart, 2002; Fick *et al.*, 2003). A chemical class of terpenoid - 1,5-Hexadiene, 1,1,2,5,6,6-hexachloro was detected and shown in Table 1a. It has a 1.29% concentration and a 3.834 retention time (RT). Also, an alkaloid - 2,6-Dibromobenzoquinone commonly called Quinone, 2,6-dibromo- had 2.98% at 4.403 RT. 2,6-Dibromoquinone-4-chloroimide is a reagent for the determination of phenols (Wagner *et al*., 2007). Katherine (2016) study the effect of halobenzoquinone on human neural stem cells (hNSCs), a flow cytometric analysis revealed that hNSCs exposed to 0.5 µM of 2,6-dichlorobenzoquinone (2, 6- DCBQ), for 96 hours which occasioned greater quantities of cells in S-phase. This proposes the arrest of the cell cycle in the S-phase where deoxyribonucleic (DNA) replication ensues. In Table 1b, 4-benzoxazole, 2-(trifluoromethyl) which belongs to the Chlorzoxazone family of drugs was detected in the *D. stramonium* leave extract. Its concentration was 7.68% at 4.892 RT. This class of chemical is an alcohol derivative that acts as a muscle relaxant bearing tranquilizing properties. It is claimed to prevent muscle twinge by causing an effect mostly on the spinal cord and subcortical areas (Martindale, https://www.drugbank.ca/drugs/DB00356). A series of ten different oxadiazole analogs were appraised for their *in vitro* activities against cancer in a single-dose assay. The oxadiazole equivalents exhibited reasonable activity against cancer on several cell lines. The oxadiazole analogs increase their anticancer activities (Mohamed *et al.,* 2013). Another alkaloid - 4-Phenyl-2-(pyrrolidine-2-yl)-1H-imidazole whose IUPAC name is 5-phenyl-1H-imidazole was detected and estimated as 1.41% at 5.641 RT. 5-phenyl-1H-imidazole 4.41% at 5.641 RT; 1,3,4-Oxadiazol-2-amine 1.09% at 5.609 RT and s-Triazole-3-carboxaldehyde, 5-chlorophenyl were detected. There are supplemented as azole antifungal agents. They work by obstructing the making of ergosterol, a vital constituent of cell membranes in fungal. Its action is by disrupting the cytochrome p450 51 (Lanosterol 14-alpha demethylase) in fungal. This is crucial in the structure of the cell membranes of fungus. Its inhibition resulted in cell lysis (Tassaneeyakul *et al*., 1998). The inhibition in the production of ergosterol, causes holes to appear in the cell membrane. This is because cell membranes are necessary for the survival of fungi. Their general functions include Steroid hydroxylase action, which breaks down more than a few carcinogens, tablets, and diluents to reactive metabolites (Tassaneeyakul *et al*., 1998; Monostory *et al.,* 2004). Furazan, nitrophenyl-, 5-oxide 0.92% at 5.696 RT. This compound is an organic compound - nitrobenzenes. They contain a nitrobenzene moiety, this bioactive plays a vital role in metalloaminopeptidase activity by removing the N-terminal of methionine from an emerging protein. The N-terminal of methionine is repeatedly sliced when the second residue in the primary sequence is lesser and uncharged (Met-Ala-, Cys, Gly, Pro) Berman *et al*. (2000). 5 -Bromo-6-methoxy-2-methyl-8-nitroquinoline (Quinoline *alkaloid*) 1.22% at 6.587 RT. This is an organic compound known as nitroquinolines. It contains a nitro group bonded to a quinoline (Pelletier *et al*., 1994) see Table 1c. This phytochemical had exhibits antitumor activity via inhibiting the type-2 methionine of aminopeptidase (MetAP2) protein involved in angiogenesis. Its antibacterial action originates from the metal ion complexion that is useful for bacterial growth (Pelletier *et al.*, 1995; Shim *et al*., 2010). In Table 1d, the most important bioactive were detected and estimated. For example, androstane-4, 16-dien-3-one,17-formyl 1.14% at 6.947 RT is categorize as androstanes. This compound belongs to androgens and derivatives, they are 3-hydroxylated C19 steroid hormones. Known to service the development of masculine characteristics, this accounted for its utilization as an esoteric cannabinoid by some youths (Chen *et al*., 2000). These same properties corroborate the use of this plant extract for the treatment of hair loss in humans, and function in Steroid hormone receptors - ligand-activated transcription factors that control the expression of a eukaryotic gene and affect cellular proliferation and differentiation in target tissues (Takahashi *et al*., 2004). 2, 5-Cyclohexadiene-1,4-dione with 0.95% at 8.191 RT is also called RH-1. These are organic compounds known as p-benzoquinones. Benzoquinones have two C=O groups attached to carbon 1- and 4-positions, respectively. RH-1 has been used in trials, to study the handling of Progressive Hard Cancers and Non-Hodgkin's Lymphoma (Tudor *et al.,* 2005). At the superoxide dismutase activity, the enzyme helps as a quinone reductase by linking with conjugation reactions of hydroquinone that are involved in detoxification corridors and biosynthetic routes including the vitamin (Overington *et al.,* 2006; Imming *et al.,* 2006). l]piperidine o-Veratramide 1.59% at 8.525 RT. This compound belongs to aminopiperidines. They contain piperidine that carries an amino group. At the triglyceride lipase activity pathway, l]piperidine is applied in the decontamination of xenobiotics and activation prodrugs containing ester and amide. In Table 1e, tricyclic dibenzodiazepine, categorized as an uncommon antipsychotic agent (5H-

Dibenzo[c,f][1,2]diazepine,3,-dichloro-6,11-dihydro-) was detected and quantified – 1.78% at 8.590 RT. This compound binds to some receptors in the central nervous system and displays a distinctive pharmacological effect. 5H - Dibenzo[c,f][1,2]diazepine is a serotonin antagonist, with high binding to 5-HT 2A/2C receptor subtype (Berman *et al*., 2000; Weizman *et al*., 2003;). It also displays high affinity to numerous dopaminergic receptors but expresses weak antagonism at the dopamine D2 receptor, a receptor that controls neuroleptic activity (Guarrera, 1999). The major adverse effect associated with the administration of this agent is agranulocytosis (an acute febrile condition noticeable by severe reduction in blood granulocytes and often linked with the use of certain drugs). Dibenzo[c,f][1,2]diazepine is a psychotropic agent belonging to benzisoxazole derivatives indicated for the treatment of schizophrenia (a mental disorder that is characterized by disturbances in thought in the case of hallucination). 5H - Dibenzo[c,f][1,2]diazepine is a discriminating monoaminergic antagonist with a strong affinity for the serotonin Type-2 ($5HT_2$), dopamine Type-2 (D2), 1 and 2 adrenergic, and H1 histaminergic receptors (Young *et al*., 2004). 5H-Dibenzo[c,f][1,2]diazepine serves as an antagonist to other receptors sites, but with lesser potency. Antagonism at receptors other than dopamine and $5HT_2$ with similar receptor affinities explain the side effect of 5H-Dibenzo[c,f][1,2] diazepines (Stonehouse and Jones, 2005). 5H-Dibenzo[c,f][1,2]diazepine's antagonism of muscarinic M1-5 receptors explains its anticholinergic outcome after administration or ingestion. 5H-Dibenzo[c,f][1,2]diazepine's antagonism of histamine H1 receptors elucidate the somnolence experience with this drug. 5H-Dibenzo[c,f][1,2]diazepine's antagonism of adrenergic-1 receptors could clarify the orthostatic hypotension observed with this bioactive (Takano *et al*., 2006). 5H-Dibenzo[c,f][1,2]diazepine's antipsychotic action is prospectively regulated via a combination of antagonistic effects at D2 receptors in the mesolimbic pathway and 5-HT2A receptors in the frontal cortex (Chen *et al*., 2002). The D-2 antagonism could relieve a helpful symptom while 5-HT2A antagonism alleviates harmful symptoms.

A 1.61% at 9.352 RT of 1(2H)-naphthalenone, 3,4-dihydro-5 was detected. It is called 2-[4-(4-Chlorophenyl) Cyclohexylidene]-3,4-Dihydroxy-1(2h)-Naphthalene. Its mechanism of action deals with ubiquinone binding to catalyzes the transformation of dihydroorotate to orotate, while quinone will remain an electron acceptor (Berman *et al*., 2000). Phenyl-2H-chromene derivatives are derivatives to synthesize triazole and biotin-containing chromene derivatives, to facilitate the purification of protein targets (Bhaskar *et al*., 2010). These organic compounds are phenol ethers. They are aromatic compounds having an ether group substituted with a benzene ring. It derivatives is 6-(2-phenoxy ethoxy)-1, 3, 5-triazine-2, 4-diamine. Its function deals with the acetylation of the coenzyme-A carboxylase complex. Whereat first, biotin carboxylase will catalyze the carboxylation of the carrier protein and then the transcarboxylase transfers the Ca^+ (Berman *et al*., 2000), find Table 1f. A flavonoid named 4-(1-Benzofuran-2-yl)-7-methoxychromen-2-one had 1.21% at 9.988 RT was detected in *D. stramonium* leaves. This compound is a flavone whose backbone is 2-phenylchromen-4-one (2-phenyl-1-benzopyran-4-one) (Shimada *et al.*, 2009). It has antibiotic activity (for Gram-positive bacteria) and antitumor activity (for some mouse tumors). It binds non-covalently to a chromophore which is the cytotoxic and mutagenic component of the antibiotic. The chromophore in turn binds to DNA as a weak intercalator and reasons a single - and double-strand breakdown (Shimada *et al*., 2010). 2-Chloro-5-methyl-4, 6-bis (2-thienyl) pyrimidine 1.25% at 10.001 RT was obtained from *D. stramonium* leaves and presented in Table 1g. This organic compound is known as aminobenzenesulfonamides (Derewlany *et al*., 1994). They contain benzenesulfonamide moiety with an amine group bonded to the benzene ring. This amide is directed for the treatment of bacterial infections which cause bronchitis, prostatitis, and urinary tract infections. The role of 2-Chloro-5-methyl-4,6-bis(2-thienyl) pyrimidine is to inhibit the enzymatic conversion of pteridine and p-aminobenzoic acid (PABA) to dihydropteroate acid by opposing PABA from binding to dihydrofolate synthetase, an intermediate of tetrahydrofolic acid (THF) synthesis. THF is usually needed to synthesize purines and dTMP. Any disruption of its synthesis will inhibit the growth of bacterial. Pyrimethamine and trimethoprim inhibit dihydrofolate reductase, additional pace in THF synthesis, and act in synergy with 2-Chloro-5-methyl-4,6-bis(2-thienyl) pyrimidine. 2-Chloro-5-methyl-4,6-bis(2-thienyl) pyrimidine as a side effect which may be nausea, vomiting, diarrhea, and hypersensitivity reactions (Friaza *et al*., 2010). Hematologic effects such as anemia, agranulocytosis, thrombocytopenia, and hemolytic anemia in patients with glucose-6-phosphate dehydrogenase insufficiency may arise (Bratlid and Bergan, 1976). 2-Chloro-5-methyl-4,6-bis(2-thienyl) pyrimidine might dislodge bilirubin from albumin binding sites triggering jaundice or kernicterus in newborns (Angelakou *et al*., 1993). In Table 1h, 5-Bromo-6-methoxy-2-methyl-8-nitroquinoline 1.33% at 11.664 RT was obtained. This compound is nitroquinolines and their derivatives. They contain a nitro group bonded to a quinoline. It is indicated for dealing with Schistosomiasis affected by *Schistosoma mansoni (*Filho *et al*., 2006*).* 5-Bromo-6-methoxy-2-methyl-8-nitroquinoline is an anthelmintic with schistosomicidal activity against *Schistosoma mansoni*, but not against other Schistosoma spp. 5-Bromo-6-methoxy-2-methyl-8-nitroquinoline causes worms to move from the mesenteric veins to the liver where the male worms are

retained; the female worms return to the mesentery, but can no longer release eggs (Overington *et al.*, 2006). 5-Bromo-6-methoxy-2-methyl-8-nitroquinoline may link with an irreversible inhibitor of nucleic acid metabolism. A premise has been put forth that the drug is activated by a single step, in which a schistosome sulfotransferase enzyme converts 5-Bromo-6-methoxy-2-methyl-8-nitroquinoline into an ester (probably acetate, phosphate, or sulfate group). Successively, the ester suddenly dissociates, the resultant electrophilic reactant is capable of alkylating the schistosome DNA (Imming *et al.*, 2006; Pica-Mattoccia *et al.*, 2006). The phytochemistry and therapeutic elucidation of *Datura stramonium* leave extract have been well recognized in this investigation. Because of its multiple uses, more bioactive screening and structural elucidation studies are yet to be explored. The information presented in this work would help promote research aiming at the development of methods for isolation and application of new agents for medical applications and agro-industries based on natural products derived from plants.

Conclusion: The information about jimson weed (leaves) covers many aspects including botanical, chemical, pharmaceutical, and medical. The objectives of this study were to (a) develop an improved GC-MS procedure for the analysis of bioactive components of jimson weed leaves to show the known and unknown alkaloids, Flavonoids, Terpenoids, saponins, amide, amines, and alcohols using the GC-MS technique. These bioactive were identified, classified, characterized, and estimated. They were blasted against the synthetic drug bank to ascertain their therapeutic relevance, correlation, and relativity. Much of their pharmacological relevance was describe together with their mechanism of action. This was performed with the hope that drugs producers, researchers, and herbal technicians will find a better understanding in redirecting their treatment synthesis of novel therapies.

Competing interests: Authors have declared that no competing interests exist. The products used for this research are commonly and predominantly use products in our area of research and country. There is no conflict of interest between the authors and producers of the products because we do not intend to use these products as an avenue for any litigation but the advancement of knowledge. Also, the research was not funded by the producing company rather it was funded by the personal efforts of the authors.

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