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'The GC MS Analysis of Ethyl Acetate Extract of One Herbal Plant, '*Justicia Simplex*'

Ganesan Muruga Perumal[1], Prabhu K[2], Rao MRK[3*]. Janaki C. S.[4], Kalaivannan J[5], Kavimani M[1]

[1]Professor, Department of Anatomy, Sree Balaji Medical College and Hospital, Chennai, Tamil Nadu, India.
[2] Associate Professor, Department of Anatomy, Sree Balaji Medical College and Hospital, Chennai, Tamil Nadu, India.
[3] Consultant Scientist, M/s. Noahs Laboratories, No, 8/1, Old Mahabalipuram Road, Thiruporur, Tamil Nadu 603110, India.
[4] Associate Professor, Department of Anatomy, Bhaarath Medical College and Hospital, Chennai, Tamil nadu, India.
[5]Associate Professor, Department of Anatomy, Vinayaka Mission's Medical College and Hospital, Karikal, Vinayaka Mission's Research foundation, Salem, Tamil nadu, India.

ABSTRACT

The present study deals with the GC MS analysis of one medicinal plant*, Justicia simplex*. The plant is diuretic, stomachic, expectorant, anthelmintic, diaphoretic and aperient. It gives relief from indigestion, biliousness, fever and burning of the body. It strengthens the lungs, the teeth and helps stop vomiting. It is also used for spleen disorders. The plant was collected from nearby hills of Chengalpattu, Tamilnadu. The ethyl acetate extract of the aerial parts of the plant was subjected to GC MS study following standard protocols. It was observed that some very important molecules such as 17-Octadecynoic acid, 2H-Pyran-2,6(3H)-dione, 2-Furancarboxylic acid, Benzoic acid, 4(1H)-Pyridone , trans-3-Methyl-2-n-propylthiophane, Catechol, 3-Hydroxydecanoic acid, .alpha.-D-Xylofuranoside, methyl, Methyl .beta.-d-galactopyranoside, .beta.-l-Arabinopyranoside, methyl, n-Hexadecanoic acid, Shikimic acid and Inositol were found in the GC MS profile which has far reaching medicinal roles, thereby supporting the medicinal value of this plant.

Key words: GC MS, Ethyl acetate, *Justicia simplex'*, 17-Octadecynoic acid, 2H-Pyran-2,6(3H)-dione, 2-Furancarboxylic acid, Benzoic acid, 4(1H)-Pyridone, n-Hexadecanoic acid, Shikimic acid, Inositol

INTRODUCTION

The plant, *Justicia simplex,* is widely used traditionally to cure some diseases. Very few reports on the medicinal role of this plant are available. The leaves contain a bitter and slightly toxic alkaloid, some aromatic amines and α and β sitosterol, the roots contain β sitosterol (Ghani, 2003). The leaves give strength to the body. The plant is diuretic, stomachic, expectorant, anthelmintic, diaphoretic and aperient. It gives relief from indigestion, biliousness, fever and burning of the body. It strengthens the lungs, the teeth and helps stop vomiting.It is also used for spleen disorders. Leaf juice drops are used to treat ophthalmia (Ghani, 2003). Eswari et al, 2014, have reported the antibacterial role of this plant on dental pathogens. The present work reports the GC MS pattern of the ethyl acetate extracts of Justicia simplex whole plant. This is in continuation of our endeavour to establish the medicinal efficacy of the herbal and traditional systems of Ayurveda, Sidhha and Unani systems of medicine (Priyadarshini *et al,* 2017; Jayakumari *et al*, 2017; Rao *et al,* 2018; Vijayalakshmi and Rao, 2019; Yuvaraj *et al*, 2019; Muttevi *et al,* 2019, Rao *et al*, 2019; Muttevi *et al,* 2020; Vijayalakshmi and Rao, 2020; Janaki *et al*, 2021).

MATERIALS AND METHODS

The plant *Justicia simplex*was collected from the nearby paddy fields at Chengalpattu, Tamil Nadu. The plant was identified by a qualified botanist at Chennai. The ethyl acetate extract of the shade dried whole plant was collected after 48 h of soaking. The extract was evaporated and the dried powder was used for GC-MS analysis by standard procedures.

GC-MS Procedure

Instrument: GC (Agilent: GC: (G3440A) 7890A. MS/MS: 7000 Triple Quad GCMS) was equipped with MS detector.

Sample Preparation

About 100 ml sample was dissolved in 1 ml of suitable solvents. The solution was stirred vigorously using vortex stirrer for 10 s. The clear extract was determined using GC for analysis.

GC-MS Protocol

Column DB5 MS (30 mm × 0.25 mm ID ×0.25 µm, composed of 5% phenyl 95% methylpolysiloxane), electron impact mode at 70 eV; helium (99.999%) was used as carrier gas at a constant flow of 1 ml/min injector temperature 280°C; auxilary temperature: 290°C ion-source temperature 280°C.

The oven temperature was programmed from 50°C (isothermal for 1.0 min), with an increase of 40°C/min, to 170°C C (isothermal for 4.0 min), then 10°C/min to 310°C (isothermal for 10 min) fragments from 45 to 450 Da. Total GC running time is 32.02 min. The compounds are identified by GC-MS Library (NIST and WILEY).

RESULTS AND DISCUSSION

The results of the GC-MS analysis of the whole plant ethyl acetate extract, along with the possible medicinal role of each molecule of*Justicia simplex*extract are tabulated in Table 1. Figure 1 represents the GC-MS profile of ethyl acetate extract of the whole plant of *Justicia simplex.* The identification of metabolites was accomplished by comparison of retention time and fragmentation pattern with mass spectra in the NIST spectral library stored in the computer software (version 1.10 beta, Shimadzu) of the GC-MS along with the possible pharmaceutical roles of each bio molecule as per Dr. Duke's Phytochemical and ethno-botanical data base (National Agriculture Library, USA) and others as shown in Table 1.Table no. 1 indictes the presence of a wide range of molecules having important medicinal roles, such as, 17-Octadecynoic acid, 2H-Pyran-2,6(3H)-dione, 2-Furancarboxylic acid, Benzoic acid, 4(1H)-Pyridone , trans-3-Methyl-2-n-propylthiophane, Catechol, 3-Hydroxydecanoic acid, .alpha.-D-Xylofuranoside, methyl, Methyl .beta.-d-galactopyranoside, .beta.-l-Arabinopyranoside, methyl, n-Hexadecanoic acid, Shikimic acid and Inositol were present suggestive of their role in support of the medicinal value of this plant. Further work to isolate, purify and characterize them is going on.

CONCLUSION

It is concluded that the types of medicinal values the molecules have, as is shown in the Table, *Justicia simplex* can prove itself as an important medicinal plant.

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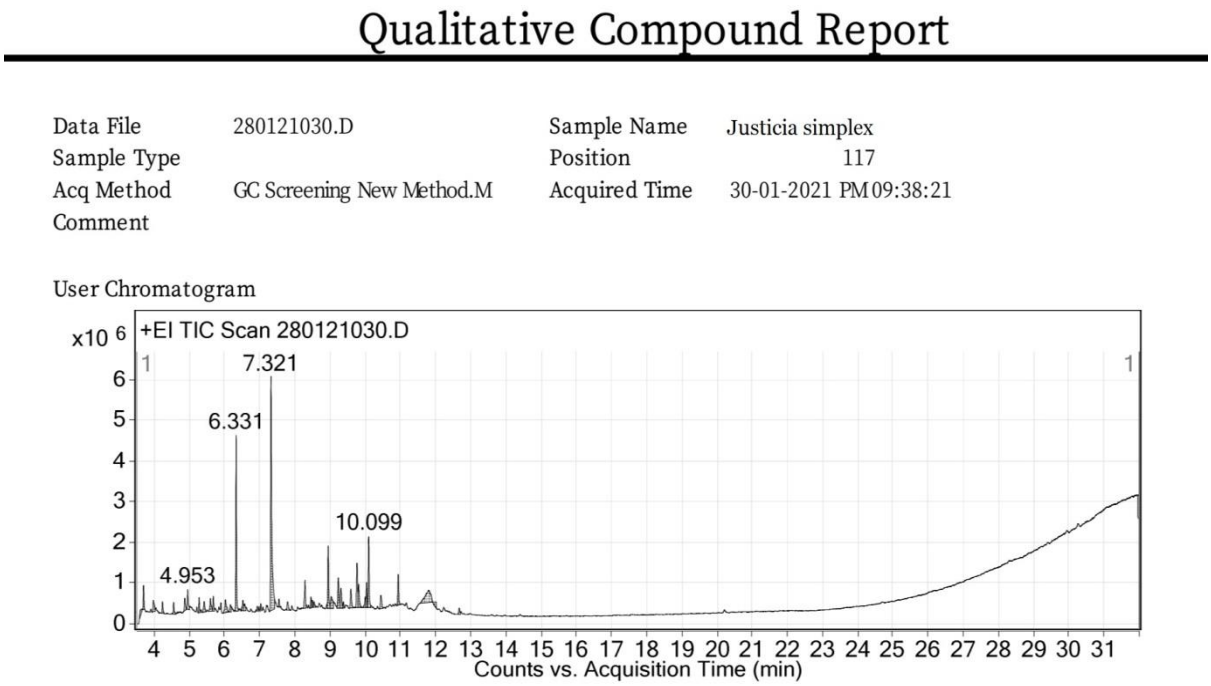

Figure 1. Represents the GC MS graph of ethyl acetate extract *Justicia simplex'*.

Table 1. Indicates the retentions time, types of possible compound, molecular formula, molecular mass, percentage peak area and the possible medicinal roles of each compound as shown in the GC MS profile of*Justicia simplex'*.

Ret. Time	Compound	Mol. formula	Mol. Mass	% peak Area	Possible Medicinal Role
3.63	17-Octadecynoic acid	C18H32O2	280.2	0.86	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
3.70	2H-Pyran-2,6(3H)-dione	C5H4O3	112	1.60	11Beta HSD inhibitor, 17-beta-hydroxysteroid dehydrogenase inhibitor, 5 HETE inhibitor, 5 HT inhibitor, 8 HETE inhibitor, Anti 5-HT, Anti HIV integrase, Aryl hydrocarbon hydroxylase inhibitor, HDL genic, Hematopoietic
3.98	2-Furancarboxylic acid	C5H4O3	112	1.43	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
4.24	Thymine	C5H6N2O2	126	0.93	Nucleotide
4.55	4(1H)-Pyridone	C5H5NO	95	0.93	11Beta HSD inhibitor, 17-beta-hydroxysteroid dehydrogenase inhibitor, 5 HETE inhibitor, 5 HT inhibitor, 8 HETE inhibitor, Anti 5-HT, Anti HIV integrase, Aryl hydrocarbon hydroxylase inhibitor, HDL genic, Hematopoietic
4.87	Benzoic acid	C7H6O2	122	1.27	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
4.95	trans-3-Methyl-2-n-propylthiophane	C8H16S	144.1	1.60	Catechol-O-Methyl-Transferase-Inhibitor, Increases Glutathione-S-Transferase (GST) Activity, Decreases Glutamate Oxaloacetate Transaminase, Decreases Glutamate Pyruvate Transaminase, Glucosyl-Transferase-Inhibitor, Glutathione-S-Transferase-Inhibitor, Increases Glyoxalate Transamination, Reverse-Transcriptase-Inhibitor, Transdermal
5.28	3-Cyclobutene-1,2-dicarboxylic acid, dimethyl ester	C8H10O4	170.1	1.05	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
5.42	Catechol	C6H6O2	110	1.27	Catechol-O-Methyl-Transferase-Inhibitor, Catecholaminogenic, Catecholaminolytic
5.60	Benzofuran, 2,3-dihydro-	C8H8O	120.1	1.49	Not known
5.68	Furane-2-carboxaldehyde, 5-(4-nitrophenoxymethyl)-	C12H9NO5	247	1.08	Not known
6.02	3-Hydroxydecanoic acid	C10H20O3	188.1	2.06	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
6.17	Cyclopentanone, 2-(1-methylpropyl)-	C9H16O	140.1	0.77	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
6.33	Cyclopentanecarboxylic acid, 4-nitrophenyl ester	C12H13NO	235.1	11.48	Acidifier, Arachidonic acid Inhibitor,

		4			Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
6.52	2-Methoxy-4-vinylphenol	C9H10O2	150.1	0.97	Not known
7.32	1,2,3-Benzenetriol	C6H6O3	126	25.58	Not known
7.55	.alpha.-D-Xylofuranoside, methyl	C6H12O5	164.1	0.58	5, alpha-reductase inhibitor, alpha-amylase inhibitor, alpha-glucosidase inhibitor, alpha-reductase inhibitor, HIF 1 alpha inhibitor, increases alpha-N-mannosidase activity, interleukin-1 alpha inhibitor, testosterone 5-alpha reductase inhibitor TNF-alpha inhibitor, Catechol-O-Methyl-Transferase-Inhibitor, methyl donar, methyl guanidine inhibitor, smart drug
7.79	(3-Nitrophenyl) methanol, n-propyl ether	C10H13NO3	195.1	1.03	Anaphylactic, Antitumor, Arylamine-N-Acetyltransferase-Inhibitor, Decreases Norepinephrine Production, Down regulates nuclear and cytosol androgen reuptake, GABA-nergic, Increases natural killer cell activity, Inhibits Production of Tumor Necrosis Factor, Myo-neuro-stimulant, N-Cholinolytic, NADH-Oxidase-Inhibitor, NADH-Ubiquinone-Oxidoreductase-Inhibitor
8.29	Ethyl pipecolinate	C8H15NO2	157.1	2.47	Not known
8.46	Ethylene glycol, O,O-di(pivaloyl)-	C12H22O4	230.2	0.92	Not known
8.50	Methyl (+-)-2-hydroxy-3-butenoate	C5H8O3	116	0.67	Not known
8.54	Propylparaben	C10H12O3	180.1	0.66	Not known
8.95	.beta.-D-Glucopyranose, 1,6-anhydro-	C6H10O5	162.1	5.27	17-beta-hydroxysteroid dehydrogenase inhibitor, Antiamyloid-Beta, Anti TGF-Beta, Beta-2-Receptor-Agonist, Beta-Adrenergic receptor blocker, Beta Galactosidase inhibitor, Beta-Glucuronidase inhibitor
9.03	17-Octadecynoic acid	C18H32O2	280.2	2.15	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
9.24	Methyl .beta.-d-galactopyranoside	C7H14O6	194.1	3.48	17-beta-hydroxysteroid dehydrogenase inhibitor, Antiamyloid-Beta, Anti TGF-Beta, Beta-2-Receptor-Agonist, Beta-Adrenergic receptor blocker, Beta Galactosidase inhibitor, Beta-Glucuronidase inhibitor
9.31	.beta.-l-Arabinopyranoside, methyl	C6H12O5	164.1	2.27	17-beta-hydroxysteroid dehydrogenase inhibitor, Antiamyloid-Beta, Anti TGF-Beta, Beta-2-Receptor-Agonist, Beta-Adrenergic receptor blocker, Beta Galactosidase inhibitor, Beta-Glucuronidase inhibitor

9.38	tert-Hexadecanethiol	C16H34S	258.2	0.59	Not known
9.77	1,6-Anhydro-.beta.-D-glucofuranose	C6H10O5	162.1	4.18	17-beta-hydroxysteroid dehydrogenase inhibitor, Antiamyloid-Beta, Anti TGF-Beta, Beta-2-Receptor-Agonist, Beta-Adrenergic receptor blocker, Beta Galactosidase inhibitor, Beta-Glucuronidase inhibitor
9.81	Myo-Inositol, 4-C-methyl-	C7H14O6	194.1	2.56	Catechol-O-Methyl-Transferase-Inhibitor,, Myo neuro stimulant
10.00	Scyllo-Inositol, 1-C-methyl-	C7H14O6	194.1	0.95	Catechol-O-Methyl-Transferase-Inhibitor, methyl donar, Actyl choline antagonist, acetyl COA Carboxylase inhibitor, adenylate cyclase activator, anticancer, antidote
10.04	3-Hydroxydecanoic acid	C10H20O3	188.1	1.99	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
10.10	Dodecane, 1-fluoro-	C12H25F	188.2	5.73	Not known
10.44	n-Hexadecanoic acid	C16H32O2	256.2	1.56	Anaphylactic, Antitumor, Arylamine-N-Acetyltransferase-Inhibitor, Decreases Norepinephrine Production, Down regulates nuclear and cytosol androgen reuptake, GABA-nergic, Increases natural killer cell activity, Inhibits Production of Tumor Necrosis Factor, Myo-neuro-stimulant
10.94	Shikimic acid	C7H10O5	174.1	2.66	Acidifier, Arachidonic acid Inhibitor, Increases Aromatic Amino acid decarboxylase activity, Inhibits production of uric acid, Urine acidifier
11.80	Inositol	C6H12O6	180.1	5.28	Pain killer, controls cholesterol, used to treat insomnia, schizophrenia, Alzheimer
12.67	Ethyl 6,9,12-hexadecatrienoate	C18H30O2	278.2	0.61	Not known