Section A -Research paper

THE GC MS STUDY OF ONE AYURVEDIC DRUG, GUGGULU PANCHAPALA CHURNAM

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ABSTRACT
The present study deals with the GC MS analysis of one Ayurvedicmedicine, Guggulu Panchapalam Churnam which is a digestive formulation. The medicine was procured form standard Ayurvedic vendor at Chennai and was subjected to GC MS analysis after proper processing. As many as 57 compounds were shown in the GC MS profile. Some of the molecules such as Cinnamaldehyde, (E)-, Benzoic acid, 4-isopropyl-, ethyl ester, Undecanoic acid, 10-methyl-, methyl ester, Caryophyllene oxide, Tridecanoic acid, 12-methyl-, methyl ester, 1-Heptatriacotanol, .beta.-Sitosterol, 5H-Cyclopropa(3,4)benz(1,2-e)azulen-5-one, 1,1a-.alpha.,1b-.beta.,4,4a,7a-.alpha.,7b,8,9,9a-decahydro-4a-.beta.,7b-.alpha.,9a-.alpha.-trihydroxy-3-(hydroxymethyl)-1,1,6,8-.alpha.-tetramethyl-, 9a-isobutyrate, trans(2-Chlorovinyl)triethylsilane indicated many medicinal roles which correspond to that of GugguluPanchapalamChurnam. The medicinal roles of some compounds are not known and warrant further research on them. It is concluded form the above results and discussion that,the role of GugguluPanchapalamChurnam as digestive medicine augurs well with the roles of the molecules present in it.
Key words Guggulu Panchapalam Churnam, GC MS, Ayurvedic, Cinnamaldehyde, (E)-, Benzoic acid, Caryophyllene oxide, Tridecanoic acid.

INTRODUCTION
To understand the molecular role of traditional and alternative medicines GC MS technique is one tool. The knowledge so gained could give us an insight about the possible medicinal roles of the medicine itself as is claimed by the Ayurvedic literature. This is another report by the authors who are working on this aspect of standardization and efficacy evaluation of

Ayurvedic, sidhhha and Unanidrugs.[1-28]The present study deals with the GC MS analysis of one Ayurvedic drug, Guggulu Pachapala Churnam. This medicine is prescribed for problems like fistula, abdominal tumours, bloating, worm infestation, piles, skin diseases, abscess and worm infestation etc.The ingredients of this powder are 230 g of Shuddhaguggulu (*Commiphoramukul*), 46 g each of Pippali (*Piper longum*), *Haritaki (Terminaliachebula),* Vibitaki (*Terminaliabellirica*), Amalaki (*Emblicaofficinalis*), 12 g each of Twak (*Cinnamomumzeylanicum)* and Ela (Elettariacardamomum). These dry ingredients are powdered and mixed in the ratio as mentioned and stored to be used as medicine. This medicine is administered ½ to 1 teaspoon mixed in hot water or honey, two or three times a day or as directed by physician along with a dilute alkaline solution prepared by the ashes of dry plants such as *Buteamonosperma, Erythrinaindica, Terminaliabelerica, Cassia fistula, Plumbagozeylanica, Holarrhenaantidysenterica* etc.along with some salt for the management of digestive system related problems. This medicine finds its reference in the AyurvedictreatiseAstangahrudayamUttarastanam 27:40. This is manufactured by AryaVaidyaNilayam, Ashoka pharmaceuticals, AryaVaidyaSala Kottakkal, AryaVaidya Pharmacy, SNA Oushadhasala Pvt Ltd, Sitaram Ayurveda Pharmacy, NagarjunaAyurvedic Group among others.

MATERIALS AND METHODS

Guggulu Panchapala Churnam was obtained from standard Ayurvedic vendor at Chennai and was subjected to GC MS analysis by standard procedure.

Instrument:

Gas chromatography (Agilent: GC: (G3440A) 7890A. MS MS: 7000 Triple Quad GCMS,) was equipped with Mass spectrometry detector.

Sample Preparation

100 micro lit sample Dissolved in 1 ml of suitable solvents. The solution stirred vigorously using vortex stirrer for 10 seconds. The clear extract was determined using gas-chromatography for analysis.

GC-MS protocol

The GC MS Column consisted of DB5 MS (30mm×0.25mm ID ×0.25 μm , composed of 5% phenyl 95% methyl poly siloxane), Electron impact mode at 70 eV; Helium (99.999%) was used as carrier gas at a Constant flow of 1ml/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 10min) fragments from 45 to 450 Da. Total GC running time is 32.02 min. The compounds are identified by GC-MS Library (NIST & WILEY).

RESULTS

The GC MS profile of GugguluPanchapalaChurnamis represented in Figure 1. Table1 indicates the retentions time, types of possible compound, their molecular formulae,

molecular mass, percentage peak area and the medicinal roles of each compound as shown in the GC MS profile of GugguluPanchapalaChurnam. 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 ethnobotanical data base (National Agriculture Library, USA) and others as shown in Table 1.

Figure 1. Indicates the GC MS profile of Guggulu Panchapala Churnam

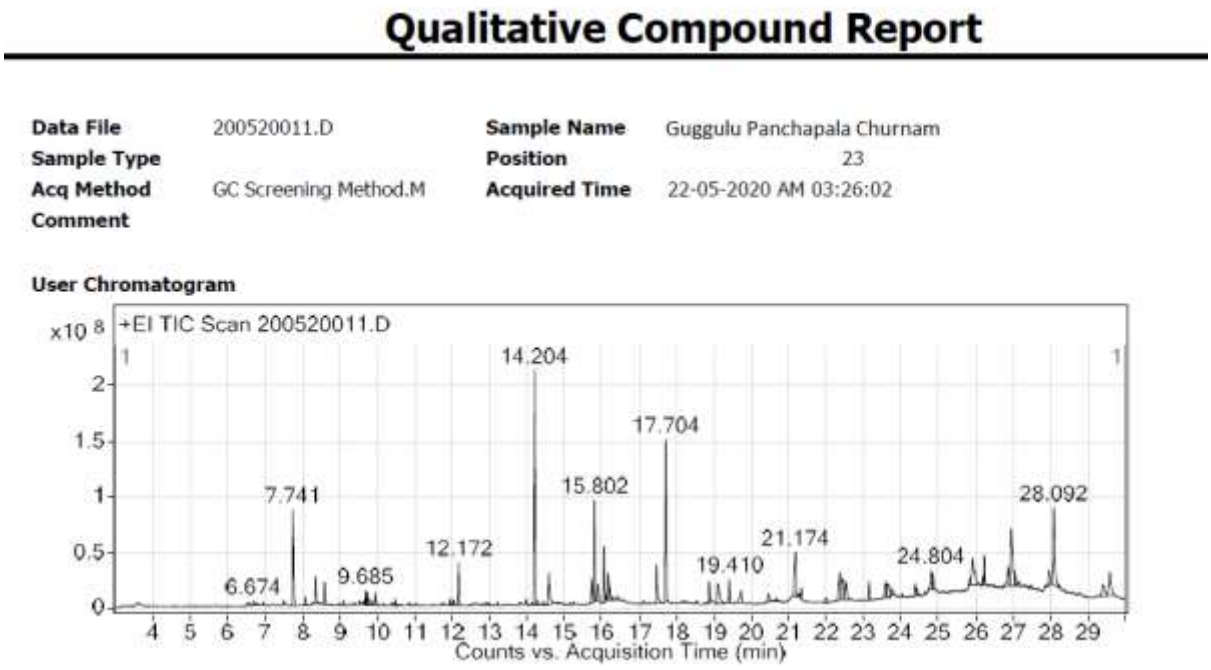

Table1. Indicates the retentions time, types of possible compound, their molecular formulae, molecular mass, percentage peak area and their medicinal roles of each compound as shown in the GC MS profile of GugguluPanchapalamChurnam.

Sl. No	Retention Time	Compound Name	Mol. Formula	Mol. Weight	% Peak Area	Possible medical Role
1	6.67	Cinnamaldehyde, (E)-	C9H8O	132.1	0.57	Antibacterial, anti caries for teeth, anticancer.[30]
2	7.74	Cyclohexene, 3-methyl-6-(1-methylethylidene)-	C10H16	136.1	5.16	Not known
3	8.07	Copaene	C15H24	204.2	0.40	Not known
4	8.34	Benzoic acid, 4-isopropyl-, ethyl ester	C12H16O2	192.1	1.38	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid

						Decarboxylase activity
5	8.58	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	C15H24	204.2	1.28	Not known
6	9.09	Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	C15H24	204.2	0.26	Not known
7	9.69	Pentadecane	C15H32	212.3	0.59	Not known
8	9.72	.beta.-Bisabolene	C15H24	204.2	0.55	17 beta hydroxysteroid dehydrogenase inhibitor, Antiamyloid beta, Anti TGF beta, Beta receptor agonist, Beta-adrenergic receptor blocker, beta blocker, beta galactosidase inhibitor, beta glucuronidase inhibitor, ER beta binder
9	9.77	Phenol, 2,4-bis(1,1-dimethylethyl)-	C14H22O	206.2	0.31	Not known
10	9.86	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	C15H24	204.2	0.23	Not known
11	9.94	Undecanoic acid, 10-methyl-, methyl ester	C13H26O2	214.2	0.59	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor, Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
12	10.48	Caryophyllene oxide	C15H24O	220.2	0.32	Nitric oxide synthatase inhibitor
13	11.94	Heptadecane	C17H36	240.3	0.34	Not known
14	12.05	7-Ethyl-6-tridecanone	C15H30	226.2	0.24	Not known

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15	12.17	Tridecanoic acid, 12-methyl-, methyl ester	C15H30O2	242.2	1.96	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor, Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
16	13.98	Methyl hexadec-9-enoate	C17H32O2	268.2	0.23	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
17	14.20	Methyl 8-methyl-decanoate	C12H24O2	200.2	11.42	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
18	14.27	1-Heptatriacotanol	C37H76O	536.6	0.95	It has Antibacterial, Anticancer, antiprotozoal, chemopreventive and anti-inflammatory, Antimalarial, Antiflu, Antiviral, antiprotozoal, Antioxidant, Antiperoxidant, Antitumor, anticancer, Enzyme inhibitor, anti-hypercholesterolemic effects
19	14.45	Phthalic acid, butyl tridec-2-yn-1-yl ester	C25H36O4	400.3	0.27	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
20	14.59	n-Hexadecanoic acid	C16H32O2	256.2	2.18	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity

21	15.73	12,15-Octadecadienoic acid, methyl ester	C19H34O2	294.3	1.55	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
22	15.80	6-Octadecenoic acid, methyl ester, (Z)-	C19H36O2	296.3	4.62	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
23	15.90	Phenol, 4-(3,7-dimethyl-3-ethenylocta-1,6-dienyl)-	C18H24O	256.2	1.21	Not known
24	16.06	Methyl stearate	C19H38O2	298.3	2.50	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
25	16.11	Methyl 7,12-octadecadienoate	C19H34O2	294.3	0.28	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
26	16.17	6-Octadecenoic acid	C18H34O2	282.3	1.79	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
27	16.28	Methyl 5,9-heptadecadienoate	C18H32O2	280.2	0.24	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
28	16.40	Oleic Acid	C18H34O2	282.3	0.29	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
29	17.47	15-Hydroxypentadecanoic acid	C15H30O3	258.2	2.21	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
30	17.70	4-Butylbenzoic acid, 1-adamantylmethyl ester	C22H30O2	326.2	8.34	Acidifier, Arachidonic acid inhibitor, Increases Aromatic

						Amino acid Decarboxylase activity
31	18.87	9-Octadecenoic acid, (E)-	C18H34 O2	282.3	1.16	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
32	19.11	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	C19H38 O4	330.3	2.32	17 beta hydroxysteroid dehydrogenase inhibitor, Aryl hydrocarbon hydroxylase inhibitor, testosterone hydroxylase inducer, Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
33	19.41	Phthalic acid, di(2-propylpentyl) ester	C24H38 O4	390.3	1.26	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity, coronary dilator, antidote, diuretic
34	19.72	Tetradecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	C17H34 O4	302.2	1.26	7 beta hydroxysteroid dehydrogenase inhibitor, Aryl hydrocarbon hydroxylase inhibitor, testosterone hydroxylase inducer, Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
35	20.45	2,3-Dihydroxypropyl elaidate	C21H40 O4	356.3	0.68	Not known
36	20.65	Hexadecanedioic acid	C16H30 O4	286.2	0.27	Acidifier, Arachidonic acid inhibitor,

						Increases Aromatic Amino acid Decarboxylase activity
37	21.17	Phosphine, bis[2-(piperidin-1-yl)ethyl]-	C14H29N2P	256.2	3.88	Not known
38	21.33	Decanedioic acid, bis(2-ethylhexyl) ester	C26H50O4	426.4	0.50	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
39	21.98	5aH-3a,12-Methano-1Hcyclopropa[5',6']cyclodeca[1',2':1,5]cyclopenta[1,2-d][1,3]dioxol-13-one, 1a,2,3,9,12,12a-hexahydro-9-hydroxy-10-(hydroxymethyl)-1,1,3,5,7,7-hexamethyl-, [1aR-(1a.alpha.,3.alpha.,3a.alpha.,5a.alpha.,8aR*,9.beta.,12.alpha.,12a.alpha.)]-	C23H32O5	388.2	0.33	Not known
40	22.36	2,3-Dihydroxypropyl elaidate	C21H40O4	356.3	2.46	Not known
41	22.44	Eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester	C27H50O6	470.4	2.33	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
42	22.53	Docosanoic anhydride	C44H86O3	662.7	8.66	Not known
43	23.14	Cholesterol	C27H46O	386.4	1.02	Precursor for steroid synthesis
44	23.59	1-Glyceryl ricinoleate	C21H40O5	372.3	1.32	Not known
45	23.64	Oxiranedodecanoic acid, 3-octyl-, cis-	C22H42O3	354.3	2.04	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid

						Decarboxylase activity
46	23.76	16-Nitrobicyclo[10.4.0]hexadecan-1-ol-13-one	C16H27NO4	297.2	0.35	Oligosaccharide provider
47	24.38	.beta.-Sitosterol	C29H50O	414.4	0.77	17 beta hydroxysteroid dehydrogenase inhibitor, Antiamyloid beta, Anti TGF beta, Beta receptor agonist, Beta-adrenergic receptor blocker, beta blocker, beta galactosidase inhibitor, beta glucuronidase inhibitor, ER beta binder
48	24.43	2,3-Dimethoxy-5-methyl-6-dekaisoprenyl-chinon	C59H90O4	862.7	0.39	Catechol-O-methyl-Transferase Inhibitor, methyl Donar, Methyl Guanidine Inhibitor
49	24.80	Oxiranedodecanoic acid, 3-octyl-, cis-	C22H42O3	354.3	1.29	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
50	24.85	Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	C35H68O5	568.5	1.03	Acidifier, Arachidonic acid inhibitor, Increases Aromatic Amino acid Decarboxylase activity
51	25.92	Dodecyl cis-9,10-epoxyoctadecanoate	C30H58O3	466.4	5.19	Not known
52	26.20	Octanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclod	C28H42O6	474.3	0.36	Not known

		ecen-6-yl ester, [1aR-(1a.alpha.,2.alpha.,5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10 a.alpha.)]-				
53	26.22	trans(2-Chlorovinyl)triethylsilane	C8H17ClSi	176.1	1.32	Catechol O Methyl transferase, Decreases glutamate oxaloacetate transaminase, Glucosyltransferase inhibitor, Glutathione S Transferase activity inhibitor, Increases glyoxalate transamination, Reverse transcriptase inhibitor
54	26.95	Lauric anhydride	C24H46O3	382.3	5.83	Not known
55	27.14	5H-Cyclopropa(3,4)benz(1,2-e)azulen-5-one, 1,1a-.alpha.,1b-.beta.,4,4a,7a-.alpha.,7b,8,9,9a-decahydro-4a-.beta.,7b-.alpha.,9a-.alpha.-trihydroxy-3-(hydroxymethyl)-1,1,6,8-.alpha.-tetramethyl-, 9a-isobutyrate	C24H34O6	418.2	0.44	Benzodiazepine-receptor agonist, antileukotrine B4, angiotensin-receptor, 17 beta hydroxysteroid dehydrogenase inhibitor, Antiamyloid beta, Anti- TGF beta, Beta receptor agonist, Beta-adrenergic receptor blocker, beta blocker, beta galactosidase inhibitor, beta glucuronidase inhibitor, ER beta binder, anticancer, antidote
56	27.47	Clocortolonepivalate	C27H36ClFO5	494.2	0.29	Not known
57	29.41	Cholestan-3-one, cyclic 1,2-ethanediyl aetal, (5.beta.)-	C29H50O2	430.4	1.56	Not known

DISCUSSION

Table 1 indicates 57 compounds that are shown in the GC MS profile of GugguluPanchapalamChurnam. Among them some compounds such as Cinnamaldehyde, (E)-, Benzoic acid, 4-isopropyl-, ethyl ester, Undecanoic acid, 10-methyl-, methyl ester, Caryophyllene oxide, Tridecanoic acid, 12-methyl-, methyl ester, 1-Heptatriacotanol, .beta.-Sitosterol, 5H-Cyclopropa(3,4)benz(1,2-e)azulen-5-one, 1,1a-.alpha.,1b-.beta.,4,4a,7a-.alpha.,7b,8,9,9a-decahydro-4a-.beta.,7b-.alpha.,9a-.alpha.-trihydroxy-3-(hydroxymethyl)-1,1,6,8-.alpha.-tetramethyl-, 9a-isobutyrate, trans(2-Chlorovinyl)triethylsilane etc. have medicinal properties ranging from steroid metabolism, adrenal function, antibacterial, antiviral, anticancer, Beta blocking and alpha blocking roles which could contribute to the medicinal activity of GuggluPanchapalamChurnam. Sruthi and Sindhu, 2013, have reported primary phytochemical and antioxidant potential.[31]

The activities of some of the molecules which are present in good percentage are not known yet and it would be worthwhile to probe into it.

CONCLUSION

It is concluded that the medicine Guggulu Panchapalam Churnam, although made of only of seven medicinal plant ingredients revealed 57 compounds in the GC MS profile. The various medicinal roles of the molecules support the role of Guggulu Panchapalam Churnam as a digestive formulation. Further work is warranted go have a better understanding of the role of this medicine.

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