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GAS Chromatography Mass Spectroscopic Analysis Ayyappala Kera Thailam

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ABSTRACT

The Gas Chromatography Mass Spectroscopic analysis of one skin care oil Ayyappala Kerathailamand to correlate its medicinal activity with the biomolecules present in it. Some important biomolecules such as Octanoic Acid, n- Octanoic acid, cycobutyl ester, Tetra decanoic acid, Dodecanoic acid, n-Butyl laurate, Dodecanoic acid, pentafluorophenyl ester, Dodecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester, Sarcosine, N-(1-naphthoyl)-, butyl ester, trans-3-Trifluoromethyl cinnamic acid, 4-nitrophenyl ester, 1,3,2-Dioxaphosphorinan-2-amine, 4-methyl-N-phenyl-, 2-oxide, trans-, Dodecanoic acid, ethenyl ester, Acetic acid, cesium salt etc. which have properties supporting the skin treatment role of this oil.

Key words: Ayyappala kera thailam, GC MS, Ayurvedic, Octadecanoic acid, Octanoic acid, Sarcosine, N-(1-naphthoyl)

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INTRODUCTION

The validation of traditional and alternative medicines like, Ayuveda, Sidhha, Unani, Chinese etc. by modern scientific parameters is very important to establish their authenticity. This has become all the more pertinent due to the failures of modern day molecular medicines at various fronts. The uses of traditional medicines are in vogue around the globe but due to lack of proper validation they are not coming into the main stream of medicinal practice. Since last decade or so there has been some studies in this regard which is heartening [1-17]. Use of Ayurvedic, Sidhha and other complementary and alternative medicines is an age old practice. The process of preparing of these medicines is also quite elaborate strictly as per the standard procedures and protocols present in the respective literatures.

This report indicates the phytochemicals present in Ayurvedic oil, AyyappalaKerathailam, used for treating psoriasis, chronic exfoliating dermatitis, allergic dermatitis, dermatophytosis, eczema, fungal infections etc. which is used by external application.

The ingredients of this medicine:

KeraTaila: Coconut (*Cocos nucifera*) oil: 10 ml.

ShwetaKutaja: *Wrightia tinctoria* leaves: 40 gm.

Nimba: Neem: *Azadirachta indica* leaves: 1.250 gm.

The oil is applied on the affected skin ½ to one hr. and washed off with warm water. The shelf life is mentioned to be 3 years.

The three ingredients are known for their medicinal values and are in use in various compositions in many Ayurvedic and Sidhha medicines. A brief description of the medicinal potential of each is mentioned hereunder.

Coconut: *Cocos nucifera*

Coconut is an important cash crop and widely used as a part of food and its beneficial roles are reported by many research articles [18-29]. The use of coconut oil as

dietary oil is a common practice in all he countries where coconut is available in plenty. Coconut oil is an important ingredient in most of the Ayurvedic and Sidhha medicines both for intake as well for topical application and one of the most used hair oils. It is considered as one of the best antiseptic for any skin injury.

Wrightia tinctoria

Nimba (Neem): *Azadirachta indica*

Neem is also a known medicinal plant with wide range of curative roles [30,31]. Thus is it interesting that the Ayurvedic proponents have chosen these three plants to formulate one skin oil for various types of skin ailments only for topical use. The present study is to find the molecular profile of this thailam by Gas Chromatography Mass Spectroscopic analysis. This knowledge could indicate the underlying medicinal properties of this medicine.

MATERIALS AND METHODS

The medicine Ayyappalakerat hailam was procured from standard Ayurvedic vendor at Chennai, India. 50 ml of Ayyappala kera thailam was taken and extracted with ethyl acetate solvent in separating funnel. The extracted material was filtered and concentrated in water bath at low temperature and was charged to have GC MS patterns by standard procedures.

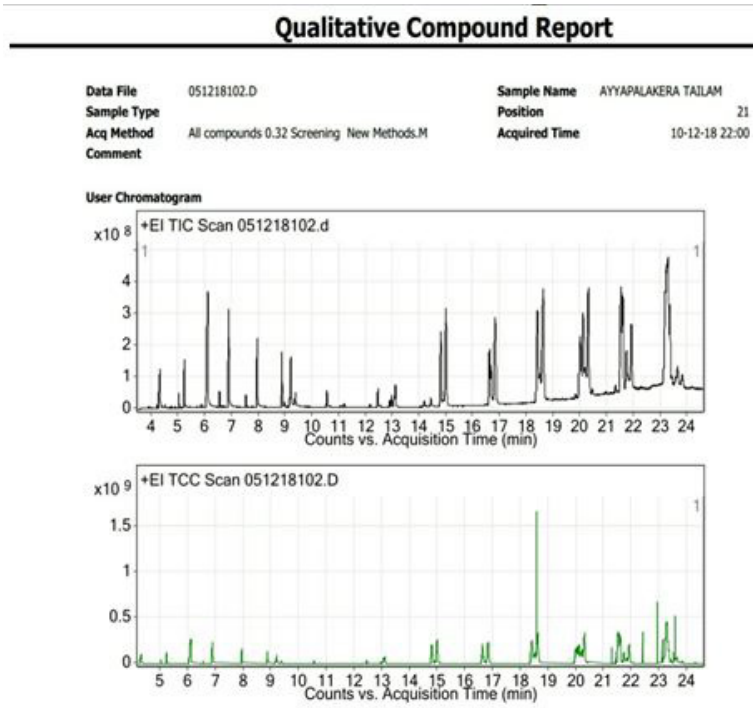

Figure 1: Indicates the GC MS profile of Ayyappala kera Thailam.

Table 1: Indicates the retentions values, the types of possible compound, their molecular formulae, molecular mass, peak area and their medicinal roles of each compound as shown in the GC MS profile of Ayyappala Kera Thailam.

Sl. No	Retention Time	Compound Name	Mol. Formula	Mol. Weight	Peak Area	Medicinal Role
1	4.32	Octanoic acid	$C_8H_{16}0_2$	144	321692208	Acidifier, Acidulant, Arachidonic acid inhibitor, Inhibits production of uric acid
2	5.02	4-Acetoxy-3-methoxystyrene	$C_{11}H_{12}0_3$	192.1	37195742	Not Known
3	5.23	n-Decanoic acid	$C_{10}H_2O_2$	172.1	229614364	Increases production of Uric acid, Anaphylactic, Antitumor, Decreases nor epinephrine production, GABAerigic, Increases NK cell Activity, Myoneuron stimulant
4	6.11	Dodecanoic acid	$C_{12}H_{24}O_2$	200.2	948463036	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid
5	6.55	Octanoic acid, cycobutyl Ester	$C_{12}H_{22}O_2$	198.2	32880864	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid,
6	6.83	Tetra decanoic acid	$C_{14}H_{29}O_2$	228.2	528148778	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid
7	7.94	Dodecanoic acid	$C_{12}H_{24}O_2$	200.2	319253420	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid,
8	8.87	Dodecanoic acid, 2,3-dihydropropyl ester	$C_{15}H_{30}O_4$	274.2	218939823	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid
9	9.2	1,1'-Bicyclopropyl, 2,2,3,',2'-tetramethyl-	$C_{10}H_{18}$	138.1	207289051	Not known

10	9.36	3-methylpenta-3-yl propyl carbonate	$C_{10}H_{20}O_3$	188.1	70596240	Not Known
11	12.45	Heptane,4-ethyl-	C_9H_{20}	128.2	55568269	Not Known
12	13.06	1,2-Benzenediol,O-(5-chlorovaleryl)-o'-(1-nephthoyl)-	$C_{22}H_{19}ClO_4$	382.1	40675250	Not Known
13	14.79	n-Butyl laurate	$C_{16}H_{32}O_2$	256.2	580692387	Anaphylactic, antitumor, Decreases Norepinephrine production, Down regulates nuclear and cytosol androgen production, GABA-ergic, Increases NK cell activity, Inhibits production of Tumor necrosis factor, Myoneuro stimulant, N-Cholinolytic, NADH-Oxidase inhibitor, NADH-Ubiquinone-Oxidoreductase Inhibitor, Narcotic, CNS depressant
14	14.8	Acetic anhydride	$C_4H_6O_3$	102	36264325	Not known
15	16.61	Dodecanoic acid, pentafluorophenyl ester	$C_{18}H_{23}F_5O_2$	306.2	363369333	Increases production of Uric acid
16	18.39	Dodecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	$C_{27}H_{52}O_5$	456.4	101484340	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid
17	18.42	Sarcosine, N-(1-naphthoyl)-, butyl ester	$C_{18}H_{21}NO_3$	299.2	40670803	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid, Anaphylactic, Antitumor, Decrease nor epinephrine production, GABAnerigic, Increases NK cell Activity, Myoneuron stimulant
18	18.47	Caprylic anhydride	$C_{16}H_{30}O_3$	270.2	130419195	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid,
19	18.6	Dodecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	$C_{27}H_{52}O_5$	456.4	141767308	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid,
20	19.97	trans-3-Trifluoromethylcinnamic acid, 4-nitrophenyl ester	$C_{27}H_{52}O_5$	227.1	32750819	Nitric Oxide Synthase Inhibitor, Catachol-O- Methyl Transferase Inhibitor, Decreases Glutamate Pyruvate Transaminase, Glutathione-S-Transferase Inhibitor
21	20.01	1,3,2-Dioxaphosphorinan-2-amine, 4-methyl-N-phenyl-, 2-oxide, trans-	C16H10F3NO4	227.1	81599860	Nitric Oxide Synthase Inhibitor, Catachol O Methyl Transferase Inhibitor, Increases Glutathione S transferase Activity, Catechol O Methyl Transferease Inhibitor, Arachidonic Acid Inhibitor, Decreases Glutamate Pyruvate transaminase, Inhibits Uric acid Production, Acidulant
22	20.09	Dodecanoic acid, ethenyl ester	$C_{14}H_{26}O_2$	226.2	824940857	Reverse Transcriptase inhibitor, Increases Glyoxalate transamination, Increases Glutathione S transferase Activity, Catechol O Methyl Transferease Inhibitor, Arachidonic Acid Inhibitor, Decreases Glutamate Pyruvate transaminase, Inhibits Uric acid Production, Acidulant
23	22.41	4-Methyl-2,4-bis(4'-trimethylsilyloxyphenyl) pentene-1	$C_{24}H_{36}O_2Si_2$	412.2	2958093897	Catechol-o-methyl Transferease
24	22.94	Acetic acid, cesium salt	$C_2H_3CsO_2$	195.9	107062504	Increases aromatic Amino Acid decarboxylase Activity, Increases production of Uric acid,

Mass Spectrometer is used for the determination of molecular weight of the compound and also for their structure elucidation. The compounds are identified by (NIST & WILEY) library.

RESULTS AND DISCUSSION

Figure 1 shows the Gas Chromatography Mass S graphs of Ayyapala kera thailam showing the number of peaks, their retention time etc. Table 1 indicates the presence of possible types of compounds with the retention times, molecular mass, peak areas and their medicinal roles found the GC MS profile of Ayyapala kera thailam. The identification of molecules was done NIST spectral library and the possible pharmaceutical roles of each bio-molecule as per National Agriculture Library, USA and others as shown in Table 1. [32]

From Figure 1 and Table 1 it is indicated that Ayyapala Kera Thailam contains mostly fatty acids and their esters or salts such as Octanoic Acid, n-Decanoic acid, Dodecanoic acid, Octanoic acid, cycobutyl ester, Tetra decanoic acid, Dodecanoic acid, Dodecanoic acid 2,3-dihydropropyl ester, n-Butyl laurate, Dodecanoic acid, pentafluorophenyl ester, Dodecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester, Sarcosine, N-(1-naphthoyl)-, butyl ester, trans-3-Trifluoromethyl cinnamic acid, 4-nitrophenyl ester, 1,3,2-Dioxaphosphorinan-2-amine, 4-methyl-N-phenyl-, 2-oxide, trans-, Dodecanoic acid, ethenyl ester, 4-Methyl-2,4-bis(4'-trimethylsilyloxyphenyl)pentene-1, Acetic acid, cesium salt etc.

The basic concept of Ayurvedic treatment for any disease is to correct the aberration in the three doshas, namely, Vata, Pitha and Kapha. Skin diseases, particularly inflammation and infections are caused due to imbalance in Pitta form of constitution. Coconut oil is considered best in balancing this dosha. It is a coolant andantimicrobial due to the presence of saturated fatty acids, Wrightiatinctoria helps in alleviating all the three doshas. Neem is one of the oldest medicine for skin diseases and also known to have extremely high antibacterial, antiviral and anti-inflammatory activities. The medicinal values of most of the molecules as seen in the GCMS analysis indicate antioxidant, anti-inflammatory and antibacterial properties. The possible positive role of some of the molecules are mentioned hereunder:

- ✓ N Hexadacoinc acid has been reported to have properties such as increase aromatic Amino Acid decarboxylase activity, decrease nor epinephrine production, GABA-nergic, increase NK cell activity and myo-neuron stimulant etc. Increase in aromatic Amino acid decarboxylase activity leads to decarboxylation of L-Dopa and 5-hydroxytryptophan thus increasing the production of catechol amines such as Dopamine, norepinephrine, epinephrine and Serotonin. The presence of more catechol amines cause mood elevation, stress relief and increased peripheral blood circulation. It is neither interesting that this compound decreases the neither function of nor epinephrine, which is known for peripheral vascular contraction. The capacity to stimulate myo-neurons also plays a major factor in maintaining good health of skin.
- ✓ 2-Methyl-3-93-methyl-but-2-enyl)-enyl)-oxetane, has the following biological roles: Catechol-o-methyl Transferase inhibitor, Methyl donor, Methyl Guanidine inhibitor etc. Catechol-o-methyl Transferase is as enzyme that degrades catechol amines like dopamine, nor epinephrine, epinephrine and other catechol compounds. By inhibiting its activity this compound present in AyyappalaKerathailam makes these compounds available which help in maintaining good health of skin.
- ✓ 3, 7-Decadien-2-one, 10-(3,3-dimethoxyloxiran dimethyl-, (E,E)-,+/-.- has properties such as anticancer, antidote, antitumor, Cytochrome –P450-2E1-inhibitor, decreases endothelial leukocyte adhesion, decreases epinephrine production. These properties can indirectly help in maintaining health of skin.
- ✓ 5α-reductase Inhibitors helps in stoppage of the steroid breakdown thus enabling the availability of the steroid in blood stream which in turn could help maintain the good health of skin.
- ✓ Alcohol dehydrogenase inhibitor stops the inter-conversion of alcohols and aldehydes, making them available during glucose metabolism and the presence of this enzyme can increase the energy supply to the skin. Thus it can be surmised from the above discussion it is clear that Ayyappalakerathailam is an excellent medicine for various skin diseases.

CONCLUSION

Thus it can be surmised from the above discussion it is clear that Ayyappalakerathailam is an excellent medicine for various skin diseases. The biological roles of some of the molecules such as 1,1'-Bicyclopropyl, 2,2,3,,2'-tetramethyl-, 3-methylpenta-3-yl propyl carbonate, Heptane,4-ethyl-, 1,2-Benzenediol, O-(5-chlorovaleryl)-o'-(1-nephthoyl)-, Acetic anhydride are not known. Further work in this direction is warranted.

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