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Quality Evaluation and Screening of Herbal Hair Oil Formulation Used in Personalized Healthcare by Digital Analytical Techniques

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ABSTRACT

This research investigates the potential of herb-infused virgin coconut oil (VCO), prepared by methodology using maceration under sunlight and hydroalcoholic extraction, for topical application. The findings of this study contribute valuable insights into potential applications of herb-infused VCO for skincare. Virgin coconut oil (VCO) have gained significant interest in recent years for their potential benefits in skincare and haircare. VCO, rich in medium-chain triglycerides and Lauric acid, has been reported to possess moisturizing and antimicrobial properties and also some cardiovascular negative effects. oil which has excess of omega-3 fatty acid also called as alpha-linolenic acid, is known for its anti-inflammatory and hair-conditioning effects. However, the individual effects of these oils might be limited. Herb-infused oils offer a promising approach to combine the benefits of base oils with the bioactive properties of herbs. This study investigated the potential of herb-infused VCO for the ability of to scavenge free radicals, assessing the safety of the infused oils on human skin cells and determining the efficacy of the infused oils against C. albicans & S. aureus. The herbs used in this study were specifically chosen for their well-documented properties that can synergistically benefit both skin and hair health.

The Spectrometric analysis revealed that constituents have been incorporated into the VCO and the Gas-Chromatography-Mass Spectroscopy (GC-MS) and Liquid-Chromatography-Mass Spectroscopy- Mass Spectroscopy (Time of Flight) confirms this.

Keywords:

Virgin coconut oil, Gas Chromatography Mass Spectroscopy, Liquid Chromatography Mass Spectroscopy,

INTRODUCTION

The soft portion of fully grown coconuts that are derived from the coconut palm trees is used to make its famous coconut oil[1]. There are two types based upon the type of fatty acid, coconut oil also called as copra oil and virgin coconut oil, both of them are comparable[2]. The virgin coconut oil has greater concentrations of certain nutrients e.g. vitamin E and nutritional higher fiber content amongst them are polyphenols. Also having cardiac associations[3].Because some medium-chain fatty acids are thought to have health benefits, coconut oil products are becoming more and more popular. As about coconut oil, lauric acid is highest in the main fatty acid in coconut oil, lauric acid, has been proposed to have two fatty chain acids, medium- and long properties from a biochemical perspective. Above all, coconut oil goods contain a broad type of variety of fatty acids, study based on fatty acids of medium change shall not be directly used[4]. The goal of the above story is to maintain an outline of the most recent, peer-reviewed research on the mechanisms and health impacts of coconut oil products. The topical application of oil pulling to prevent tooth cavities and for the prevention and treatment of atopic dermatitis is supported by a limited but consistent body of research. Merchandise having coconut oil prevent body from UV rays and protein loss during beautification process, in spite of this a detailed in-depth study is needed to substantiate this claim[2]. Use for glycaemic control, bone loss prevention, or Alzheimer's disease treatment is not supported by sufficient evidence. Big clinical studies are needed to be able to provide facts on weight loss and cardiovascular disease probabilities. A distinct type of fat called as Butter fat is tend to have a more prominent effect on low-density lipoprotein (LDL) cholesterol than refined, bleached, and deodorised copra oil, but not on cis unsaturated vegetable oils. So much facts have been laid on coconut oil goods, which are outcomes of *in vivo* or in vitro studies of separated medium-chain fatty acids, which quite frequently require clinical and kinetic studies to be conducted[5].

This research investigates the potential of herb-infused virgin coconut oil (VCO), prepared by maceration under sunlight, for topical application. The herbs used in this study includes *Asparagus racemosus* root powder, *Nardostachys jatamansi* root powder, *Rubia cordifolia* root powder, *Emblica officinalis* dried fruit powder, *Bacopa monnieri* and *Eclipta alba* leaf powder. *Withania somnifera* root powder, *Glycyrrhiza glabra* rhizome powder*, Trigonella foenum and Curcuma longa* rhizome powder

Table 1 List of Constituents in herbal hair formulation- VCO

Name of herb	Reported uses
***Nardostachys jatamansi* root powder**	Also known as jatamansi, this herb has been shown to promote hair growth and improve scalp health due to its potential to stimulate hair follicles and improve blood circulation[6] .
***Rubia cordifolia* root powder**	Also known as Manjistha or Madder root, contains compounds like alizarin that exhibit antimicrobial activity, atherosclerosis and may be beneficial for treating dandruff and other scalp conditions [7].
Bacopa monnieri	Traditionally used in Ayurvedic medicine to promote cognitive function[9], Brahmi also exhibits anti-inflammatory and antioxidant properties that may benefit the scalp and hair health .
Eclipta alba	This herb is revered in Ayurveda for its hair growth promoting properties[10]. It is believed to strengthen hair follicles and prevent hair loss .

Withania somnifera	*Withania somnifera* (WS), is a famous herbal plant of Solanaceae family having properties such as, antioxidant, anti-inflammatory, and anti-stress activities.[11]
Glycyrrhiza glabra	Glycyrrhizin (GLY), which is the most prominent thing of licorice, serving as a broadly used agent in pharmacokinetic drugs. GLY shows a variety of diverse medicinal aspects such as , including anti-inflammatory, antibacterial, and liver modulation effects[12]
Asparagus racemosus	Quercetin is the good polyphenolic flavonoid that fits in the classification. It is present in basically foods, like green tea, cranberry, apple, blueberry, broccoli, and coriander. It is present in alike forms, but the large quantity are quercetin derivatives such as are glycosides. Quercetin 3-O-glycoside, Quercetin 3-sulfate, and Quercetin 3'-metylether. This has some potent activities like antioxidant, anti-inflammatory[13]The plant as a whole has some serious pleiotropic therapeutic activity, neuroprotective, nootropic, antidepressant, etc.[14]
Trigonella foenum	Yamogenin is a steroidal saponin found in herbal species such as *Asparagus officinalis and Dioscorea collettii* as well as *Trigonella foenum-graecum*. It has, cytotoxic, antioxidant, and antimicrobial properties borne out of active constituent called as yamogenin[15]
Curcuma longa	Turmeric is also known as Haldi is used in Soth east Asian countries especially in India and China for the clinical uses for treatments of body illnesses also skin diseases, stress, and depression[16]

The above herbs were chosen on the basis of their effects related to hair growth. Ayurvedic literature review was done for shortlisting these herbs.

OBJECTIVES

The aim to the study was to determine whether herbs infused in coconut hair oil when exposed to sunlight, the constituents present in herbs gets infused in coconut oil and to what extent. Different herbs will behave differently releasing different types and amounts of its constituents in coconut oil.

It is also a test for coconut oil, whether it is apt for use in herbal hair oil.

MATERIALS AND METHODS

The herbs were sourced from Patanjali and were authenticated at NISCAIR Infusion of herbs in Oils. The herbs were weighed at 5 gm each, and mixed with coconut oil as the case may be in a sealed airlock glass jar and subjected to ambient temperature. The vessel of glass jar was shaken twice a day at 6 hr intervals to prevent herbs from settling down and to achieve mixing of herbs in coconut oil. This was done for 25 days. The experiment was performed in summer time June.

Filtration of oil mixture

After this process of exposing VCO mixed with herbs, it was then first filtered using muslin cloth and then passing through Whatman filter paper

After this process of exposing coconut oil mixed with herbs to sun, it was then filtered first using muslin cloth and then using Whatman filter paper. The oil thus obtained was stored in amber coloured bottles.

Infusion of herbs in alcohol

The herbs were weighed at 5 gm each, and mixed with hydroalcoholic mixture (50:50:: water: ethanol) in a sealed airlock glass jar and subjected to ambient temperature. The vessel was put on magnetic stirrer for 2 hrs continuously with a break of 5 hrs to achieve mixing of herbs. This was done for 25 days. The resultant was hydroalcoholic extract of herbs in alcohol.

Filtration and heating of hydroalcoholic extract

The hydroalcoholic extract mixed with herbs, it was then first filtered using muslin cloth and then passing through Whatman filter paper. Then extract was then heated up slightly making alcohol to evaporate. The constituents were left in beaker.

Mixing up of constituents and oil mixtures

The oil mixtures and constituents obtained from hydroalcoholic extract was mixed and resultant was final formulations of VCO.

The oil samples were then sent for qualitative analysis to Jawaharlal Nehru university JNU, Delhi for Gas-Chromatography-Mass Spectroscopy and Liquid-Chromatography-Mass Spectroscopy[17].

Table 2 Herbs and their effective concentration in VCO

S.No	Name of Drugs	Part of herbs used	Herbs concentration in VCO (w/v)
1.	*Asparagus racemosus*	root powder	5%
2.	*Nardostachys jatamansi*	root powder	5%
3.	*Rubia cordifolia*	root powder	5%
4.	*Bacopa monnieri*	leaves Powder	5%
5.	*Eclipta alba*	leaves powder	5%
6.	*Curcuma longa*	rhizome powder	5%
7.	*trigonella foenum*	Seeds and leaves powder	5%
8.	*Glycyrrhiza glabra*	Rhizome powder	5%
9.	*Withania somnifera*	root powder	5%

Method of Testing

Gas-Chromatography-Mass Spectroscopy

The herbal hair oil sample was subjected to GC-MS[18] by running the sample through Shimadzu QP-2010 Plus with Thermal Desorption System TD 20. The methodology was slightly modified as herbs were added to coconut oil and high temperatures were alter those constituents[19]. The retention time varied from 4 minutes to 45 minutes.[20]

Liquid Chromatography Mass Spectroscopy- Mass Spectroscopy

The herbal hair oil sample[21] was subjected to LCMS-MS by running the sample through MALDI MS - ABI Sciex 5800 TOF/ TOF System with LC-MALDI. The Human Metabolome Database: Spectra Search Mass Spectrum helped to identify the compounds, their name, structure and isotopic mass and formula. The methodology was slightly modified[22]

RESULTS

The results achieved were as follows: -

Gas-Chromatography-Mass Spectroscopy activity report

There was a total of 95 peaks obtained by GC-MS of coconut infused herbal oil. Out of which 26 compounds were identified which belonged to the herbs infused.

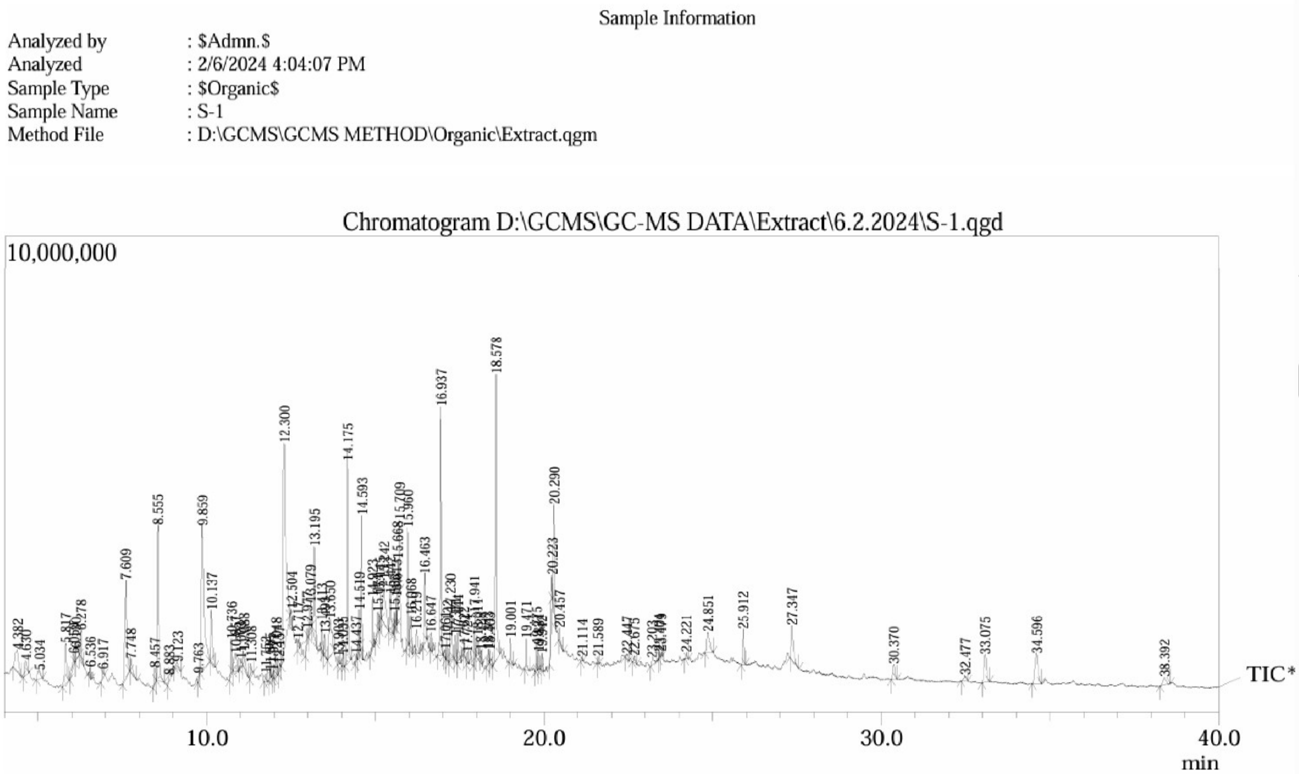

Figure 1 Peaks as expressed by GC-MS of VCO

Table 3- Peaks expressed by GC-MS and their corresponding Compounds identified

NAME OF THE COMPOUND	RETENTION TIME	AREA	AREA %	REPORTED ACTIVITY	CHEMICAL NATURE
Cycloserine	4.382	1143465	1.40	Antibiotic activity	Amino Acid
2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one	5.817	1137939	1.39	Anti-fungal	Ketone
1,3,5-Triazine-2,4,6-triamine	7.609	3001902	3.67	None	Amines
4H-Pyran-4-one, 2,3-dihydro-3,5-	8.555	33985	4.15	Excellent Antioxidan	Ketones

dihydroxy-6-methyl-		15		t	
5-Hydroxymethylfurfural	9.859	6554195	8.00	Formed by dehydration of sugars. None	aldehyde
1,2,3-Benzenetriol	12.300	9793286	11.96	Antiseptic	Cyclic alcohol
beta.-copaene	13.195	1789952	2.19	Used in fragrance	sesquiterpenoids
beta.-D-Glucopyranose, 1,6-anhydro-	13.650	1640581	2.00	Formed due to pyrolysis of carbohydrate	Sugar
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	14.175	3295055	4.02	Provides fragnance	sesquiterpenoids
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRI	14.593	2155818	2.63		sesquiterpenoids
Spirojatamol	15.145	365193	0.45	Found only in jatamansi, anti-oxidant activity	sesquiterpenoids
(-)-Globulol	15.442	947269	1.16	Anti-microbial activity	sesquiterpenoids
Ylangenal	15.668	531905	0.65		sesquiterpenoids
(3aR,4R,7R)-1,4,9,9-Tetramethyl-3,4,5,6,7,8-hexahydro-2H	15.960	1646935	2.01	Found only in Cyperus rotundus. Anti-oxidant activity	sesquiterpenoids
2-PROPENAL, 3-(2,4,5,6,7,7A-HEXAHYDRO-3,7-DIME	16.068	917147	1.12		
Corymbolone	16.463	1212166	1.48	Anti-bacterial	sesquiterpenoids

Cyclohexanol, 3-ethenyl-3-methyl-2-(1-methylethenyl)-6-(	16.937	3556160	4.34	Anti-microbial activity	sesquiterpenoids
Nootkatone	17.122	341383	0.42	fragrance	sesquiterpenoids
Neophytadiene	17.230	1421841	1.74	anti-inflammatory agent, an antimicrobial agent	diterpene
LUP-20(29)-ENE-3,28-DIOL, (3.BETA.)-	17.724	147936	0.18	anti-inflammatory	triterpenes
n-Hexadecanoic acid	18.578	5507941	6.73	anti-inflammatory	Saturated fatty acid
9,12-OCTADECADIENOIC ACID (Z,Z)-	20.223	853579	1.04		
9-Octadecenal, (Z)-	20.290	2070810	2.53	Anti-bacterial activity	Fatty aldehyde
Oleoyl chloride	24.851	987217	1.21		Acid chloride
Piperine	27.347	1206654	1.47	an antimicrobial agent	alkaloid
ERGOSTA-5,22-DIEN-3-OL, 24-METHYL-, (3.BETA.,22	33.075	1207131	1.47	Reduce serum cholesterol level	phytosterol
ERGOST-5-EN-3-OL, (3.BETA.,24R)-	34.596	1465754	1.79	Reduce serum cholesterol level	phytosterol

Liquid Chromatography Mass Spectroscopy- Mass Spectroscopy activity report

NEGATIVE MODE

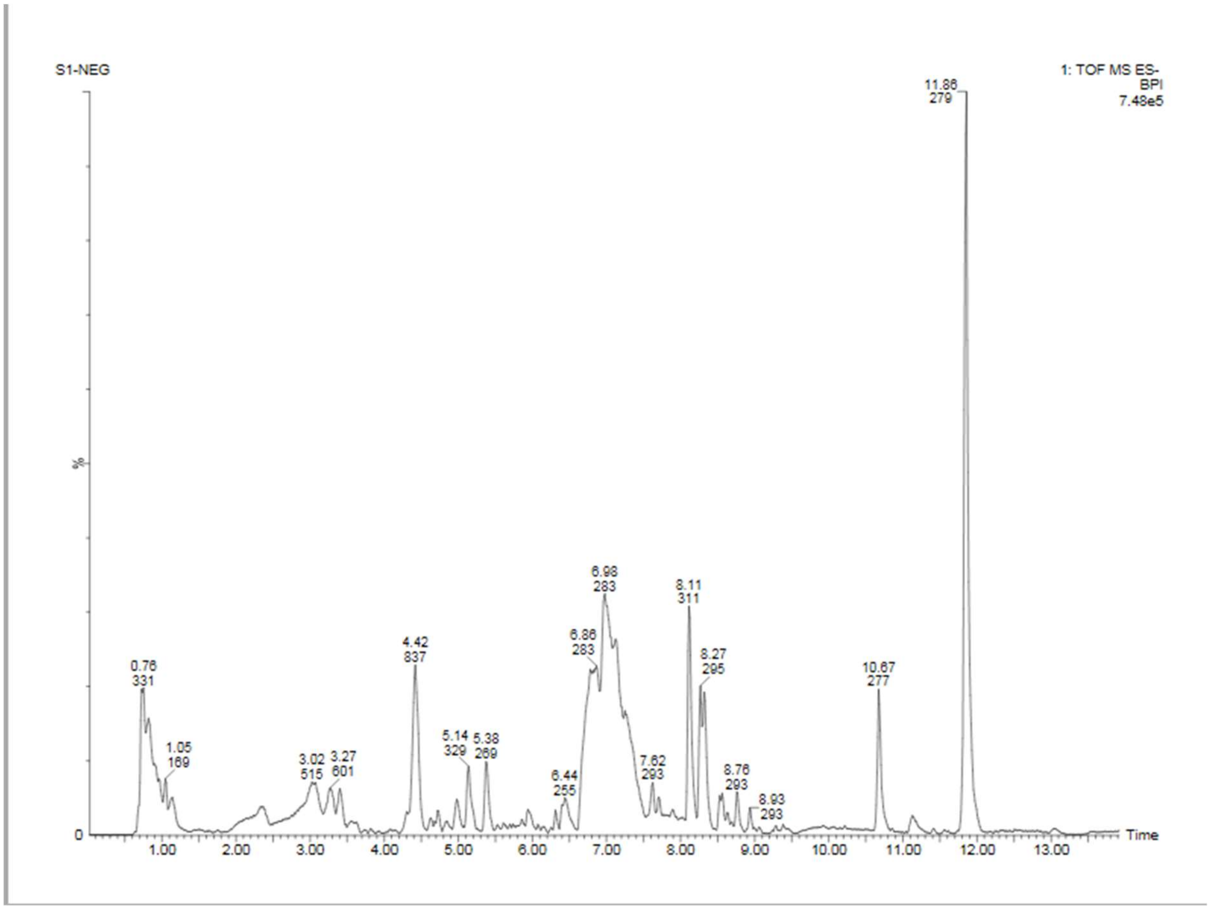

Figure 2- Peaks as expressed by negative mode of LC-MS/MS of VCO

Table 4 Compounds identified by LC-MS/MS negative mode

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0250712 (/metabolites/HMDB0250712)	Cystine	$C_6H_{12}N_2O_4S_2$	240.0238	M-H	239.0166 m/z calculator (/spectra/mzcal/HMDB0250712/calculator?chemi_formula=C6H12N2O4S2)	29	147.1
HMDB0000192 (/metabolites/HMDB0000192)	L-Cystine	$C_6H_{12}N_2O_4S_2$	240.0238	M-H	239.0166 m/z calculator (/spectra/mzcal/HMDB0000192/calculator?chemi_formula=C6H12N2O4S2)	29	147.0775
HMDB0257042 (/metabolites/HMDB0257042)	Quinizarin	$C_{14}H_8O_4$	240.0423	M-H	239.0350 m/z calculator (/spectra/mzcal/HMDB0257042/calculator?chemi_formula=C14H8O4)	48	150.5
HMDB0248144 (/metabolites/HMDB0248144)	Alizarin	$C_{14}H_8O_4$	240.0423	M-H	239.0350 m/z calculator (/spectra/mzcal/HMDB0248144/calculator?chemi_formula=C14H8O4)	48	153.4
HMDB0036006 (/metabolites/HMDB0036006)	Xanthopurpurin	$C_{14}H_8O_4$	240.0423	M-H	239.0350 m/z calculator (/spectra/mzcal/HMDB0036006/calculator?chemi_formula=C14H8O4)	48	153.2
HMDB0029752 (/metabolites/HMDB0029752)	Dantron	$C_{14}H_8O_4$	240.0423	M-H	239.0350 m/z calculator (/spectra/mzcal/HMDB0029752/calculator?chemi_formula=C14H8O4)	48	152.6

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0032324 (/metabolites/HMDB0032324)	Hexyl decanoate	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0032324/calculator?chemi_formula=C16H32O2)	45	171.4
HMDB0032249 (/metabolites/HMDB0032249)	Dodecyl butyrate	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0032249/calculator?chemi_formula=C16H32O2)	45	171.9
HMDB0033166 (/metabolites/HMDB0033166)	Octyl octanoate	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0033166/calculator?chemi_formula=C16H32O2)	45	170.7
HMDB0032065 (/metabolites/HMDB0032065)	Butyl dodecanoate	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0032065/calculator?chemi_formula=C16H32O2)	45	171.9
HMDB0036210 (/metabolites/HMDB0036210)	Dodecyl 2-methylpropanoate	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0036210/calculator?chemi_formula=C16H32O2)	45	171.6
HMDB0034153 (/metabolites/HMDB0034153)	Ethyl tetradecanoate	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0034153/calculator?chemi_formula=C16H32O2)	45	172.3
HMDB0031068 (/metabolites/HMDB0031068)	Isopalmitic acid	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0031068/calculator?chemi_formula=C16H32O2)	45	172.4
HMDB0002396 (/metabolites/HMDB0002396)	Trimethyltridecanoic acid	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0002396/calculator?chemi_formula=C16H32O2)	45	171.7
HMDB0000220 (/metabolites/HMDB0000220)	Palmitic acid	$C_{16}H_{32}O_2$	256.2402	M-H	255.2330 m/z calculator (/spectra/mzcal/HMDB0000220/calculator?chemi_formula=C16H32O2)	45	170.363

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0250962 (/metabolites/HMDB0250962)	9H-Fluorene-9-carboxamide, 9-(3-aminopropyl)-	$C_{17}H_{18}N_2O$	266.1419	M-H	265.1346 m/z calculator (/spectra/mzcal/HMDB0250962/calculator?chemi_formula=C17H18N2O)	1	167.6
HMDB0060569 (/metabolites/HMDB0060569)	Deoxyartemsinin	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0060569/calculator?chemi_formula=C15H22O4)	38	168.9
HMDB0037070 (/metabolites/HMDB0037070)	Sporol	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0037070/calculator?chemi_formula=C15H22O4)	38	170.5
HMDB0036038 (/metabolites/HMDB0036038)	1alpha,15-Dihydroxymarasmene	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0036038/calculator?chemi_formula=C15H22O4)	38	167.3
HMDB0036039 (/metabolites/HMDB0036039)	3alpha,15-Dihydroxymarasmene	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0036039/calculator?chemi_formula=C15H22O4)	38	167.7
HMDB0038148 (/metabolites/HMDB0038148)	Ipomeamaronol	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0038148/calculator?chemi_formula=C15H22O4)	38	169.3
HMDB0035210 (/metabolites/HMDB0035210)	10-Hydroxymyoporone	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0035210/calculator?chemi_formula=C15H22O4)	38	168.3
HMDB0030137 (/metabolites/HMDB0030137)	Adhumulinic acid	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0030137/calculator?chemi_formula=C15H22O4)	38	168.6
HMDB0040905 (/metabolites/HMDB0040905)	Ipomeamaronolide	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0040905/calculator?chemi_formula=C15H22O4)	38	170.3
HMDB0038476 (/metabolites/HMDB0038476)	7-Hydroxytrichodermol	$C_{15}H_{22}O_4$	266.1518	M-H	265.1445 m/z calculator (/spectra/mzcal/HMDB0038476/calculator?chemi_formula=C15H22O4)	38	169.2

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0256151 (/metabolites/HMDB0256151)	8-Quinolinol, 5,7-dichloro-2-((dimethylamino)methyl)-	$C_{12}H_{12}Cl_2N_2O$	270.0327	M-H	269.0254 m/z calculator (/spectra/mzcal/HMDB0256151/calculator?chemi_formula=C12H12Cl2N2O)	32	154.9
HMDB0258611 (/metabolites/HMDB0258611)	Sulfuretin	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0258611/calculator?chemi_formula=C15H10O5)	43	161.4
HMDB0041655 (/metabolites/HMDB0041655)	3'-Hydroxydaidzein	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0041655/calculator?chemi_formula=C15H10O5)	43	161.5
HMDB0031715 (/metabolites/HMDB0031715)	6-Hydroxydaidzein	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0031715/calculator?chemi_formula=C15H10O5)	43	161.5
HMDB0030829 (/metabolites/HMDB0030829)	Aloeemodin	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0030829/calculator?chemi_formula=C15H10O5)	43	161.7
HMDB0029372 (/metabolites/HMDB0029372)	2'-Hydroxydaidzein	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0029372/calculator?chemi_formula=C15H10O5)	43	161.5
HMDB0033860 (/metabolites/HMDB0033860)	8-Hydroxydaidzein	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0033860/calculator?chemi_formula=C15H10O5)	43	161.2
HMDB0033790 (/metabolites/HMDB0033790)	1,2,8-Trihydroxy-3-methylanthraquinone	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0033790/calculator?chemi_formula=C15H10O5)	43	161.1
HMDB0034004 (/metabolites/HMDB0034004)	3,4',7-Trihydroxyflavone	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0034004/calculator?chemi_formula=C15H10O5)	43	160.5
HMDB0034409 (/metabolites/HMDB0034409)	Rhababerone	$C_{15}H_{10}O_5$	270.0528	M-H	269.0455 m/z calculator (/spectra/mzcal/HMDB0034409/calculator?chemi_formula=C15H10O5)	43	160.8

POSITIVE MODE

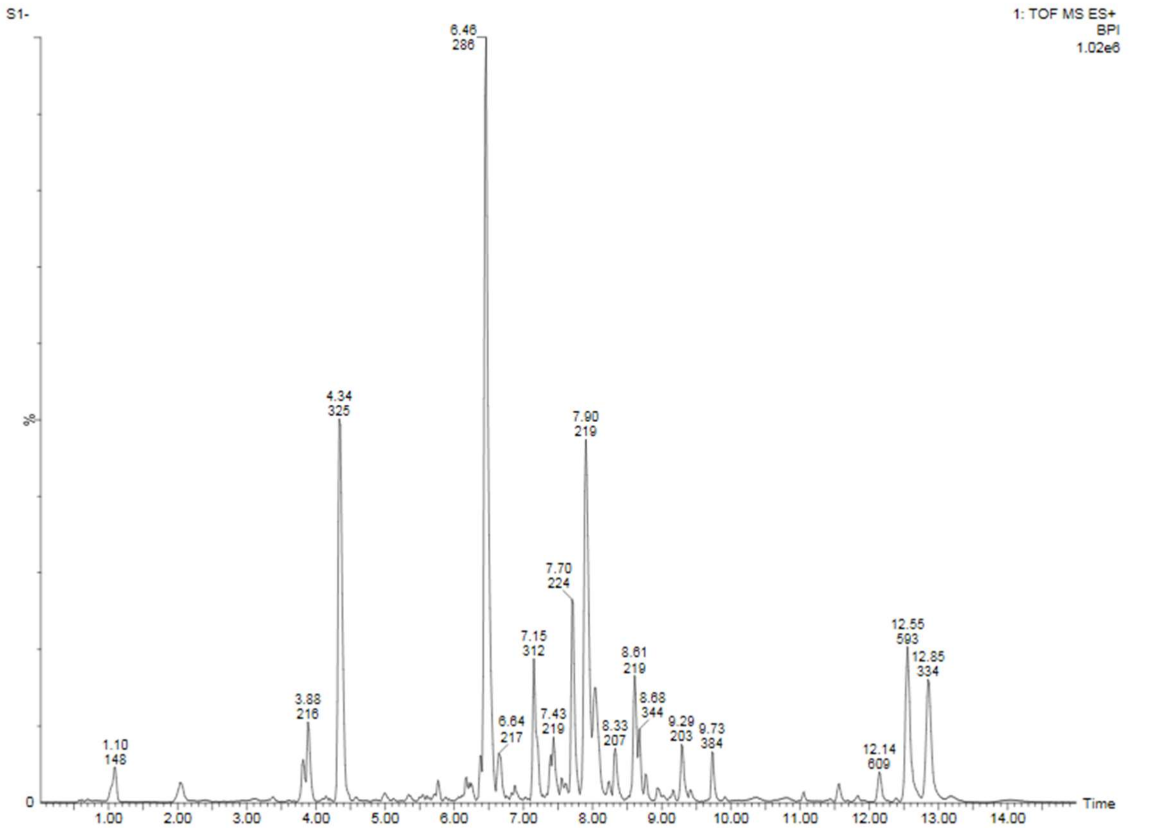

Figure 3- Peaks as expressed by positive mode of LC-MS/MS of VCO

Table 5 Compounds identified by LC-MS/MS positive mode

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0041922 (/metabolites/HMDB0041922)	Melamine	$C_3H_6N_6$	126.0654	M+Na	149.0546 m/z calculator (/spectra/mzcal/HMDB0041922/calculator?chemi_formula=C3H6N6)	22	136.8
HMDB0249105 (/metabolites/HMDB0249105)	beta-Aspartylhydroxamate	$C_4H_8N_2O_4$	148.0484	M+H	149.0557 m/z calculator (/spectra/mzcal/HMDB0249105/calculator?chemi_formula=C4H8N2O4)	29	133.5
HMDB0032332 (/metabolites/HMDB0032332)	Hydroxylated lecithin	$C_4H_8N_2O_4$	148.0484	M+H	149.0557 m/z calculator (/spectra/mzcal/HMDB0032332/calculator?chemi_formula=C4H8N2O4)	29	133.5
HMDB0243852 (/metabolites/HMDB0243852)	1-Cyclohexene-1-carboxylic acid	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0243852/calculator?chemi_formula=C7H10O2)	40	133.7
HMDB0032333 (/metabolites/HMDB0032333)	4-Hydroxy-4-methyl-5-hexenoic acid gamma lactone	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0032333/calculator?chemi_formula=C7H10O2)	40	131.0
HMDB0032067 (/metabolites/HMDB0032067)	Allyl crotonate	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0032067/calculator?chemi_formula=C7H10O2)	40	134.9
HMDB0029582 (/metabolites/HMDB0029582)	Methyl sorbate	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0029582/calculator?chemi_formula=C7H10O2)	40	134.7
HMDB0034080 (/metabolites/HMDB0034080)	3-Methyl-1,2-cyclohexanedione	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0034080/calculator?chemi_formula=C7H10O2)	40	132.0
HMDB0037027 (/metabolites/HMDB0037027)	3,5-Dimethyl-1,2-cyclopentanedione	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0037027/calculator?chemi_formula=C7H10O2)	40	131.4
HMDB0037026 (/metabolites/HMDB0037026)	3,4-Dimethyl-1,2-cyclopentanedione	$C_7H_{10}O_2$	126.0681	M+Na	149.0573 m/z calculator (/spectra/mzcal/HMDB0037026/calculator?chemi_formula=C7H10O2)	40	131.9

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0244242 (/metabolites/HMDB0244242)	1,6-Dimethoxyhexane	$C_8H_{18}O_2$	146.1307	M+H	147.1380 m/z calculator (/spectra/mzcal/HMDB0244242/calculator?chemi_formula=C8H18O2)	36	136.2
HMDB0244945 (/metabolites/HMDB0244945)	2-(Hexyloxy)ethanol	$C_8H_{18}O_2$	146.1307	M+H	147.1380 m/z calculator (/spectra/mzcal/HMDB0244945/calculator?chemi_formula=C8H18O2)	36	135.0
HMDB0302164 (/metabolites/HMDB0302164)	1,1-Diethoxy-2-methylpropane	$C_8H_{18}O_2$	146.1307	M+H	147.1380 m/z calculator (/spectra/mzcal/HMDB0302164/calculator?chemi_formula=C8H18O2)	36	135.503
HMDB0038679 (/metabolites/HMDB0038679)	1-Methoxy-1-pentyloxyethane	$C_8H_{18}O_2$	146.1307	M+H	147.1380 m/z calculator (/spectra/mzcal/HMDB0038679/calculator?chemi_formula=C8H18O2)	36	137.2
HMDB0037635 (/metabolites/HMDB0037635)	xi-1-Ethoxy-1-butoxyethane	$C_8H_{18}O_2$	146.1307	M+H	147.1380 m/z calculator (/spectra/mzcal/HMDB0037635/calculator?chemi_formula=C8H18O2)	36	137.1
HMDB0029359 (/metabolites/HMDB0029359)	(R)-1,3-Octanediol	$C_8H_{18}O_2$	146.1307	M+H	147.1380 m/z calculator (/spectra/mzcal/HMDB0029359/calculator?chemi_formula=C8H18O2)	36	136.5

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DISCUSSION

The digital analytical techniques revealed that constituents have been incorporated into the VCO and the Gas-Chromatography-Mass Spectroscopy and Liquid-Chromatography-Mass Spectroscopy- Mass Spectroscopy confirms this, , Spirojatamol found BY GC-MS or 3,4-Di-O-caffeoylquinic acid and Dicaffeoylquinic acid by LC-MS/MS only in jatamansi, which also does anti-oxidant activity. beta.-copaene provides fragrance which provides its unique smell to the herbal hair oil. Eriodictyol 7-(6- galloylglucoside) found in Amla. There were various Amino Acids, phytosterol, triterpenes, sesquiterpenoids, aldehyde and ketones were also found. The constituents found has all those activities like anti-microbial, anti- bacterial, anti-inflammatory and anti-oxidant activity which help the herbal hair oil to show its efficacy and its mode of action

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