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GC-MS ANALYSIS OF ABHAYA GUTIKA

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ABSTRACT

Introduction: Abhaya Gutika is a traditional Ayurvedic formulation referenced in the classical text Rasa Ratna Samucchaya for the management of Krimidanta (dental caries). Despite its historical use, modern analytical data regarding its chemical composition is limited. **Methodology:** The formulation was subjected to Gas Chromatography-Mass Spectrometry (GC-MS) analysis using a Clarus 680 GC system with an HP-5MS column to identify its volatile and semi-volatile bioactive compounds. **Observation and Results:** GC-MS analysis revealed a diverse array of phytochemicals at various retention times. Key compounds identified include 1,2,4-Benzenetriol (22.8%), 6-Acetyl-β-d-mannose (22.1% and 45.5% at different RTs), 5-Hydroxymethylfurfural (9.11%), and various fatty acid derivatives like n-Hexadecanoic acid and methyl esters. These compounds are known for their antimicrobial, antioxidant, and anti-inflammatory properties. **Conclusion:** The study successfully characterized the chemical profile of Abhayadi Gutika. The presence of potent bioactive molecules supports its traditional use in treating dental caries and suggests that the unique preparation method involving a copper vessel may contribute to its therapeutic efficacy.

KEYWORDS: Abhaya Gutika, Rasa Ratna Samucchaya, GC-MS, Krimidanta, Dental Caries.

INTRODUCTION

Abhaya Gutika is a herbal formulation referenced in the classical text Rasa Ratna Samucchaya with Haritaki (*Terminalia chebula*) and honey as primary ingredients. Haritaki is mixed with honey and heated on mild fire and then rolled into pills. This is indicated in dental caries. The pill must be kept on the caried tooth. In the present study GCMS analysis of Abhaya Gutika is carried out to know the phytoconstituents of the formulation.

METHODOLOGY

GC-MS analysis of Abhaya gutika was done at Chromatogen Analytical solutions Mysore.

Procedure: The Clarus 680 GC was used in the analysis employed a fused silica column, packed with HP-5MS (5% biphenyl 95% dimethyl polysiloxane, 30 m x 0.25 mm ID× 250µm df) and the components were separated using Helium as carrier gas at a constant flow of 2 ml/min. The injector temperature was set at 250°C during the chromatographic run. The 1µL of extract sample injected into the instrument the oven temperature was as follows: 50 °C (2 min); followed by 150 °C at the rate of 15 °C min-1; and 150 °C, where it was held for 1min and then followed by 240°C at the rate of 25°C min-1; it was held for 12.00 min. The mass detector conditions were: Inlet line temperature 250 °C; ion source temperature 230 °C; and ionization mode electron impact at 70 eV, a scan time 0.2 sec and scan interval of 0.1 sec. the fragments from 40 to 600 Da. The spectrums of the components were compared with the database of spectrum of known components stored in the GC-MS NIST (2014) library.

OBSERVATION AND RESULTS

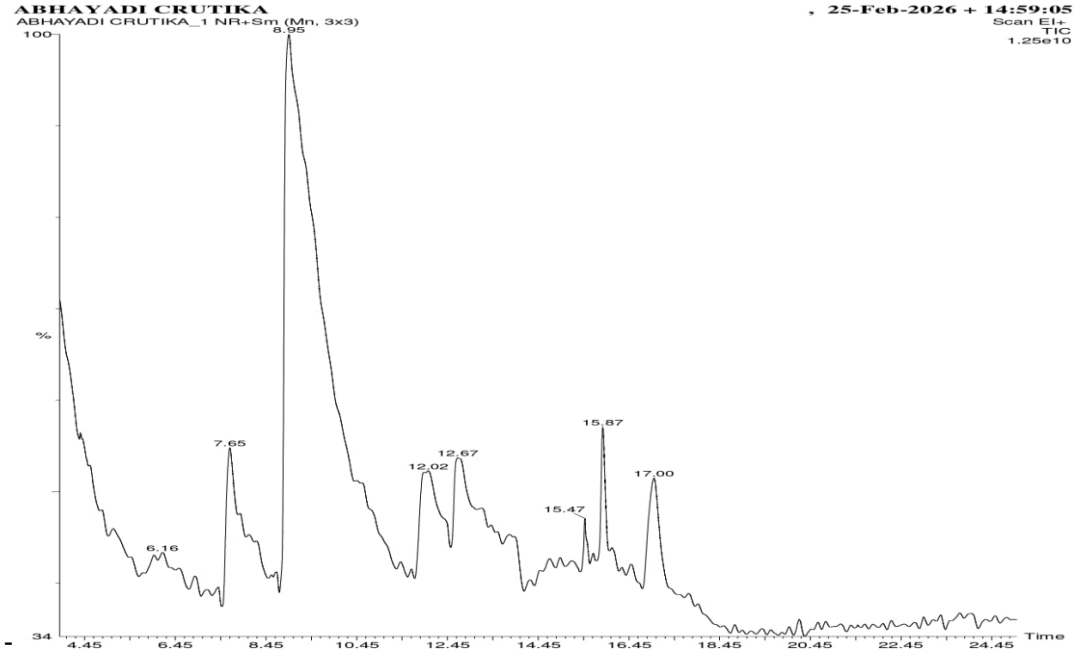

Figure 1: GC-MS plot of Abaya Gutika(TIC).

Table 1: GC-MS of Abhaya Gutika at RT=7.6

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	1-Hydroxy-2-pentanone	$C_5H_{10}O_2$	599	64502-89-2	7. 86
2	3(2H)-Furanone,dihydro-2-methyl	$C_5H_8O_2$	592	3188-00-9	6.02
3	2-propenoic acid, 2-[(1,3-dioxobutyl)amino]ethyl ester	$C_9H_{13}NO_4$	588	-	5.08
4	Glycidol	$C_3H_6O_2$	583	556-52-5	4.10
5	1,2,4-Trioxolane,3,5dipropyl	$C_8H_{16}O_3$	582	1696-03-3	3.94
6	2-Furanmethanol, tetrahydro	$C_5H_{10}O_2$	581	97-99-4	3.78
7	L-Talose,6-deoxy-3-methyl-2-O-methyl	$C_8H_{16}O_5$	581	27208-98-6	3.78
8	Aceticacid,[(aminocarbonyl)amino]oxo	$C_3H_4N_2O_4$	576	585-05-7	3.05
9	Formic acid, ethenyl ester	$C_3H_4O_2$	576	692-42-5	3.05
10	Succindialdehyde	$C_4H_6O_2$	574	638-37-9	2. 81
11	Glyceraldehyde	$C_3H_6O_3$	574	56-82-6	2. 81
12	Propanamide, N-acetyl	$C_5H_9NO_2$	571	19264-34-7	2.48
13	Oxiranemethanol, (S)	$C_3H_6O_2$	566	60456-23-7	2.00
14	Sulfurous acid, dipropyl ester	$C_6H_{14}O_3S$	566	623-9-3	2.00
15	1-Butanol, 2-nitro	C_4HgNO_3	565	609-31-4	1.92
16	Propylene oxide	C_3H_6O	565	75-56-9	1.92
17	Ethanol,2-(diethylamino)-,N-oxide	$C_6H_{15}NO_2$	565	16684-49-4	1.92
18	Bis(ethoxycarbonyl)methoxyiminomethane	$C_8H_{13}NO_5$	562	62619-46-9	1.70
19	1H-1,2,3,4-Tetrazole,5 hydrazino	CH_4N_6	561	-	1.63
20	3(2H)-Furanone,dihydro-2-methyl	$C_5H_8O_2$	561	3188-00-9	6.02
21	Propylene Carbonate	$C_4H_6O_3$	599	108-32-7	1.51
22	Hydroperoxide,1methylbutyl	$C_5H_{12}O_2$	558	14018-58-7	1.45
23	3-Buten-1-ol	C_4H_8O	557	627-27-0	1.39
24	2,2'-Bioxirane	$C_4H_6O_2$	556	1464-53-5	1.34
25	Dihydroxyacetone	$C_3H_6O_3$	556	96-26-4	1.34
26	Oxiranemethanol, (R)	$C_3H_6O_2$	555	57044-25-4	1.28
27	p-Dioxane, methylene	$C_5H_8O_2$	555	3984-19-8	1.28
28	Glycidol	$C_3H_6O_2$	552	556-52-5	4.10
29	1-Butanol, 2-nitro	$C_4H_9NO_3$	552	609-31-4	1.92
30	1,3-Dioxane, 4-methyl	$C_5H_{10}O_2$	551	1120-97-4	1.08

Table 2: GC-MS of Abhaya gutika at RT=8.9.

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	6-Acetyl-β-d-mannose	$C_8H_{14}O_7$	674	-	22.1
2	3-Methylenecyclopropane-trans-1,2-dicarboxylic acid	$C_6H_6O_4$	660	499-02-5	13.8
3	4-Pyrimidinol,5-methoxy	$C_5H_6N_2O_2$	657	695-87-4	12.2
4	2-Cyclobutene-1-carboxamide	C_5H_7NO	654	53778-54-4	10.8
5	5-Hydroxymethylfurfural	$C_6H_6O_3$	650	67-47-0	9.11
6	3-Methylenecyclopropane-trans-1,2-dicarboxylic acid	$C_6H_6O_4$	649	499-02-5	13.8
7	Bicyclo[2.2.2]octan-1-amine	$C_8H_{15}N$	626	1193-42-6	3.05
8	5-Hydroxymethylfurfural	$C_6H_6O_3$	624	67-47-0	9.11
9	5-Hydroxymethylfurfural	$C_6H_6O_3$	619	67-47-0	9.11
10	1-Azabicyclo[2.2.2]octan-3-one	$C_7H_{11}NO$	609	3731-38-2	1.66
11	N-(Furan-2-ylmethyl)-2-(5-methyl-2H-1,2,4-triazol-3-yl)acetamide	$C_{10}H_{12}N_4O_2$	606	-	1.47
12	1-(4-Hydroxy-6-methyl-2-pyrimidinyl)-2-aziridinone	$C_7H_7N_3O_2$	606	-	1.47
13	3-Methylenecyclopropane-trans-1,2-dicarboxylic acid	$C_6H_6O_4$	602	499-02-5	13.8
14	Histamine,N-trifluoroacetyl-2-amino	$C_7H_9F_3N_4O$	600	50580-60-4	1.15
15	3,6-Pyridazinedione,1,2-dihydro-4-methyl	$C_5H_6N_2O_2$	598	5754-18-7	1.06
16	1H-Pyrazole-3-aceticacid,2,5-dihydro-5-oxo	$C_5H_6N_2O_3$	596	-	0.98
17	Spiro[4.4]nonane-1,6-dione	$C_9H_{12}O_2$	596	27723-43-9	0.98
18	2H-Pyrrol-2-one,1,5-dihydro-1-methyl	C_5H_7NO	594	13950-21-5	0.90
19	3a,7a-Epoxy-1H-inden-4(5H)-one, tetrahydro	$C_9H_{12}O_2$	593	39746-31-1	0.87
20	3H-Pyrazol-3-one,2,4-dihydro-4,4,5-trimethyl	$C_9H_{10}N_2O$	592	3201-20-5	0.83
21	1,1'-Bicycloheptyl	$C_{14}H_{26}$	588	23183-11-1	0.70
22	Cyclopentane,1,1'-ethylidenebis	$C_{12}H_{22}$	587	4413-21-2	0.68
23	2H-Pyran-2-one,5,6-dihydro-6-pentyl	$C_{10}H_{16}O_2$	586	54814-64-1	0.65
24	N'-(4,5,6,7-Tetrahydro-3H-azepin-2-yl)-semicarbazide	$C_7H_{14}N_4O$	586	-	0.65
25	3-Methylenecyclopropane-trans-1,2-dicarboxylic acid	$C_6H_6O_4$	588	499-02-5	13.8
26	1-Pyrroline, 3-ethyl	$C_6H_{11}N$	583	-	0.57
27	Furan-2(3H)-one,4,5-dihydro-4-(4-acetyl-3-methylpyrazol-5-ylmethyl)-5,5-dimethyl	$C_{13}H_{18}N_2O_3$	583	-	0.57
28	Piperidine,1-(1-propenyl)	$C_8H_{15}N$	579	7182-09-4	0.48
29	9-Oxabicyclo[6.1.0]nonan-4-one	$C_8H_{12}O_2$	578	28399-88-4	0.47
30	2-Butenoicacid,2-cyano-3 methyl-, ethyl ester	$C_8H_{11}NO_2$	578	759-58-0	0.47

Table 3: GC-MS of abhaya gutika at RT=12.

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	1,2,4-Benzenetriol	$C_6H_6O_3$	575	533-73-3	22.8
2	Pyrazole-5-carboxylic acid, 3-methyl	$C_5H_6N_2O_2$	556	696-22-0	11.1
3	4-Pyrimidinol, 5-methoxy	$C_5H_6N_2O_2$	546	695-87-4	7.80
4	6-Methoxytetrazolo(b)pyridazine	$C_5H_5N_5O$	546	27062-50-6	7.80
5	1,2,4-Benzenetriol	$C_6H_6O_3$	539	533-73-3	22.8
6	6-Ethoxy-6H-[1,2]oxazine-6-carbonitrile	$C_7H_8N_2O_2$	535	-	5.35
7	3-Picoline, 4-amino-, 1-oxide	$C_6H_8N_2O$	530	4832-24-0	4.31
8	Benzeneethanamine, 3-fluoro-4-hydroxy	$C_8H_{10}FNO$	528	404-82-2	3.98
9	1,2,3-Benzenetriol	$C_6H_6O_3$	526	87-66-1	3.67
10	1,2,4-Benzenetriol	$C_6H_6O_3$	521	533-73-3	22.8
11	1,2,3-Benzenetriol	C_6H_6O3	521	87-66-1	3.67
12	6-Aminotetrazolo(b)pyridazine	$C_4H_4N_6$	517	19195-43-8	2.66
13	1-Azabicyclo[2.2.2]oct-2-ene-3-carboxylic	$C_9H_{13}NO_2$	505	31539-88-5	1.77

	acid, methyl ester				
14	Ethane	C_2H_6	504	74-84-0	1.70
15	1-Methyl-5-nitroimidazole-4-carboxaldehyde	$C_5H_5N_3O_3$	504	85012-72-2	1.70
16	3-(Furan-2-yl)propan-1-amine	$C_7H_{11}NO$	501	4428-38-0	1.50
17	1,2,3-Benzenetriol	$C_6H_6O_3$	499	87-66-1	3.67
18	2-Butenoic acid, 2-cyano-3-methyl-, ethyl ester	$C_8H_{11}NO_2$	495	759-58-0	1.18
19	3-(4-Nitropyrazol-1-yl)propanenitrile	$C_6H_6N_4O_2$	488	-	0.90
20	5-Hydroxy-5-(1-hydroxy-1-isopropyl)-2-methyl-2-cyclohexen-1-one	$C_{10}H_{16}O_3$	486	97762-08-8	0.83
21	3-Methyl-2-furoic acid	$C_6H_6O_3$	486	4412-96-8	0.83
22	Cyclohexanone, 5-(1-hydroxy-2-propenyl)-2,2-dimethyl-	$C_{11}H_{18}O_2$	486	141033-66-1	0.83
23	Acetic acid, hydroxy-, ethyl ester	$C_4H_8O_3$	484	623-50-7	0.77
24	1-Decanamine	$C_{10}H_{23}N$	484	2016-57-1	0.77
25	Dimethoxyamine	$C_2H_9NO_2$	483	7487-32-3	0.74
26	Hydroperoxide, pentyl	$C_5H_{12}O_2$	482	74-80-6	0.71
27	trans,trans-Muconic acid	$C_6H_6O_4$	481	3588-17-8	0.68
28	1,2-Cyclopentanedicarboxylic acid, 4-(1,1-dimethylethyl)-, dimethyl ester, (1α,2α,4α)	$C_{13}H_{22}O_4$	479	55044-88-7	0.63
29	(Z),(Z)-2,5-Dimethyl-2,4-hexadienedioic acid	$C_8H_{10}O_4$	478	20514-40-3	0.60
30	2-Aminoresorcinol	$C_6H_7NO_2$	477	3163-15-3	0.58

Table 4: GC-MS of Abhaya Gutika at RT=12.6.

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	6-Acetyl-β-d-mannose	$C_8H_{14}O_7$	641	-	45.5
2	2-Methyl-4,5-tetramethylene-5-ethyl-2-oxazoline	$C_{10}H_{17}NO$	566	24337-58-4	5.91
3	DL-Leucine,N-glycyl	$C_8H_{16}N_2O_3$	565	688-14-2	5.68
4	Cytidine, 5-methyl	$C_{10}H_{15}N_3O_5$	549	2140-61-6	3.27
5	2-Methyl-4,5-tetramethylene-5-ethyl-2-oxazoline	$C_{10}H_{17}NO$	543	24337-58-4	5.91
6	1-(β-d-2-Desoxyribofuranosyl)-4-O-difluormethyl-thymine	$C_{11}H_{14}F_2N_2O_5$	542	102302-63-6	2.50
7	Maltose	$C_{12}H_{22}O_{11}$	540	69-79-4	2.31
8	α-D-Mannopyranoside, methyl 3,6-anhydro	$C_7H_{12}O_5$	537	15814-56-9	2.04
9	N-Propionyl-D-glucosamine	$C_9H_{17}NO_6$	530	15475-14-6	1.56
10	1-Amino-2-butanol	$C_4H_{11}NO$	526	13552-21-1	1.32
11	Inosine, 1-methyl	$C_{11}H_{14}N_4O_5$	526	2140-73-0	1.32
12	Octane, 1-azido	$C_8H_{17}N_3$	520	7438-05-3	1.04
13	N-Cyclooct-4-enylacetamide	$C_{10}H_{17}NO$	520	170952-69-9	1.04
14	n-Butyl nitrite	$C_4H_9NO_2$	518	544-16-1	0.95
15	2-Nitro-2-ethyl-1,3-propanediol	$C_5H_{11}NO_4$	518	597-09-1	0.95
16	1-Butanol, 2-nitro	$C_4H_9NO_3$	517	609-31-4	0.92
17	(+)-N-Acetylmuramic acid	$C_{11}H_{19}NO_8$	517	10597-89-4	0.92
18	Succindialdehyde	$C_4H_6O_2$	515	638-37-9	0.85
19	β-D-Glucopyranoside, methyl 3,6-anhydro	$C_7H_{12}O_5$	514	3056-46-0	0. 81
20	n-PROPYL NONYL ETHER	$C_{12}H_{26}O$	512	-	0.75
21	Cyclohexanecarboxylic acid, 3-(acetyloxy)	$C_9H_{14}O_4$	512	105207-65-6	0.75
22	Propanamide, N-acetyl	$C_5H_9NO_2$	511	19264-34-7	0.72
23	2-Myristynoic acid	$C_{14}H_{24}O_2$	511	67587-19-3	0.72
24	Dimethoxyamine	$C_2H_7NO_2$	510	7487-32-3	0.69
25	N-Acetyl-D-glucosamine	$C_8H_{15}NO_6$	509	7512-17-6	0.66
26	Propylene Carbonate	$C_4H_6O_3$	506	108-32-7	0.59
27	N-Trifluoroacetyl-D-glucosamine	$C_8H_{12}F_3NO_6$	505	36875-26-0	0.56
28	2-propenoic acid, 2-[(1,3-dioxobutyl)amino]ethyl ester	$C_9H_{13}NO_4$	503	-	0.52
29	1-Decanamine	$C_{10}H_{23}N$	503	2016-57-1	0.52
30	Hydroperoxide, pentyl	$C_5H_{12}O_2$	502	74-80-6	0.50

Table 5: GC-MS of abhaya gutika at RT=15.4.

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	7-Hexadecenoic acid, methyl ester, (Z)	$C_{17}H_{32}O_2$	592	567875-67-3	8.10----
2	1-(β-d-2-Desoxyribofuranosyl)-4-O-difluormethyl-thymine	$C_{11}H_{14}F_2N_2O_5$	577	102302-63-6	4.91
3	Dodecanoic acid, 3-hydroxy	$C_{12}H_{24}O_3$	577	1883-13-2	4.91
4	Glycyl-D-asparagine	$C_6H_{11}N_3O_4$	576	24667-21-8	4.72
5	1,2-Cyclopentanedicarboxylic acid, 4-(1,1-dimethylethyl)-, dimethyl ester, (1α,2β,4β)	$C_{13}H_{22}O_4$	568	55044-87-6	3.52
6	Cyclopentaneundecanoic acid	$C_{16}H_{30}O_2$	568	6053-49-2	3.52
7	Methyl 11-oxo-9-undecenoate	$C_{12}H_{20}O_3$	565	53613-55-1	3.11
8	Methyl Z-11-tetradecenoate	$C_{15}H_{28}O_2$	561	-	2.62
9	DL-Leucine, N-glycyl	$C_8H_{16}N_2O_3$	555	688-14-2	2.06
10	E-9-Methyl-8-tridecen-2-ol, acetate	$C_{16}H_{30}O_2$	555	-	2.06
11	13-Tetradecynoic acid, methyl ester	$C_{15}H_{26}O_2$	550	56909-03-6	1.66
12	2-Dodecenoic acid	$C_{12}H_{22}O_2$	550	4412-16-2	1.66
13	Cyclopropanepentanoic acid, 2-undecyl-, methyl ester, trans	$C_{20}H_{38}O_2$	550	42199-20-2	1.66
14	13-Docosenoic acid, methyl ester	$C_{23}H_{44}O_2$	550	56630-69-4	1.66
15	3,6-Octadecadiynoic acid, methyl ester	$C_{19}H_{30}O_2$	549	56554-43-9	1.60
16	L-Asparagine	$C_4H_8N_2O_3$	548	70-47-3	1.53
17	Cyclopropaneoctanoic acid, 2-hexyl-, methyl ester	$C_{18}H_{34}O_2$	547	10152-61-1	1.47
18	Uric acid	$C_5H_4N_4O_3$	547	69-93-2	1.47
19	11-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	547	52380-33-3	1.47
20	Methyl 12-hydroxy-9-octadecenoate	$C_{19}H_{36}O_3$	546	-	1.42
21	1,3,2-Dioxaborolane, 2-ethyl-4-(3-oxiranylpropyl)	$C_9H_{17}BO_3$	546	74810-66-5	1.42
22	9-Hexadecenoic acid	$C_{16}H_{30}O_2$	546	2091-29-4	1.42
23	Cyclopentaneundecanoic acid, methyl ester	$C_{17}H_{32}O_2$	545	25779-85-5	1.36
24	Cyclopropanebutanoic acid, 2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-,methyl ester	$C_{25}H_{42}O_2$	544	56051-53-7	1.31
25	Methyl 10-oxo-8-decenoate	$C_{11}H_{18}O_3$	542	65114-83-2	1.21
26	Undecanedioic acid, dimethyl ester	$C_{13}H_{24}O_2$	542	4567-98-0	1.21
27	10-Undecenoic acid, methyl ester	$C_{12}H_{22}O_2$	540	111-81-9	1.11
28	Inosine, 1-methyl	$C_{11}H_{14}N_4O_5$	539	2140-73-0	1.07
29	9-Hexadecenoic acid, methyl ester, (Z)	$C_{17}H_{32}O_2$	538	1120-25-8	1.03
30	11-Dodecenoic acid, methyl ester	$C_{13}H_{24}O_2$	538	29972-79-0	1.03

Table 6: GC-MS of abhaya gutika at RT=15.8.

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	7-Methyl-Z-tetradecen-1-ol acetate	$C_{17}H_{32}O_2$	624	-	24.6
2	Estra-1,3,5(10)-trien-17β-ol	$C_{18}H_{24}O$	604	2529-64-8	11.2
3	Cyclopentaneundecanoic acid	$C_{16}H_{30}O_2$	597	6053-49-2	8.58
4	2-Methyl-4,5-tetramethylene-5-ethyl-2-oxazoline	$C_{10}H_{17}NO$	588	24337-58-4	6.23
5	E-9-Methyl-8-tridecen-2-ol, acetate	$C_{16}H_{30}O_2$	588	-	6.23
6	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	579	57-10-3	4.52
7	1-(β-d-2-Desoxyribofuranosyl)-4-O-difluormethyl-thymine	$C_{11}H_{14}F_2N_2O_5$	578	102302-63-6	4.34
8	2-Methyl-4,5-tetramethylene-5-ethyl-2-oxazoline	$C_{10}H_{17}NO$	575	24337-58-4	6.23
9	Hexanoic acid, 2-isopropyl-2-methyl-5-oxo-, methyl ester	$C_{11}H_{20}O_3$	572	33422-34-3	3.41
10	4-Hydroxy-4-methylhex-5-enoic acid, tert.-butyl ester	$C_{11}H_{20}O_3$	567	-	2.75
11	10-Methyl-8-tetradecen-1-ol acetate	$C_{17}H_{32}O_2$	567	-	2.75
12	4-Nonene, 5-nitro	$C_9H_{17}NO_2$	563	6065-01-6	2.32
13	9-Oxabicyclo[6.1.0]nonan-4-one	$C_8H_{12}O_2$	554	28399-88-4	1.69
14	Hexanoic acid, 3,5-difluorophenyl ester	$C_{12}H_{14}F_2O_2$	552	-	1.55
15	4H,5H-Pyrano[4,3-d]-1,3-dioxin, tetrahydro-8a-methyl	$C_8H_{14}O_3$	543	54340-98-6	1.13
16	Trichloroacetic acid, 3-tridecyl ester	$C_{15}H_{27}Cl_3O_2$	537	-	0.88

17	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	534	57-10-3	4.52
18	Cytidine, 5-methyl	$C_{10}H_{15}N_3O_5$	534	2140-61-6	0.78
19	4-Allyl-3-(dimethylhydrazono)-2-methylhexane-2,5-diol	$C_{12}H_{24}N_2O_2$	530	-	0.66
20	Dodecylsuccinic anhydride	$C_{16}H_{28}O_3$	529	2561-85-5	0.63
21	3-Hexen-2-one, 3,4-dimethyl-, (Z)	$C_8H_{14}O$	525	20685-45-4	0.53
22	Hexadecanoic acid, 1,1-dimethylethyl ester	$C_{20}H_{14}O_2$	525	31158-91-5	0.53
23	Tridecanoic acid, thiophen-2-ylmethylenehydrazide	$C_{18}H_{13}N_2OS$	520	-	0.43
24	Propanamide, N-acetyl	$C_5H_9NO_2$	519	19264-34-7	0.41
25	4-Cyclopentene-1,3-diol, trans	$C_5H_8O_2$	519	694-47-3	0.41
26	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	518	57-10-3	4.52
27	Hydroperoxide, heptyl	$C_7H_{16}O_2$	517	764-81-8	0.38
28	Longipinene epoxide	$C_{15}H_{24}O$	517	142792-93-6	0.38
29	1-Hydroxy-2-pentanone	$C_5H_{10}O_2$	516	64502-89-2	0.37
30	3-Oxazolepropanamide, N-(4-chlorophenyl)tetrahydro-4-hydroxy-4,5,5-trimethyl-2-oxo	$C_{15}H_{19}ClN_2O_4$	516	-	0.37

Table 7: GC-MS of abhaya gutika at RT=17.

Peak	Compound name	Formula	Match factor	CAS#	Prob%
1	Glycyl-D-asparagine	$C_6H_{11}N_3O_4$	645	24667-21-8	33.9
2	Inosine, 1-methyl	$C_{11}H_{14}N_4O_5$	632	2140-72-0	21.9
3	1,2-Cyclopentanedicarboxylic acid, 4-(1,1-dimethylethyl)-, dimethyl ester, (1α,2β,4β)	$C_{13}H_{22}O_4$	609	55044-87-6	7.99
4	1-Hydroxybicyclo[2.2.2]oct-5-en-2-yl, methyl ketone	$C_{10}H_{14}O_2$	586	-	2.9
5	Uric acid	$C_5H_4N_4O_3$	585	69-93-2	2. 80
6	8-Dodecen-1-ol, acetate, (Z)	$C_{14}H_{26}O_2$	581	28079-04-1	2.37
7	E-5-Dodecen-1-ol acetate	$C_{14}H_{26}O_2$	577	-	2.00
8	3,6,12-Trimethyl-1,4,7,10,13,16-hexaaza-cyclooctadecane-2,5,8,11,14,17-hexaone	$C_{15}H_{24}N_6O_6$	577	5519-72-2	2.00
9	DL-Leucine, N-glycyl	$C_8H_{16}N_2O_3$	576	688-14-2	1.9
10	Glycine, N-(N-glycyl-L-leucyl)	$C_{10}H_{19}N_3O_4$	576	2576-67-2	1.92
11	E-7-Dodecen-1-ol acetate	$C_{14}H_{26}O_2$	572	-	1.62
12	2(3H)-Benzofuranone, hexahydro-4,4,7a-trimethyl	$C_{11}H_1O_2$	569	1677-27-1	1.43
13	11-Dodecen-1-ol monofluoroacetate	$C_{14}H_{25}FO_2$	562	128792-44-9	1.10
14	Guanosine, 2'-O-methyl	$C_{11}H_{15}N_5O_5$	560	2140-71-8	1.01
15	1,5-Dodecadiene	$C_{12}H_{22}$	556	-	0.85
16	2-Oxa-6-azatricyclo[3.3.1.1(3,7)]decane-6-carboxaldehyde	$C_9H_{13}NO_2$	556	50267-24-8	0.85
17	9-Dodecen-1-ol, acetate, (Z)	$C_{14}H_{26}O_2$	555	16974-11-1	0.82
18	1(2H)-Naphthalenone, octahydro-4a-methyl-, trans	$C_{11}H_{18}O$	549	937-99-5	0.64
19	6-Ethyl-5-[4-morpholinyl]-2,4(1H,3H)-pyrimidinedione	$C_{10}H_{15}N_3O_3$	549	177941-50-3	0.64
20	2-Amino-4-dimethylaminomethylenepentanedinitrile	$C_8H_{12}N_4$	546	-	0.57
21	Dodecanal	$C_{12}H_{24}O$	544	112-54-9	0.52
22	Azacyclotridecan-2-one	$C_{12}H_{23}NO$	544	947-04-6	0.52
23	[1,2,5]Oxadiazolo[3,4-b][1,4]diazocine-5,7(4H,6H)-dione, 8,9-dihydro	$C_6H_6N_4O_3$	543	-	0.50
24	4,5-Tetramethylenetetrahydro-1,3-oxazine-2-thione	$C_8H_{13}NO_5$	542	104893-74-5	0.48
25	4H,5H-Pyrano[4,3-d]-1,3-dioxin, tetrahydro-8a-methyl	$C_8H_{14}O_3$	539	54340-98-6	0.43
26	Spiro[5.6]dodecane	$C_{12}H_{22}$	539	181-15-7	0.43
27	E-3-Tetradecen-1-ol acetate	$C_{16}H_{30}O_2$	538	-	0.41
28	Hydroxycyprazine	$C_9H_{15}N_5O$	537	39095-60-4	0.39
29	1-Decanamine	$C_{10}H_{23}N$	537	2016-57-1	0.39
30	Z-3-Tetradecen-1-ol acetate	$C_{16}H_{30}O_2$	535	-	0.36

The GC-MS chromatogram of Abhaya Gutika displayed multiple peaks, indicating a complex mixture of bioactive compounds. The major constituents identified across different retention times (RT) are summarized below.

Retention Time (RT)	Major Compounds Identified	Relative Abundance / Probability (%)
7.6	1-Hydroxy-2-pentanone, 3(2H)-Furanone, dihydro-2-methyl,	1.08% - 7.86%

	Glycidol	
8.9	6-Acetyl-β-d-mannose, 3-Methylenecyclopropane-trans-1,2-dicarboxylic acid, 5-Hydroxymethylfurfural	9.11% - 22.1%
12.0	1,2,4-Benzenetriol, Pyrazole-5-carboxylic acid, 3-methyl, 1,2,3-Benzenetriol (Pyrogallol)	3.67% - 22.8%
12.6	6-Acetyl-β-d-mannose, DL-Leucine, N-glycyl, Maltose	2.31% - 45.5%
15.4	7-Hexadecenoic acid methyl ester, Dodecanoic acid, 3-hydroxy, L-Asparagine	1.53% - 8.10%
15.8	7-Methyl-Z-tetradecen-1-ol acetate, n-Hexadecanoic acid (Palmitic acid)	4.52% - 24.6%
17.0	Glycyl-D-asparagine, Inosine, 1-methyl, Uric acid	2.80% - 33.9%

The presence of 1,2,4-Benzenetriol and Pyrogallol (1,2,3-Benzenetriol) is particularly noteworthy, as these are potent phenolic antioxidants derived from the tannins in Haritaki. 5-Hydroxymethylfurfural (HMF) is a common product of the Maillard reaction, likely formed during the heating of honey with the herbal powder.

DISCUSSION

The GC-MS analysis of Abhayadi Gutika reveals a sophisticated chemical profile that validates its traditional therapeutic claims. The high concentration of phenolic compounds like Benzenetriols and Pyrogallol suggests strong antioxidant and antimicrobial activities, which are essential for inhibiting the growth of cariogenic bacteria such as Streptococcus mutans.

The identification of 6-Acetyl-β-d-mannose and other sugar derivatives indicates the role of honey not just as a binding agent, but as a source of bioactive glycoconjugates. The formation of 5-Hydroxymethylfurfural (HMF) confirms the chemical transformation occurring during the heating process in the copper vessel. While HMF is often discussed in the context of food quality, in small quantities within medicinal formulations, it can exhibit certain biological activities.

Furthermore, the presence of fatty acids like n-Hexadecanoic acid (Palmitic acid) and its esters provides anti-inflammatory benefits, which could help reduce the gingival inflammation associated with Krimidanta. The unique preparation method—heating in a copper vessel—potentially introduces trace amounts of copper ions or facilitates specific catalytic reactions that enhance the stability and bioavailability of these phytochemicals.

The synergy between the astringent (Kashaya) and bitter (Tikta) properties of Haritaki and the soothing, healing nature of honey, processed under controlled heat, results in a formulation that is chemically equipped to tackle the microbial and inflammatory aspects of dental decay.

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CONCLUSION

This study provides the first comprehensive GC-MS characterization of Abhayadi Gutika prepared according to Rasa Ratna Samucchaya. The results confirm the presence of diverse bioactive molecules, including phenolics, fatty acids, and sugar derivatives, which collectively contribute to its anti-cariogenic properties. The traditional method of preparation is scientifically sound, as it facilitates the extraction and formation of key therapeutic compounds. These findings lay the groundwork for further clinical trials and the standardization of this traditional Ayurvedic remedy for modern dental care.

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