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A COMPARISON OF VOLATILE COMPOUNDS IN DIFFERENT GENOTYPES OF *SESAMUM INDICUM* L. BY GC-MS

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ABSTRACT: The aim of the present study was to investigate the oil composition extracted from *Sesamum indicum* seeds. The oil was extracted from seeds by soxhlet method and analyzed by gas chromatography-mass spectrometry (GC-MS). A total of 84 different components were identified and out of which 12 are fatty acid components. The principal compounds identified and present in all samples were silane, trimethyl[5-methyl-2-(1-me thylethyl)phenoxy]-; silicic acid, diethyl bis (trimethylsilyl)ester; stearic acid; oleic acid; n-Hexadecanoic acid; myristic acid; indole-2-one 2,3-dihydro-N-hydroxy-4-methoxy-3,3-dimethyl-; cyclotrisiloxane, hexamethyl-; acetamide, N-[-4-(trimethylsilyl)phenyl]-; benzene, 2-[(tert-butyldimethylsilyl)oxy]-1-isopropyl-4-methyl-; benzo[h]quinoline, 2,4-dimethyl-, trichloroacetic acid undec-2-enyl ester and 2-Ethylacridine. Among fatty acids, palmitic acid and oleic acid were identified in highest concentration. In comparison, myristic acid and stearic acid were present in lesser amount. Variation was found between chemical compositions of different genotypes of sesame. The obtained results supported the use of seed oil as edible oil and in pharmaceuticals. This study is also important as identification of volatile compounds in Indian genotypes of *Sesamum indicum* was done for the first time.

INTRODUCTION: Sesame (*Sesamum indicum* L.) belongs to Pedaliaceae family, is one of the most ancient oilseeds crop. It was domesticated on the Indian subcontinent during Harappan era [1] but now in all tropical and subtropical countries.

India is the leading producer in the world and sesame is the third most important Indian oil seed crop [2].

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It is known by different names in different countries such as til (Hindi), huma (Chinese), sesame (French), goma (Japanese), gergelim (Portuguese) and ajonjoli (Spanish). It is cultivated for its high edible oil content and protein.

The edible oil is highly valuable and has certain industrial applications including human nutrition such as pharmaceuticals, cosmetics, perfumery, soaps, paints and insecticides, hair oil, hydrogenated oil and certain medicines [3].

It is called queen of the oilseeds crops because of its high oil content, mildness and pleasant taste [4]. The oil is free of unwanted odors and rancidity resistant and has high level of unsaturated fatty-acids which makes it suitable for cooking [5].

Sesame oil contains 20% saturated fatty-acids mainly palmitic (7.9-12%) and stearic (4.8-6.1%) and more than 80% unsaturated fatty-acids (oleic acid 35.9-42.3%, linoleic acid 41.5-47.9%). Other fatty acids are also present in minor amount (less than 1%) viz. myristic (~0.1), palmitoleic (~0.1-0.2), heptadecanoic (~0.2) and fatty acid composition varies with the sesame's species [6]. Sesame oil has good amount of unsaponification matter (~2%) which includes sterols, triterpenes, triterpene alcohols, tocopherols and lignans. It is an annual, erect herb and has indeterminate growth which grows best at 25-27°C temperature and neutral pH.

From medicinal point of view, sesame oil has numerous functions such as antiaging, lowers serum lipid, blood pressure and other functions[7]. The genetic and environmental factors affect oil content and fatty acid composition in sesame[8]. GC/MS appears an ideal technique for the detection of fatty acids and their concentrations. There are few reports on fatty acid composition analysis of sesame oil in India [9-11]. But there is not any report on chemical characterization of sesame oil so far in India. The purpose of the present study was to investigate the chemical compounds present in sesame oil and comparison of chemical composition of sesame oil between different Indian sesame genotypes. This will further increase its medicinal and cosmetic importance and resultant its production.

MATERIAL AND METHODS:

Plant Material: Seeds of *Sesamum indicum* were collected from different states (Rajasthan, Uttar Pradesh, Madhya Pradesh, Punjab, Tamil Nadu and Gujarat) of India as illustrated in **Table 1**. Seeds were made clear of foreign particles like dust particles and sand.

TABLE 1: LIST OF *SESAMUM INDICUM* L. GENOTYPES USED ALONG WITH THEIR PLACE OF ORIGIN

Genotypes	Place of origin
DT-46	Uttar Pradesh
RT-46	Rajasthan
RT-346	Rajasthan
RT-127	Rajasthan
T-12	Uttar Pradesh
T-13	Uttar Pradesh
TMV3	Tamil Nadu

Oil extraction: 5 gram grounded seeds were placed into a cellulose paper cone and extracted using light petroleum ether (b.p. 40-60°C) in a Soxhlet extractor for 8 hrs [12]. The oil was then recovered by evaporating of the solvent using rotary vacuum evaporator and residual solvent was removed by drying in an oven at 60°C for 1 hour.

GC-MS analysis: Agilent 6890 gas chromatograph coupled with 5975B mass spectrometer was used for GC-MS analysis. The chromatographic separation of analytes occurred on a capillary column of fused silica HP-5ms (0.25mm x 30m x 0.25 µM). The oven programming was maintained at 50°C [13]. 1 µl of extract was injected in the split mode (1:50) at 280°C. The mass spectrometer was operated in electron impact mode. The mass scan range was *m/z*- 40 to150 atom mass units (amu). All the mass spectra of the identified peaks were compared with the spectra from the NIST'05 and WILAY spectral library. The compounds were reported as percentage of the total area of their peaks in the total ion chromatogram.

RESULT AND DISCUSSION: The GC-MS chromatogram of volatile oil samples revealed the presence of 84 compounds, which were identified in comparison to the fragmentation patterns in the resulting mass spectra with those published in literature and using the National Institute of Standards and Technology (NIST), Mass Spectral Database of the gas chromatograph–mass spectrometer. A number of other compounds were also detected but not of good quality. The maximum number of compounds was found in T13 genotype. The chemical names with retention time (RT) and peak area (%) of the compounds which were detected was given in **Table 2**.

The mass spectra of different samples were shown in **Fig. 1**. The major compounds identified and present in almost each genotype were silane, trimethyl[5-methyl-2-(1-me thylethyl)phenoxy]-; silicic acid, diethyl bis (trimethylsilyl)ester; stearic acid; oleic acid; n-Hexadecanoic acid; myristic acid; indole-2-one 2,3-dihydro-N-hydroxy-4-methoxy-3,3-dimethyl-; cyclotrisiloxane, hexa methyl-; acetamide, N-[-4-(trimethylsilyl) phenyl]; benzene, 2-[(tert-butyldimethylsilyl)oxy]-1-iso propyl-4-methyl-; benzo[h]quinoline, 2,4-dimethyl-, trichloroacetic acid undec-2-enyl ester

and 2-Ethylacridine. The fatty acids identified in sesame oil were given in **Table 3**.

TABLE 2: LIST OF CHEMICAL COMPOUNDS IDENTIFIED IN SESAME OIL BY GC-MS.

Compound	CAS	RT (min)	Peak Area (%)						
			DT46	RT46	RT127	T12	T13	RT346	TMV3
1-(4-Methoxy-phenyl)-5,5-dioxo-hexahydro-5.lambda.(6)-thieno[3,4-b]pyrrol-2-one	1000297-17-8	24.249	-	-	-	1.64	-	-	-
1,1,1,3,5,5,5-Heptamethyltrisiloxane	001873-88-7	34.491	0.13	-	-	2.49	2.08	-	0.04
1,2-Benzisothiazole-3-propanoic acid	050565-45-2	31.869	-	13.03	-	-	0.41	-	-
1,2-Bis (trimethylsilyl) benzene	017151-09-6	41.712	0.16	0.13	-	0.27	0.17	0.41	-
1,3-Benzodioxole, 5,5'-(tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bis-, [1S-(1.alpha.,3a.alpha.,4.beta.,6a.alpha.)]-	000133-03-9	30.792	-	-	-	20.04	-	-	-
1,3-Dioxolane, 4-ethyl-5-octyl-2,2-bis (trifluoromethyl)-, trans-	038274-73-6	24.171	-	-	-	-	1.65	-	-
1-Eicosanol	000629-96-9	22.782	-	-	-	-	0.20	-	-
1-Octadecanol	000112-92-5	20.783	-	-	-	5.87	-	-	-
2-(Acetoxymethyl)-3-(methoxycarbonyl) biphenylene	093103-70-9	41.945	-	-	-	-	0.25	-	-
2-(Acetoxymethyl)-3-(methoxycarbonyl) biphenylene	093103-70-9	29.148	-	-	-	-	0.46	-	-
2,4-Decadienal	025152-84-5	11.463	-	-	-	-	-	-	0.04
2,4-Decadienal, (E,E)-	025152-84-5	11.118	-	-	-	-	0.18	-	0.04
2-Cyclohexen-1-ol	000822-67-3	10.596	-	-	-	-	-	-	0.08
2-Decenal, (E,)-	003913-81-3	10.596	-	-	-	-	0.37	-	-
2-Ethylacridine	055751-83-2	31.858	5.84	0.46	-	0.89	0.29	2.15	-
2-Heptenal	1000143-48-6	21.327	-	-	-	-	0.34	-	-
2-Heptenal, (E)-	018829-55-5	5.186	-	-	-	-	0.09		-
2-Methoxybenzoic acid, 2-methylpropyl ester	081763-24-8	31.858	-	-	-	11.55	-	-	0.04
2-Nonanone	000821-55-6	18.206	-	-	0.19	-	-	-	-
2-undecanone	000112-12-9	14.196	-	-	0.22	-	-	-	-
3-Amino-4-piperonyl-5-pyrazolone	014731-77-2	31.891	-	-	-	-	3.55	-	-
3-Carboxy-2-piperidone	003731-16-6	10.383	-	-	-	-	-	-	0.01
3-Hexanol	000623-37-0	4.953	-	-	-	0.79	0.07	-	0.01
4-Methylthieno[2,3-b]pyridine	013362-81-7	30.792	-	-	-	20.04	-	-	0.01
5-Octadecenal	056554-88-2	20.961	-	-	-	0.88	-	-	-
6-Methylthieno[2,3-b]pyridine	001759-30-4	30.792	-	-	-	20.04	-	-	-
6-Octadecanoic acid, (Z)-	000593-39-5	20.805	-	-	-	-	5.47	-	-
9, 17-Octadecadienal, (Z)-	056554-35-9	22.027	-	-	-	-	-	-	14.07
9,12-Octadecadienoic acid (Z,Z)-	000060-33-3	20.728	-	-	-	1.83	-	5.47	1.44
9H-Fluorene-2-carboxylic acid, 9-oxo-, (2-hydroxyethyl) (methyl) amide	1000316-02-1	32.183	-	-	-	-	0.75	-	0.25
9-Octadecenoic acid, (E)-	000112-79-8	20.805	-	-	-	-	5.47	-	-
Acetamide, N-[-4-(trimethylsilyl)phenyl]-	000541-05-9	45.155	0.16	0.41	-	-	0.41	1.27	14.07
Benzene, 2-[(tert-butyldimethylsilyl)oxy]-1-isopropyl-4-methyl-	330455-64-6	24.449	0.91	-	-	2.27	0.57	-	-
Benzeneamine, 4-(2-phenylethenyl)-N-(3,5-dimethyl-1-pyrazolylmethyl)-	1000260-49-5	25.337	-	-	-	-	1.16	-	-
Benzo[h]quinoline, 2,4-dimethyl-	000605-67-4	34.424	0.30	0.48	-	-	0.98	0.21	-
Beta-Sitosterol	000083-46-5	34.036	-	13.59	-	-	4.16	-	-
Chloromethyl 9-chloroundecanoate	080418-95-7	19.861	-	-	-	-	-	-	0.84
Cyclohexane,1-(1,5-dimethylhexyl)-4-(4-methylpentyl)-	056009-20-2	22.738	-	-	-	-	-	-	1.66
Cyclopentanol, 1-(1-methylene-2-propenyl)-	078158-11-983	21.527	-	-	-	-	-	3.17	-

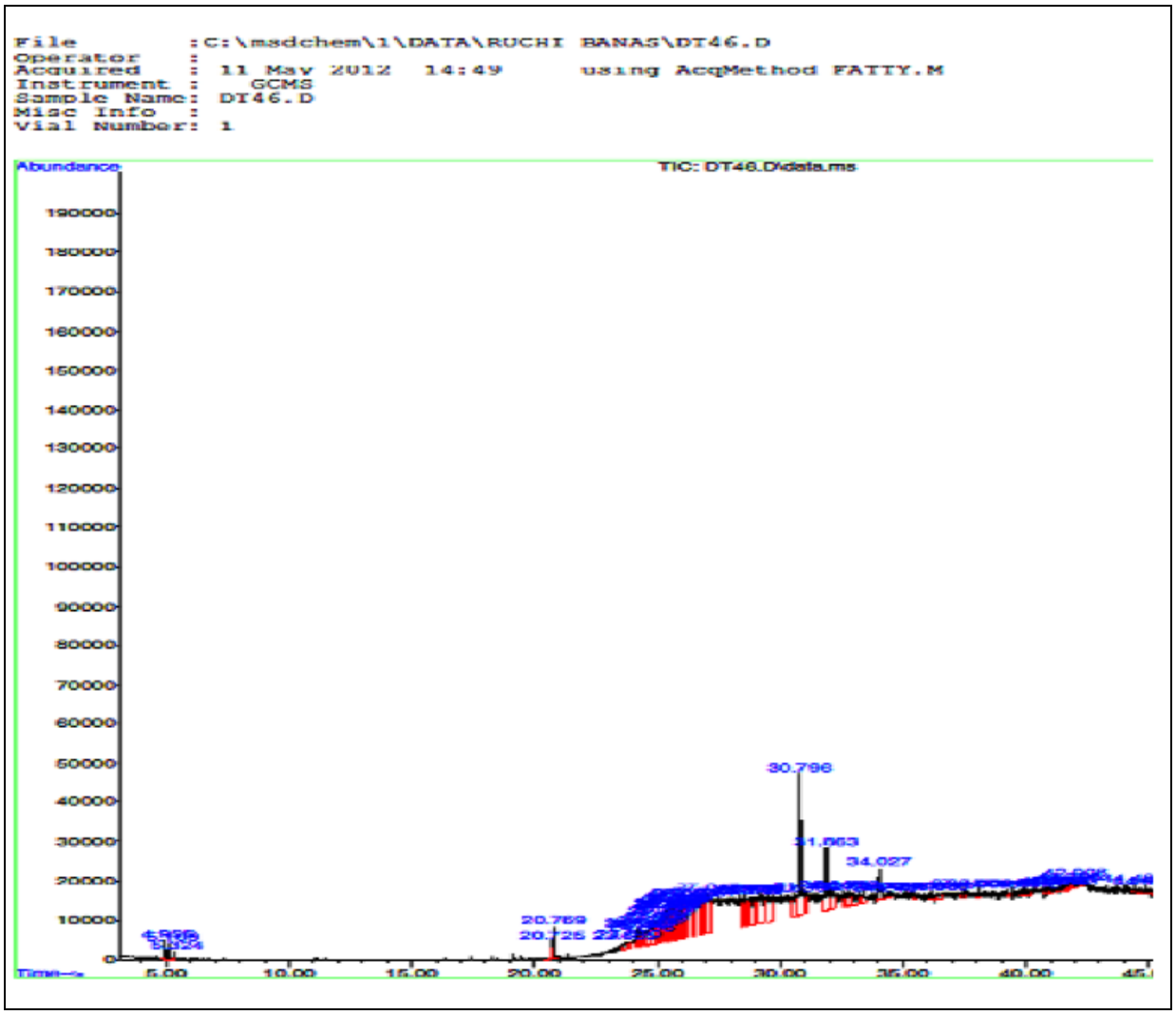
cis-6-Nonen-1-ol	035854-86-5	21.238	-	-	2.97	-	-	-	0.04
Cyclopropaneoctanal, 2-octyl-	056196-06-6	21.783	-	-	-	-	-	-	0.39
Cyclotrisiloxane, hexamethyl-	000541-05-9	25.338	1.36	1.32	-	2.60	1.06	2.15	0.65
Cycloundecane, 1-methyl-	088828-82-4	20.727	2.55	0.91		0.84	-	-	-
Dodecanoic acid	000143-07-7	19.072	-	-	-	0.55	-	-	0.04
Erucic acid	000089-81-6	22.416	-	-	-	0.55	-	-	18.63
Ethyladamantane-1-carboxylate	002094-73-7	31.858	-	-	-	11.55	-	-	-
Fenchyl alcohol	001632-73-1	17.673	-	-	0.44	-	-	-	-
Furfuryl alcohol	000098-00-0	25.549	-	-	4.96	-	-	-	18.63
Furo [2,3-c]pyridine, 2,3-dihydro-2, 7-dimethyl-	069022-82-8	19.194	-	-	-	-	0.06	-	-
Gamma-Sitosterol	000083-47-6	34.058	-	13.59	-	-	4.16	-	0.84
Heptadecanoic acid, heptadecyl ester	036617-50-2	22.182	-	-	-	-	0.25	-	-
Indole	029812-79-1	21.316	0.63	0.08	0.39	-	4.16	-	-
Indole-2-one, 2,3-dihydro-N-hydroxy-4-methoxy-3,3-dimethyl-	000120-72-9	25.149	1.17	0.26	-	2.14	0.42	0.80	0.19
Isopulegol	059905-50-2	21.583	-	-	2.09	-	-	-	-
Lauric acid	000143-07-7	22.738	-	-	2.01	-	-	-	-
Lauric aldehyde	000112-54-9	18.050	-	-	0.30	-	-	-	-
Lauryl acetate	000112-66-3	25.916	-	-	0.18	-	-	-	-
Lauryl alcohol	000112-53-8	16.417	-	-	0.15	-	-	-	-
Methyl 3-(1-pyrrolo)thiophene-2-carboxylate	074772-16-0	24.249	-	-	-	1.64	-	-	-
Myristic acid (Tetradecanoic acid)	000544-63-8	20.983	1.65	0.55	2.01	1.97	0.47	-	1.66
N-(2-Acetylcyclopentylidene) cyclohexylamine	1000100-48-5	22.716	-	-	-	-	0.24	-	-
n-decanal	000112-44-7	25.916	-	-	8.26	-	-	-	-
n-Decanoic acid	000334-48-5	20.983	-	-	-	-	-	17.17	-
n-Eicosane	000112-95-8	19.461	-	3.38	-	-	-	-	-
n-Hexadecanoic acid (Palmitic acid)	000057-10-3	15.195	0.14	0.32	-	5.87	5.47	45.20	2.08
N-Methyl-1-adamntaneacetamide	013897-93-5	32.169	-	-	-	-	2.08	-	-
n-Octadecane	000593-45-3	17.439	-	-	-	-	-	4.62	-
Nonahexacontanoic acid	040710-32-5	21.316	-	-	-	0.52	-	-	-
n-Teracosane	000646-31-1	22.994	-	1.75	-	-	-	-	-
Oleic Acid (9-octadecenoic acid (Z)-	000112-14-1	3.343	-	-	-	5.87	5.47	45.20	14.07
Omega-6-Hexadecalactone, Ambrettol	007779-50-2	17.806	-	-	0.85	-	-	-	-
Oxycyclotetradecan-2-one	000112-14-1	3.343	-	-	-	-	-	17.17	-
Pentadecanoic acid	001002-84-2	21.016	-	-	-	-	-		2.08
Pentafluoropropionic acid, hexadecyl ester	006222-07-7	22.560	-	-	-	-	-	1.97	-
Pentanoic acid, 10-undecenyl ester	001002-84-2	21.016	-	0.40	8.26	-	-	-	0.02
Silane, trimethyl[5-methyl-2-(1-methylethyl)phenoxy]-	055012-80-1	23.216	1.37	0.31	-	1.93	1.16	0.25	0.40
Silicic acid, diethyl bis (trimethylsilyl)ester	003555-45-1	29.148	4.83	0.57	-	2.23	0.62	0.32	0.07
Stearic acid (Octadecanoic acid)	000057-11-4	20.983	4.83	0.73	8.40	2.23	0.29	0.15	-
Stigmasterol, 22,23-dihydro-	003555-45-1	29.148		-	-	-	0.26	-	-
Tetrasiloxane, decamethyl-	1000214-20-7	34.047	4.83	0.31	-	1.93	1.16	0.25	-
Trichloroacetic acid, undec-2-enyl ester	1000299-26-1	22.860	4.83	0.57	-	2.23	0.62	0.32	0.40
Tridecanoic acid	000638-53-9	19.094	-	0.73	8.40	2.23	0.45	0.15	0.07
Trimethyl[4-(2-methyl-4-oxo-2-pentyl)phenoxy]silane	1000283-54-9	25.404	-	-	-	-	-	1.68	-
Undecanoic acid, monoethyl ester	003927-60-4	18.472	-	-	-	-	-	-	0.01

(RT: Retention time).

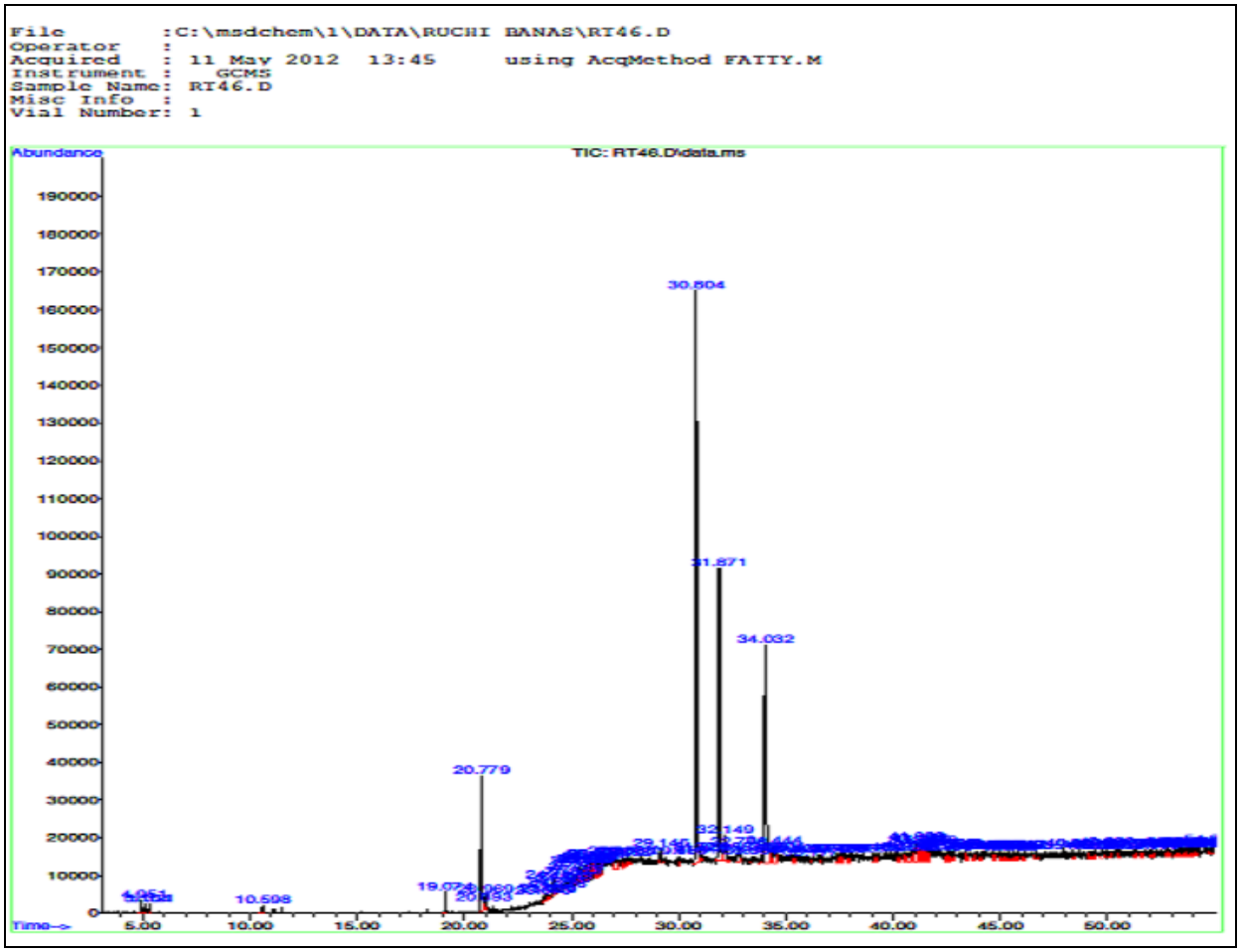
TABLE 3: LIST OF FATTY ACIDS PRESENT IN SESAME OIL OBTAINED BY GC-MS.

Compound	CAS	RT (min)	Peak Area (%)						
			DT46	RT46	RT127	T12	T13	RT346	TMV3
6-Octadecanoic acid, (Z)-	000593-39-5	20.805	-	-	-	-	5.47	-	-
Dodecanoic acid	000143-07-7	19.072	-	-	-	0.55	-	-	0.04
Erucic acid	000089-81-6	22.416	-	-	-	0.55	-	-	18.63
n-Decanoic acid	000334-48-5	20.983	0.38	-	8.40	-	0.33	17.17	-
Heptadecanoic acid, heptadecyl ester	036617-50-2	22.182	-	-	-	-	0.25	-	-
n-Hexadecanoic acid (Palmitic acid)	000057-10-3	15.195	0.14	0.32	-	5.87	5.47	45.20	2.08
9-octadecenoic acid (Z)- (Oleic Acid)	000112-14-1	3.343	-	-	-	5.87	5.47	45.20	14.07
Pentadecanoic acid	001002-84-2	21.016	-	-	-	-	-		2.08
Pentafluoropropionic acid, hexadecyl ester	006222-07-7	22.560	-	-	-	-	-	1.97	-
Pentanoic acid, 10-undecenyl ester	001002-84-2	21.016	-	0.40	8.26	-	-	-	0.02
Octadecanoic acid (Stearic acid)	000057-11-4	20.983	4.83	0.73	8.40	2.23	0.29	0.15	-
Tetradecanoic acid (Myristic acid)	000544-63-8	20.983	1.65	0.55	2.01	1.97	0.47	-	1.66

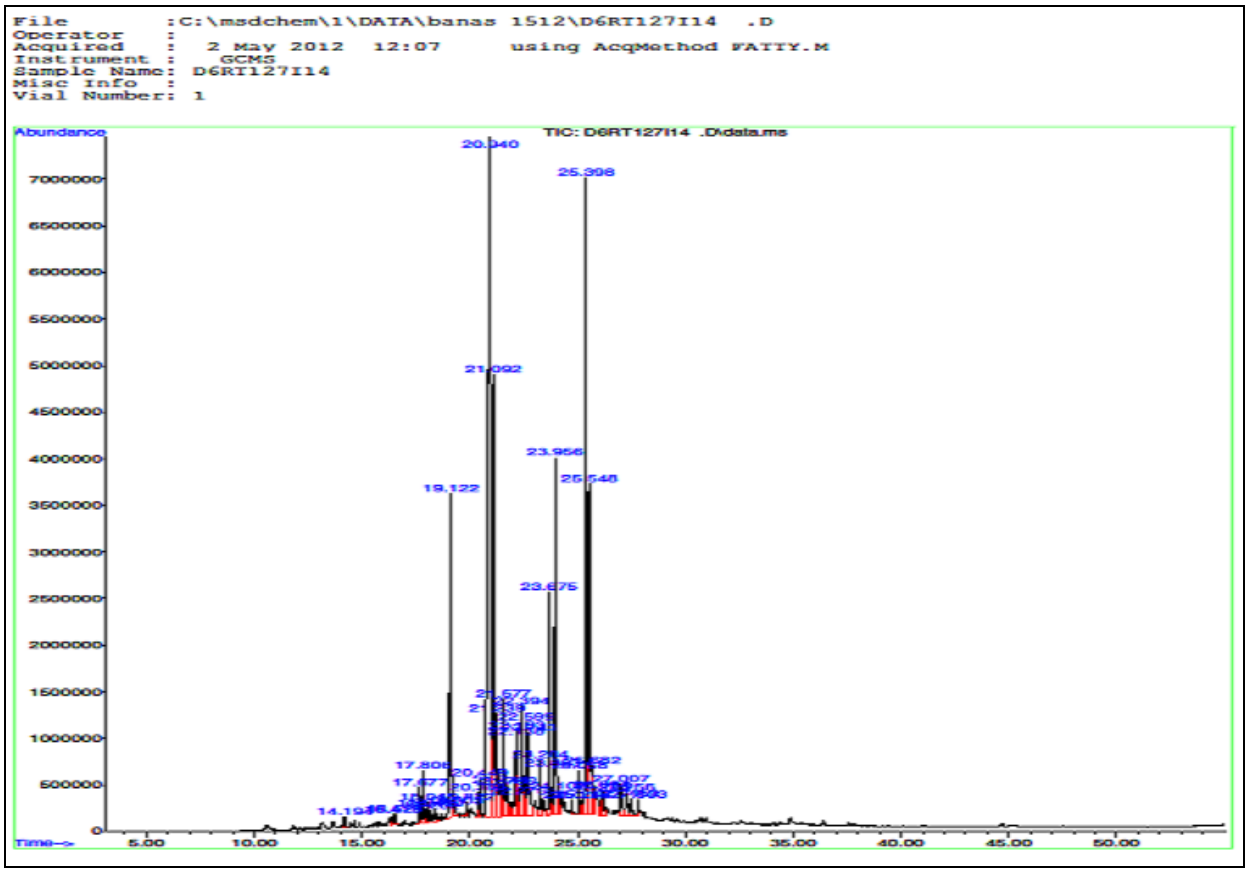
(RT: Retention time).



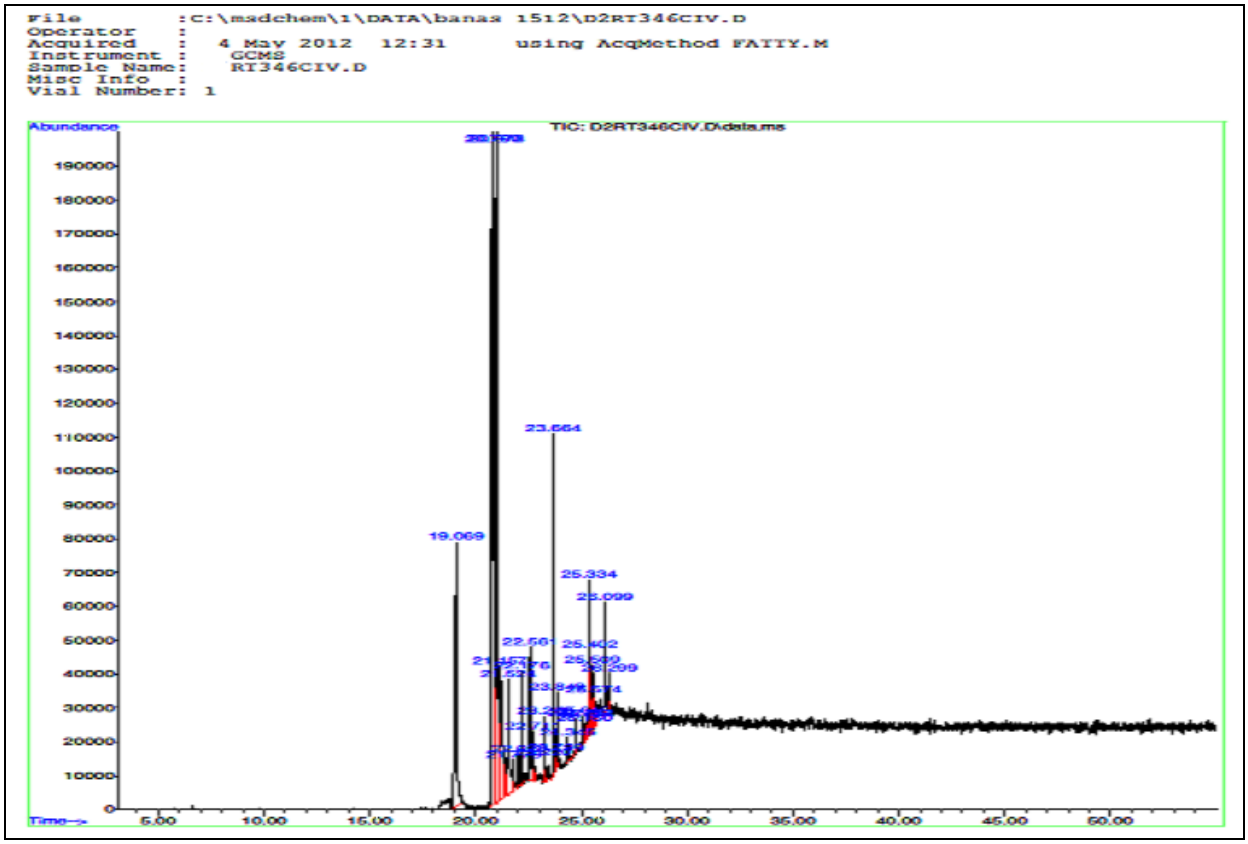
A) DT46



B) RT46



C) RT127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Acquired : 4 May 2012 12:31 using AcqMethod FATTY.M
Instrument : GCMS
Sample Name: RT346CIV.D
Misc Info :
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Abundance
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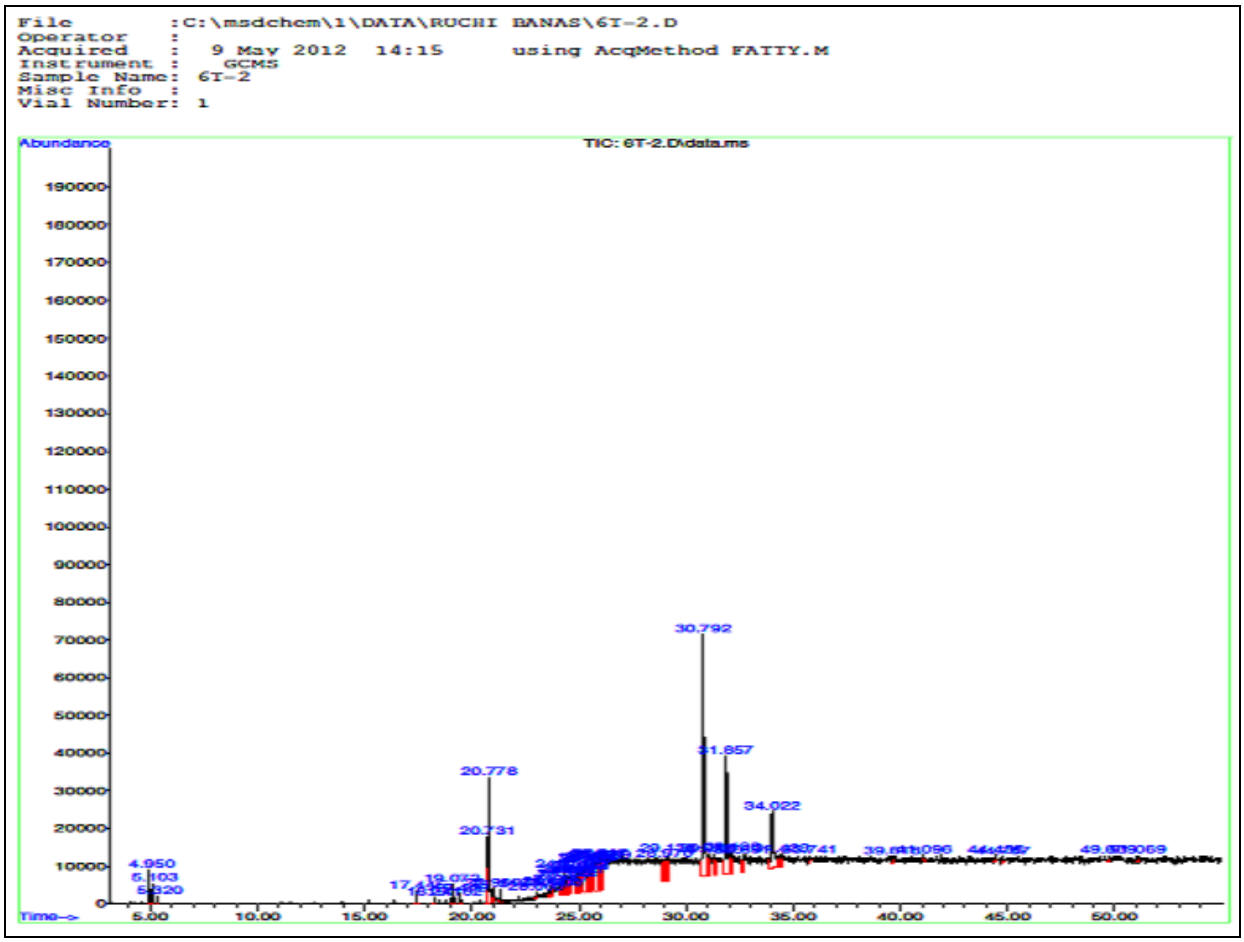
23.664
25.334
25.099
Time-->

D) RT346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Operator :
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Instrument : GCMS
Sample Name: 6T-2
Misc Info :
Vial Number: 1
Abundance
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20.778
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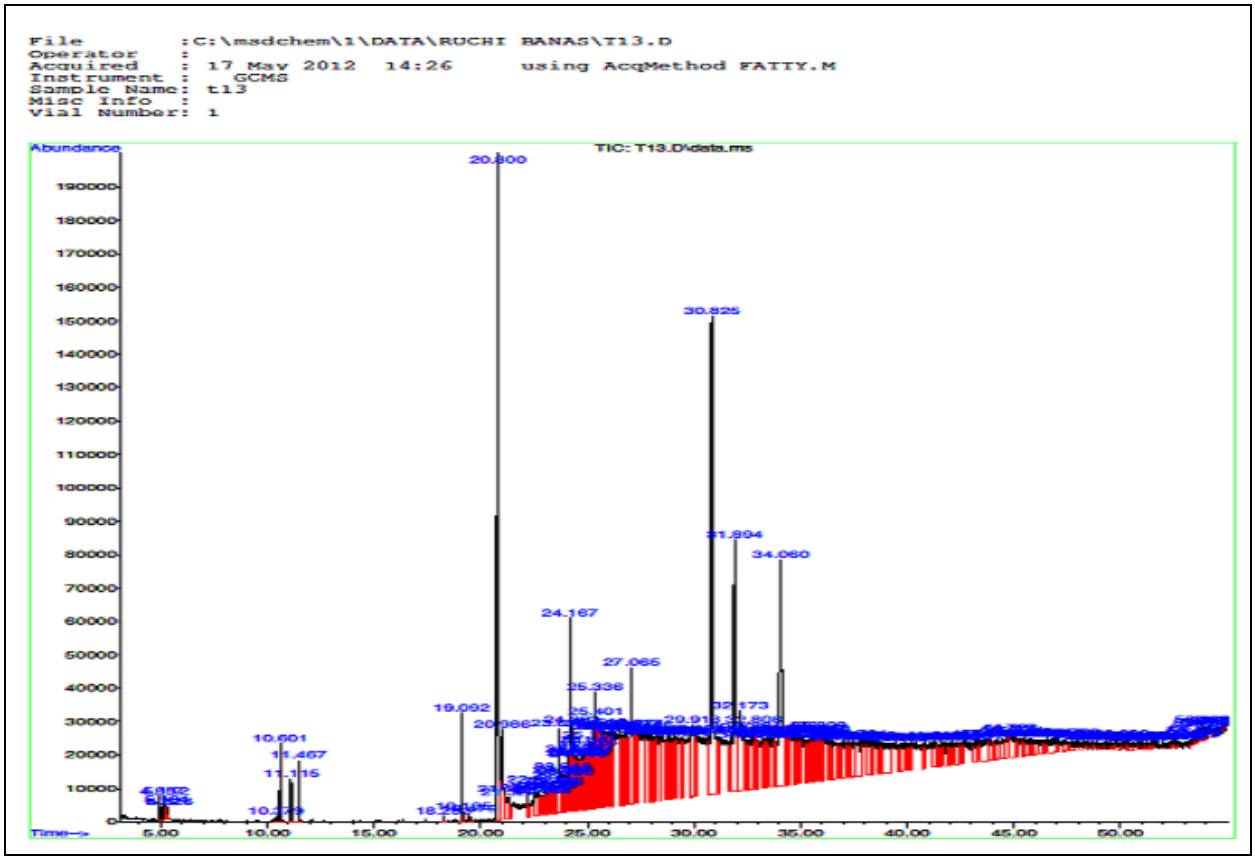
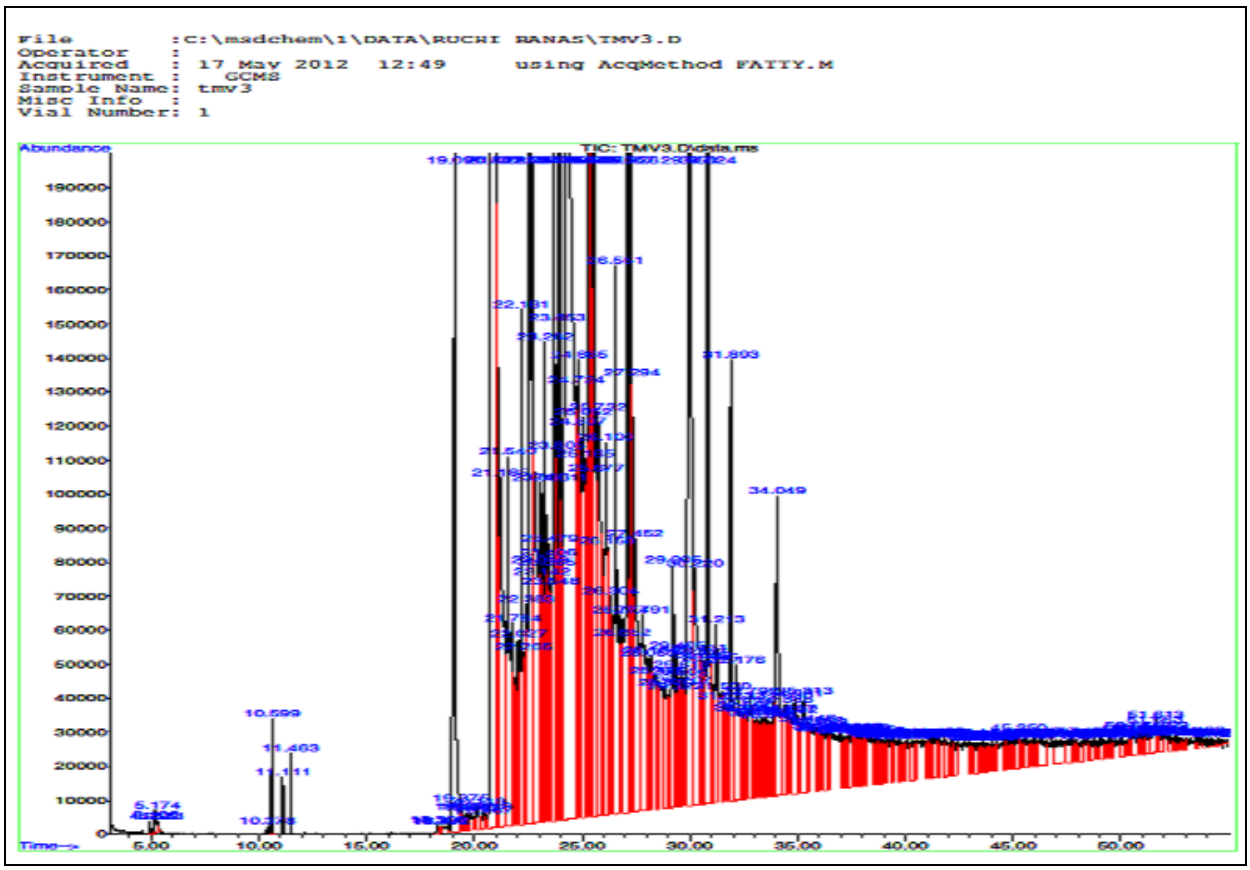
Time-->

E) T12



F) T13



G) TMV3

Fig. 1: THE MASS SPECTRA OF DIFFERENT GENOTYPES OF *SESAMUM INDICUM* A) DT5; B) RT46; C) RT127; D) RT346 E) T12; F) T13; G) TMV3

Likewise, the oil content and fatty acid composition of eleven genotypes of pot marigold (*Calendula officinalis* L.) seeds were determined[14]. In the present study a wide variation was found between chemical compositions of different genotypes of sesame. It was supported by literature which stated that chemical composition of volatile oils could differ widely within the same species depending on several factors such as the ecological niches, climatic conditions and trophic level [15, 16].

Similar studies had been done previously in sesame oil and more than 400 components have been isolated and identified including pyrazines, pyridines, pyrroles, furans, thiophens, thiazoles, carbonyl compounds and others [17, 18].

Recently, in 2010 GC-MS analysis performed on white sesame seeds in Germany and novel aroma-active thiols were found. It includes 2-furfurylthiol, 4-hydroxy-2, 5-dimethyl-3(2h)-furanone, 2-thenylthiol (thiophen-2-yl-methylthiol), and 2-methoxy-4-vinylphenol.

In addition, 9 odor-active thiols were also identified for the first time in roasted sesame seeds including 2-methyl-1-propene-1-thiol, (Z)-3-methyl-1-butene-1-thiol, (E)-3-methyl-1-butene-1-thiol, (Z)-2-methyl-1-butene-1-thiol[19]. Fatty acid analysis was done in different plants by GC-MS including *Sterculia foetida* Linn.[20], L*awsonia inermis* [21], *Tabernaemontana divaricate* [22], *Ziziphus mauritiana* [23], *rocket seed oil* [24], *Datura alba* [25]. In similar manner, seed oil of *Ferulago trachycarpa* Boiss. collected from two different localities was analyzed for their fatty acids by GC-MS.

In this study 9-octadeceneoic acid, 9, 12-octadecadienoic acid, 9-hexadeceneoic acid and 11-octadecenoic acid were found as main components [26]. A comparative analysis of essential oil components of two *Daucus* species from Algeria was done and a total of 67 compounds were found [27].

But this study is important as comparison of genotypes for volatile compounds was done for the first time in sesame. And also important as volatile compounds identification in Indian genotypes of *Sesamum indicum* was done first time.

CONCLUSION: In the present study, total 84 volatile chemical compounds were identified in sesame oil of *Sesamum indicum* by help of GC-MS. Although the number of compounds vary between individual genotypes. The volatile compounds present in almost all genotypes were n-hexadecanoic acid, myristic acid; indole-2-one 2,3-dihydro-N-hydroxy-4-methoxy-3,3-dimethyl-; cyclotrisiloxane, hexamethyl-; acetamide, N-[-4-(trimethylsilyl)phenyl]-; benzene, 2-[(tert-butyldimethylsilyl)oxy]-1-isopropyl-4-methyl-; benzo[h]quinoline, 2,4-dimethyl- and 2-Ethylacridine.

The current study will offer a sound basis of selection of genotypes which are chemically complex and help in effective utilization of sesame. And it laid a foundation for searching chemical compound's nature and application for pharmaceutical, cosmetics and food industry.

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