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GC- MS ANALYSIS OF HEXANE EXTRACTS OF TWO VARIETIES OF SESAME (*SESAMUN INDICUM* L.*)* SEED OIL

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ABSTRACT

The qualitative determination fatty acids from hexane extract of two varieties of sesame seed oil using GC-MS analysis revealed the following fatty acids or white sesame seed oil; 11-octadecenoic acid, Oleic acid, Decanoic acid, Tridecanoic acid, Hexadecanoic acid, Stearic acid, Linolelaidic acid, Arachidic acid, Methyl ricinoleate, Nonenoic acid. While for brown sesame seed oil; Oleic acid, Palmitic acid, Decanoic acid , Stearic acid, Erucic aci , Arachidic acid, Methyl ricinoleate, 11-octadecenoic acid, 10-undecenoic acid, 7-Nonenoic acid were detected. The results were in favour of the utilization of the seed oils in cosmetic industry.

Keywords: Sesame, seed oil, GC-MS, fatty acids, cosmetics.

INTRODUCTION

Sesame, *Sesamum indicum* L. is one of the oldest and important oil seed crop in the world [1]. There are various methods of extracting sesame oil from its seeds from traditional to laboratory scale [2]. There was also a literature report on comparative study of fatty acid extraction methods of sesame (*sesamum indicum* l.) varieties grown under mediterranean environment [3]. Extraction and Characterization of Oil from Sesame Seed was reported [4]. An optimization study for Biodiesel production from Sesamum indicum L. seed oil was also reported [5]. Similarly, Glycerine Analysis of Beniseed (Sesanum Indicum) Oil,Biodiesel and Blends was reported [6]. In this work fatty acid profile of Hexane Extracts of Two Varieties of Sesame (*Sesamun indicum* L.*)* Seed Oil was determine qualitatively using GC-MS analysis in other to show the cosmetic potential of the two seed varieties.

EXPERIMENTAL

SAMPLE COLLECTION, IDENTIFICATION AND PREPARATION

The dried seeds of the two varieties of sesame were deshelled and crushed into powder using mortar and pestle and were stored in a plastic container prior to oil extraction.

OIL EXTRACTION PROCEDURE

The hexane extract was obtained by complete extraction using the Soxhlet extractor (GG-17, SHUNIU). The 50 g of each powdered kernel sample was put into a porous thimble and placed in a Soxhlet extractor, using 150 cm3 of n-hexane (with boiling point of 40- 60°C) as extracting solvent for 6 hours repeatedly until required quantity was obtained. The oil was obtained after evaporation using Water bath at 70^0C to remove the excess solvent from the extracted oil. The oil was then stored in refrigerator prior to GC-MS analysis.

GC-MS ANALYSIS

The analysis of the fatty acids in the *Thevetia peruviana* seed oil sample was done at National Institute of Chemical Technology (NARICT), Zaria, Nigeria, a Shimadzu QP2010 plus series gas chromatography coupled with Shimadzu QP2010 plus mass spectroscopy detector (GCMS) system was used. The temperature programmed was set up from 70°C to 280°C. Helium gas was used as carrier gas. The injection volume was 2 µL with injection temperature of 250°C and a column flow of 1.80 mL/min for the GC. For the mass spectroscopy ACQ mode scanner with scan range of 30-700 amu at the speed of 1478 was used. The mass spectra were compared with the NIST05 mass spectral library [7].

RESULTS

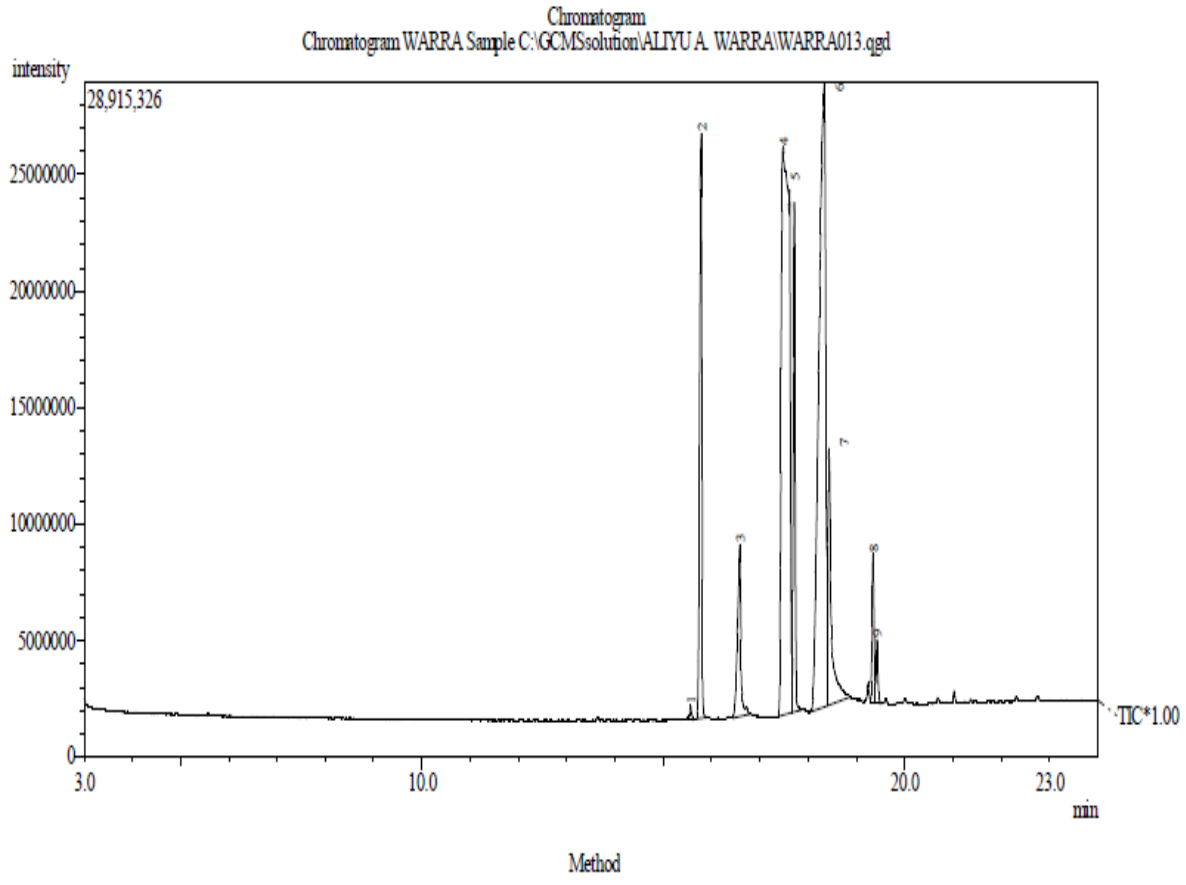
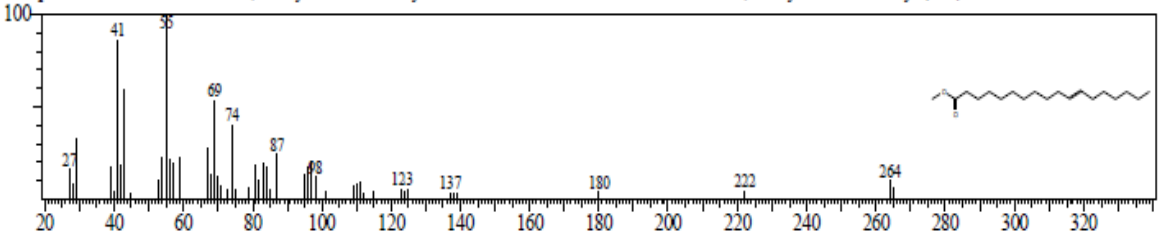


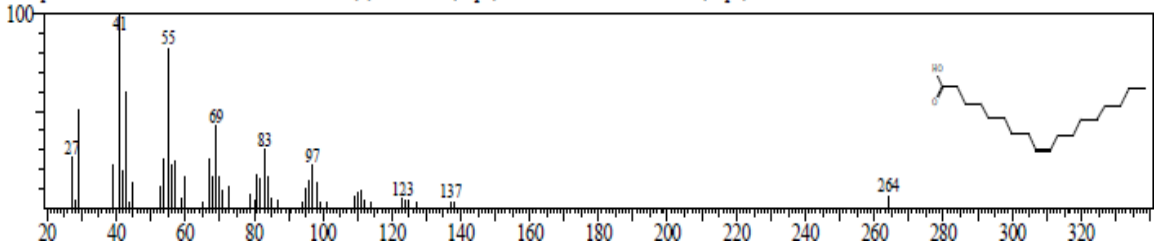
Figure 1: Typical GC-MS total ionic chromatogram (TIC) of hexane extract of white sesame seed oil.

GC-MS Fragments of white sesame seed oil

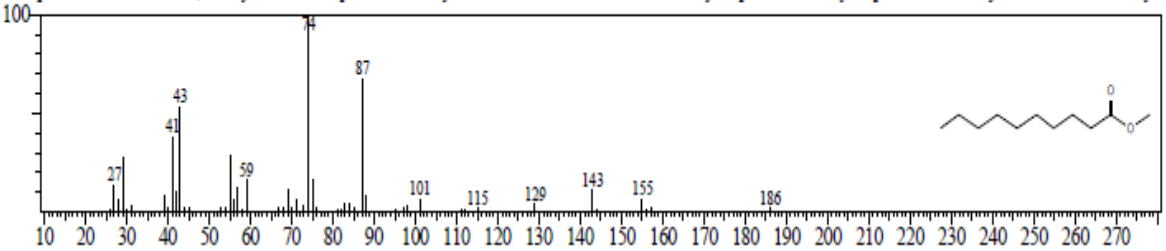
Hit#:1 Entry:98778 Library:NIST05.LIB
SI:91 Formula:C19H36O2 CAS:52380-33-3 MolWeight:296 RetIndex:2085
CompName:11-Octadecenoic acid, methyl ester $$ Methyl 11-octadecenoate $$ Octadec-11-enoic acid, methyl ester $$ Methyl (11E)-11-octadecenoate # $$



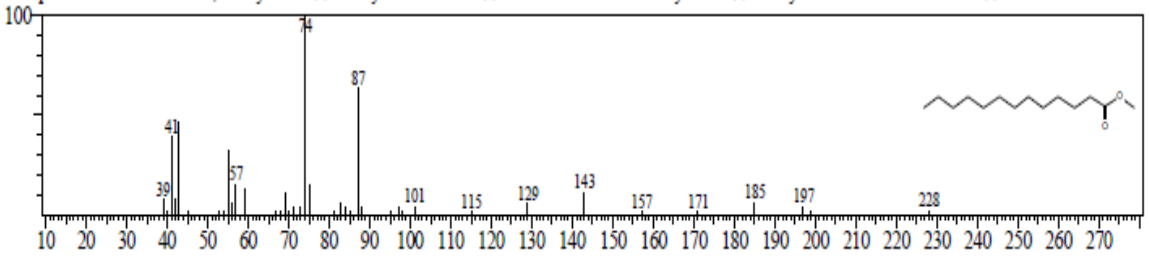
Hit#:3 Entry:22869 Library:NIST05s.LIB
SI:87 Formula:C18H34O2 CAS:112-80-1 MolWeight:282 RetIndex:2175
CompName:Oleic Acid $$ 9-Octadecenoic acid (Z)- $$ .delta.(Sup9)-cis-Oleic acid $$ cis-.delta.(Sup9)-Octadecenoic acid $$ cis-Oleic Acid $$ cis-9-Octadecer



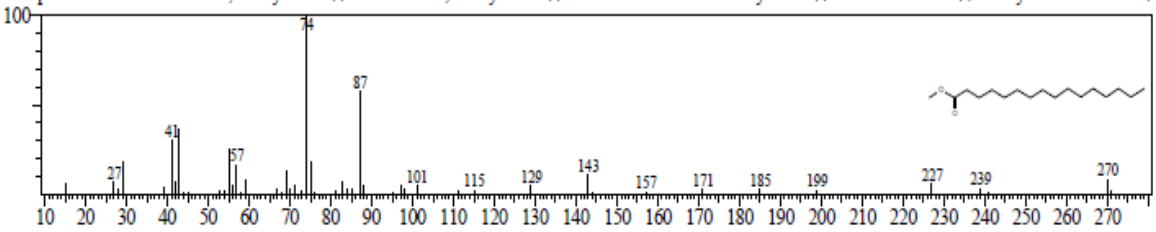
Hit#:2 Entry:14361 Library:NIST05s.LIB
SI:92 Formula:C11H22O2 CAS:110-42-9 MolWeight:186 RetIndex:1282
CompName:Decanoic acid, methyl ester $$ Capric acid methyl ester $$ Metholene 2095 $$ Methyl caprate $$ Methyl caprinate $$ Methyl decanoate $$ Methyl-



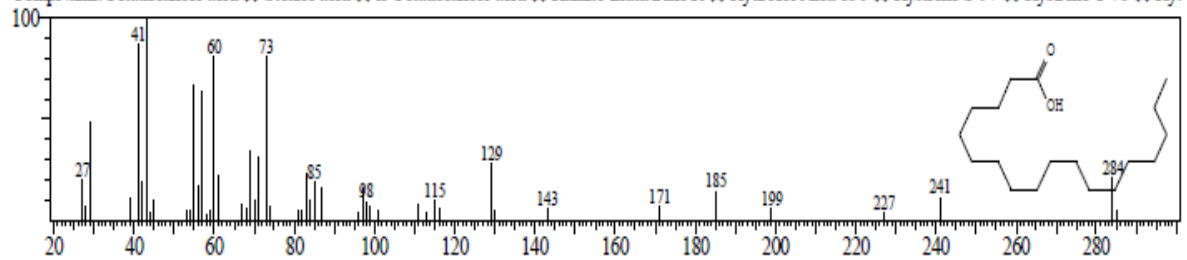
Hit#:4 Entry:19255 Library:NIST05s.LIB
SI:91 Formula:C14H28O2 CAS:1731-88-0 MolWeight:228 RetIndex:1580
CompName:Tridecanoic acid, methyl ester $$ Methyl tridecanoate $$ n-Tridecanoic acid methyl ester $$ Methyl ester of tridecanoic acid $$



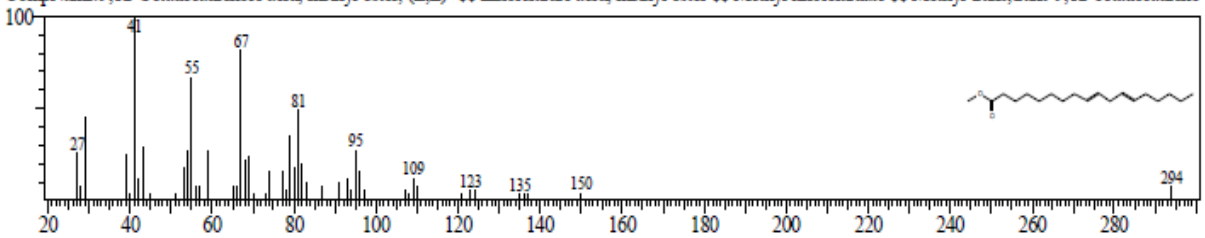
Hit#:5 Entry:22219 Library:NIST05s.LIB
SI:91 Formula:C17H34O2 CAS:112-39-0 MolWeight:270 RetIndex:1878
CompName:Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 2216 $$ Methyl hexadecanoate $



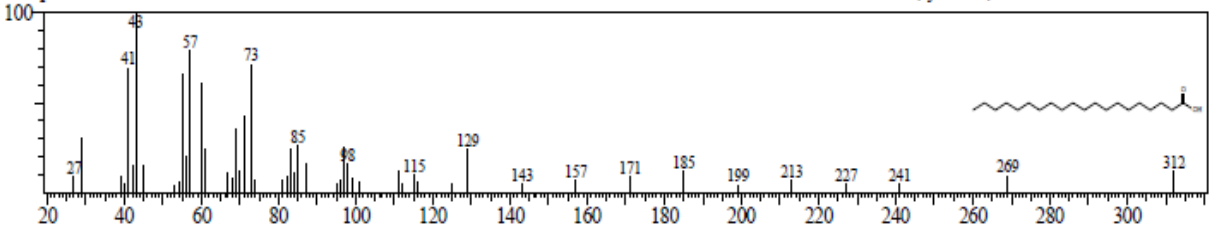
Hit#:4 Entry:22977 Library:NIST05s.LIB
SI:89 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Hunko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $$ Hy



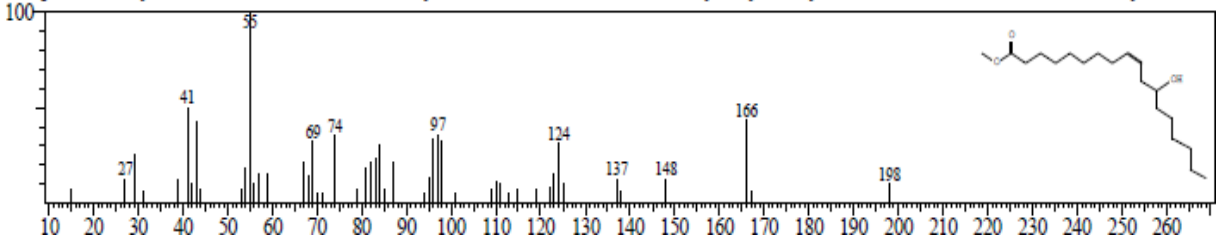
Hit#:3 Entry:97647 Library:NIST05.LIB
SI:89 Formula:C19H34O2 CAS:2566-97-4 MolWeight:294 RetIndex:2093
CompName:9,12-Octadecadienoic acid, methyl ester, (E,E)- $$ Linolelaidic acid, methyl ester $$ Methyl linolelaidate $$ Methyl trans,trans-9,12-octadecadieno



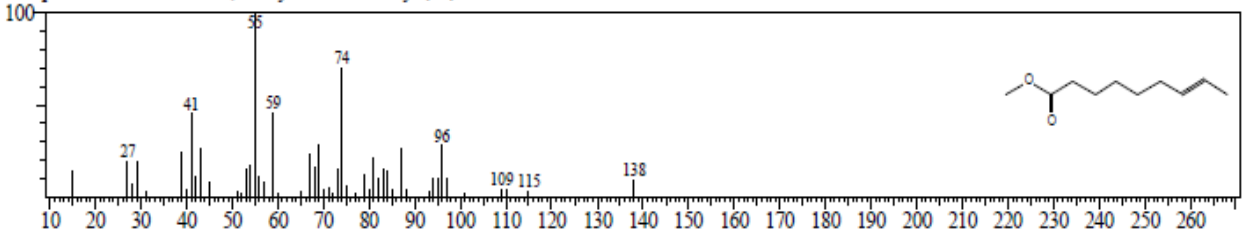
Hit#:5 Entry:108054 Library:NIST05.LIB
SI:87 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic) $$



Hit#:1 Entry:24270 Library:NIST05s.LIB
SI:87 Formula:C19H36O3 CAS:141-24-2 MolWeight:312 RetIndex:2247
CompName:Methyl ricinoleate $$ Ricinoleic acid methyl ester $$ 9-Octadecenoic acid, 12-hydroxy-, methyl ester, [R-(Z)]- $$ Flexricin P-1 $$ Methyl ricinolat



Hit#:5 Entry:24729 Library:NIST05.LIB
SI:85 Formula:C10H18O2 CAS:20731-22-0 MolWeight:170 RetIndex:1191
CompName:7-Nonenoic acid, methyl ester $$ Methyl (7E)-7-nonenoate # $$



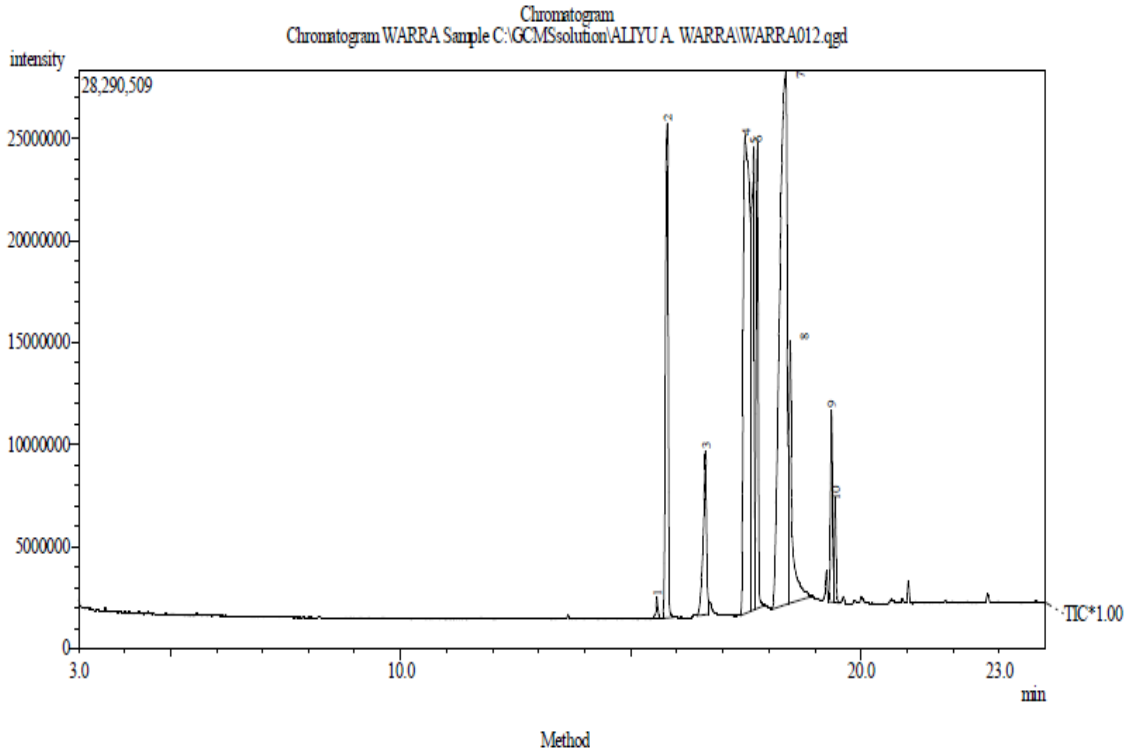
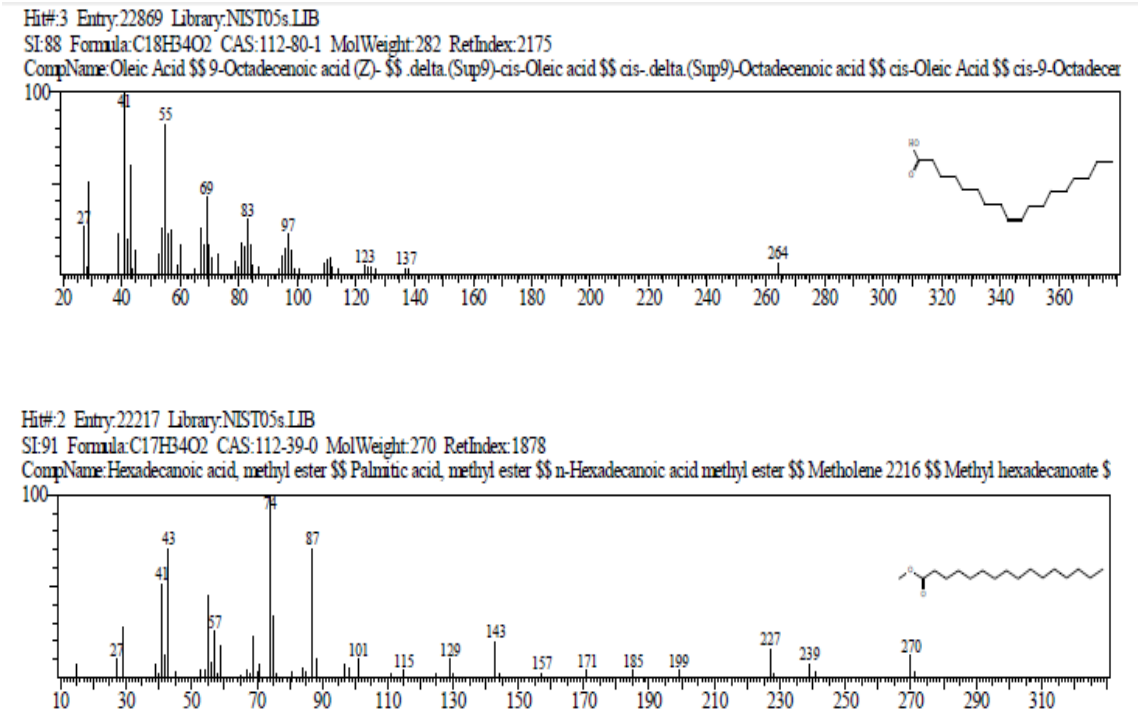
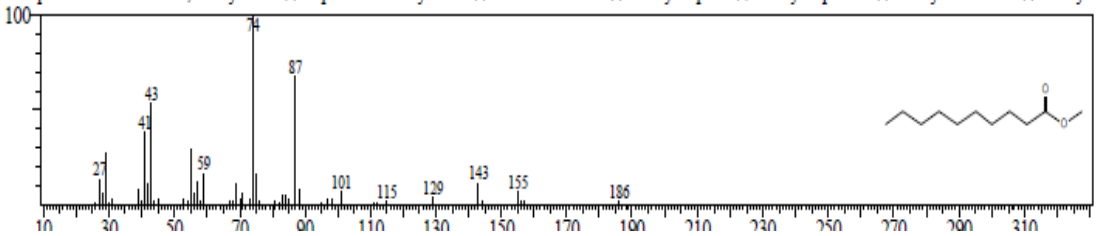


Figure: 2 Typical GC-MS total ionic chromatogram (TIC) of hexane extract of brown sesame seed oil

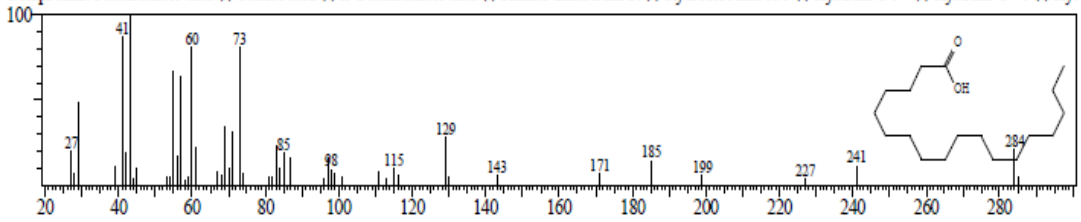
GC-MS fragments of brown sesame seed oil



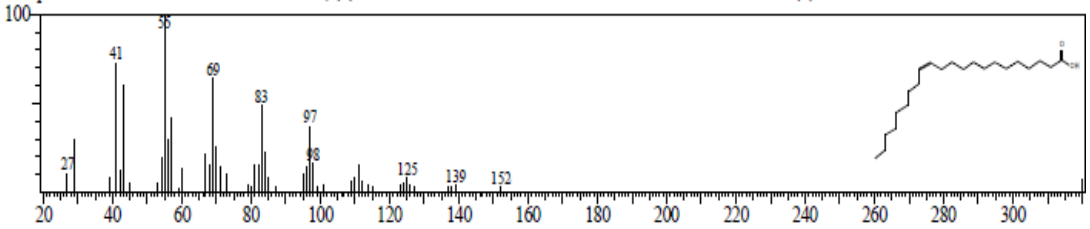
Hit#:4 Entry:14361 Library:NIST05s.LIB
SI:90 Formula:C11H22O2 CAS:110-42-9 MolWeight:186 RetIndex:1282
CompName:Decanoic acid, methyl ester $$ Capric acid methyl ester $$ Metholene 2095 $$ Methyl caprate $$ Methyl caprinate $$ Methyl decanoate $$ Methyl-



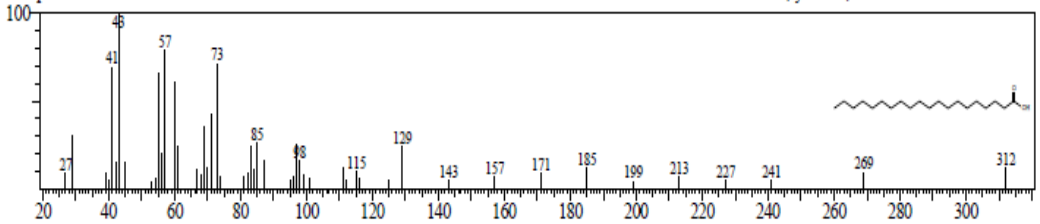
Hit#:4 Entry:22977 Library:NIST05s.LIB
SI:89 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $$ Hys



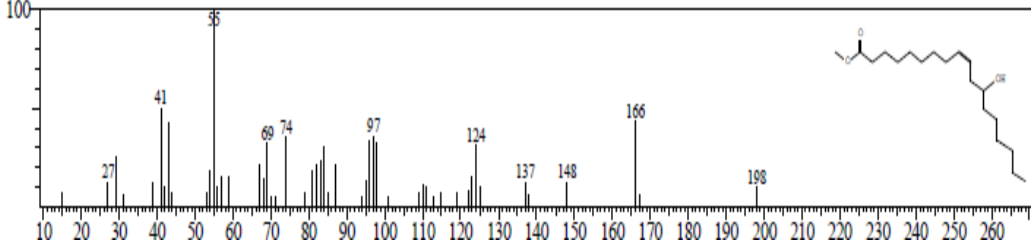
Hit#:2 Entry:121691 Library:NIST05.LIB
SI:91 Formula:C22H42O2 CAS:112-86-7 MolWeight:338 RetIndex:2572
CompName:Erucic acid $$ 13-Docosenoic acid, (Z)- $$ .delta.13-cis-Docosenoic acid $$ cis-13-Docosenoic acid $$ (Z)-13-Docosenoic acid $$ Prifrac 2990 $$



Hit#:5 Entry:108054 Library:NIST05.LIB
SI:87 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic) $$



Hit#:1 Entry:24270 Library:NIST05s.LIB
SI:87 Formula:C19H36O3 CAS:141-24-2 MolWeight:312 RetIndex:2247
CompName:Methyl ricinoleate $$ Ricinoleic acid methyl ester $$ 9-Octadecenoic acid, 12-hydroxy-, methyl ester, [R-(Z)]- $$ Flexricin P-1 $$ Methyl ricinolat



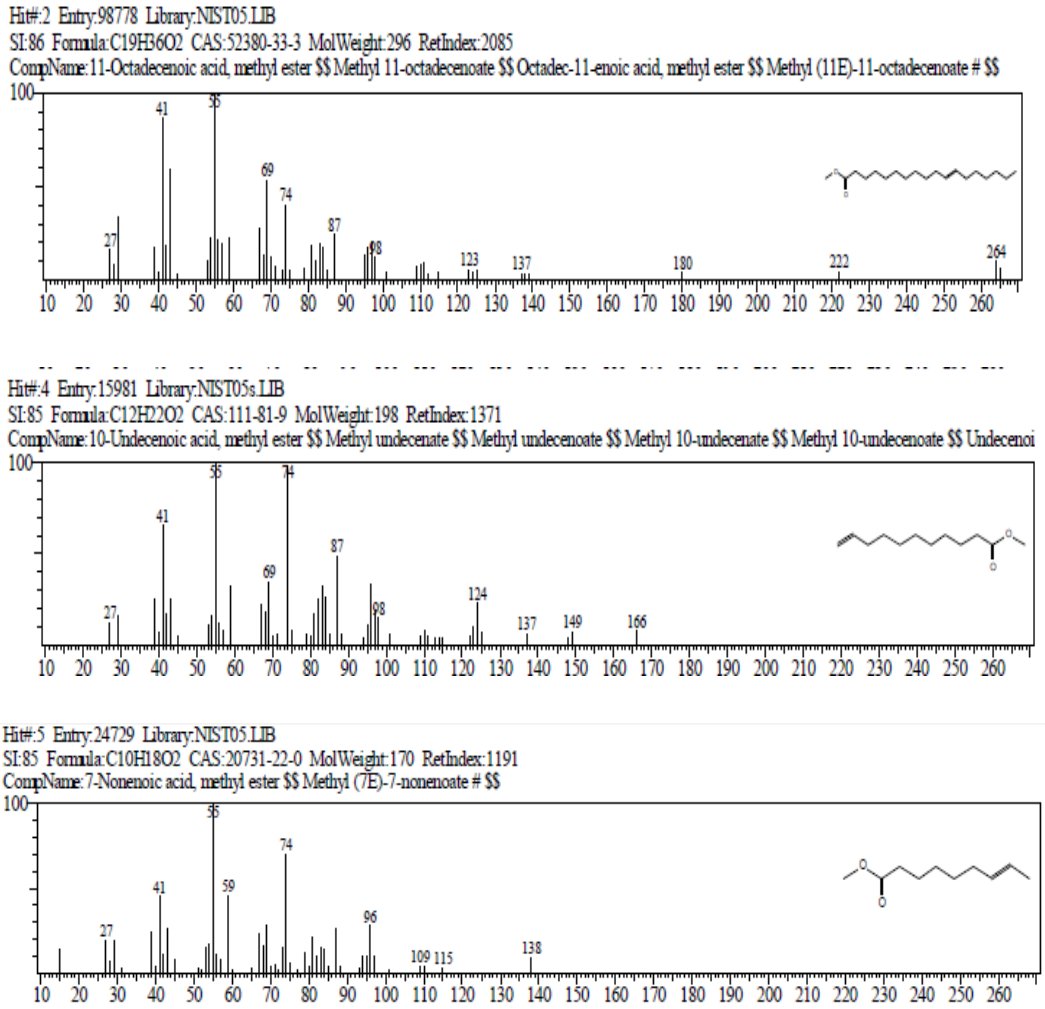


Table: 1 Major fatty acids derived from hexane extract of white sesame seed oil

S. No.	Name of fatty acid	MF	MW	RI	SI% to T.C.
1.	11-octadecenoic acid	$C_{19}H_{36}O_2$	296	2085	91
2.	Oleic acid	$C_{18}H_{34}O_2$	282	2175	87
3.	Decanoic acid	$C_{11}H_{22}O_2$	186	1282	92
4.	Tridecanoic acid	$C_{14}H28O_2$	228	1580	91
5.	Hexadecanoic c acid	$C_{17}H_{34}O_2$	270	1828	91
6.	Stearic acid	$C_{18}H_{36}O_2$	284	2169	89
7.	Linolelaidic acid	$C_{19}H_{34}O_2$	294	2093	89
8.	Arachidic acid	$C_{20}H_{40}O_3$	312	2366	87
9.	Methyl ricinoleate	$C_{19}H_{36}O_2$	312	2247	87
10.	7-Nonenoic acid	$C_{10}H_{18}O_2$	170	1191	85

Note: S/N = Serial number, M.F.= Molecular formula, M.W. = Molecular weight, RI= Retention index SI% = Similarity index, T.C. = Target compound.

Table: 2 Major fatty acids derived from hexane extract of brown sesame seed oil

S. No.	Name of fatty acid	MF	MW	RI	SI% to T.C.
1.	Oleic acid	$C_{18}H_{34}O_2$	282	2175	88
2.	Palmitic acid	$C_{17}H_{34}O_2$	270	1875	91
3.	Decanoic acid	$C_{11}H_{22}O_2$	186	1282	90
4.	Stearic acid	$C_{18}H_{36}O_2$	284	2167	81
5.	Erucic acid	$C_{22}H_{42}O_2$	338	2572	91
6.	Arachidic acid	$C_{20}H_{40}O_2$	312	2366	87
7.	Methyl ricinoleate	$C_{14}H_{36}O_3$	312	2492	92
8.	11-octadecenoic acid	$C_{19}H_{36}O_3$	312	2247	87
9.	10-undecenoic acid	$C_{12}H_{22}O_2$	198	1371	85
10.	7-Nonenoic acid	$C_{10}H_{18}O_2$	170	1191	85

Note: S/N = Serial number, M.F.= Molecular formula, M.W. = Molecular weight, RI= Retention index SI% = Similarity index, T.C. = Target compound.

DISCUSSION

The following major fatty acids were qualitatively identified form the GC-MS analysis; 11-Octadecenoic acid, reported for the first time in a seed oil of *Asclepias syriaca* L. (common milkweed). 11-Octadecenoic acid differs from most natural unsaturated fatty acids in having the double bond at the seventh carbon atom from the methyl end of the chain [8]. Oleic Acid's high lipid count makes it a great moisturizer, and a number of cosmetic companies add it to lotions and soaps in order to boost their ability to nourish the skin [9]. Palmitic acid a natural saturated acid, present in plants, animals, and microorganisms [10]. It is among the fatty acids that is used in concentration in cosmetics [11]. Stearic acid a saturated fatty acid with an 18- carbon chain and the IUPAC name octadecanoic acid was found, Stearic acid is mainly used in the production of detergents, soaps, and cosmetics such as shampoos and shaving cream products. Soaps are not made directly from stearic acid, but indirectly by saponification of triglycerides consisting of stearic acid esters. Esters of stearic acid with ethylene glycol, glycol stearate, and glycol distearate are used to produce a pearly effect in shampoos, soaps, and other cosmetic products. They are added to the product in molten form and allowed to crystallize under controlled conditions. Detergents are obtained from amides and quaternary alkylammonium derivatives of stearic acid. Surfactants, cosmetics and personal hygiene products are in fact prospects of stearic acid [12]. Linolelaidic was also found. Stearolic acid was detected, a fatty acid which supports the growth of anaerobic yeast [13]. Arachidic acid also called eicosanoic acid is a saturated fatty acid was detected. It is found in appreciable quantities only in some vegetable fats and oils where it occurs as glycerol ester [14]. Erucic acid was also found, products produced using erucic acid include cosmetics [15].

CONCLUSION

The results of the fatty acid composition of the two varieties of sesame seed oil through GC-MS analysis indicated their suitability for industrial production of cosmetic products

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