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GC-MS analysis of *Majidea zanquebarica J.Krikex Oliv.* (Sapindaceae) seed extract

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Abstract

Introduction: To identify the various phyto constituents present in the unexplored plant *Majidea zanquebarica* by using gas chromatography and mass spectrometry.

Methods: Hexane seed extract of this plant was analyzed using Gas Chromatography–Mass Spectrometry, while the mass spectra of the compounds found in the extract was matched with the National Institute of Standards and Technology (NIST) library.

Result: Gas chromatography mass spectrometry (GC-MS) analysis revealed the presence of eight compounds. In GC-MS analysis, some of the phytocomponents screened were 10- Undecanal, 2-methyl-2, 2,6,10,15,19,23-Hexamethyl, 2,6,10,14,18,22-Tetracosa, 9,12- Octadecadienoic acid, Methylester, Hexadecanoic acid, ethylesters Ethylpalm. The compounds were identified by comparing their retention time and peak area with that of literature and by interpretation of mass spectra. Many of them are used in industry for various applications like flavor, antioxidant, anti-inflammatory, antimicrobial, pesticide and cancer preventive.

Keywords: *Majidea zanquebarica*, GC-MS, Hexadecanoic acid and various applications

INTRODUCTION

Presences of bioactive secondary metabolites in the medicinal plants are more responsible to cure several diseases in mankind[1]. Plants are described as "nature's chemical factories" which may contain natural substances that exhibit bioactive properties by producing a definite physiological action on the human body when administered[2].

Herbal medicine, based on their traditional uses in the form of powders, liquids or mixtures, has been the basis of treatment for various ailments in India since ancient times[3]. The medicinal plants are reliable sources for the treatment of many health problems. Man has depended a lot on herbs in the past, and even at the present. For future health challenges, plants are reasonably prepared to serve man. The only need is to develop the isolation and purification techniques. The medicinal value of plants is due to the phytochemical constituents they produce. Several studies have reported elemental contents in plant extracts, which are consumed by us either as an herbal health drink or medicine[4]. In general, these secondary metabolites are an important source with a variety of structural arrangements and properties[5].

A knowledge of the chemical constituents of plants is desirable not only for the discovery of therapeutic agents, but also because such information may be of great value in disclosing new sources of economic phytocompounds for the synthesis of complex chemical substances and for discovering the actual significance of folkloric remedies[6]. Hence a thorough validation of the herbal drugs has emerged as a new branch of science emphasizing and prioritizing the standardization of the natural drugs and products because several of the phytochemicals have complementary and overlapping mechanism of action. Chromatography is the term used to describe a separation technique in which a mobile phase carrying a mixture is caused to move in contact with a selectively absorbent stationary phase. It also plays a fundamental role as an analytical technique for quality control and standardization of phyto therapeuticals[7].

In recent years GC-MS studies have been increasingly applied for the analysis of medicinal plants as this technique has proved to be a valuable method for the analysis of non polar components and volatile essential oil, fatty acids, lipids[8] and alkaloids[9].

(GC–MS) has been applied unambiguously to identify the structures of different phytoconstituents from plant extracts and biological samples with great success[11-12] Gas chromatography and mass spectrum is a reliable technique to identify the phytoconstituents of volatile matter, long chain branched hydrocarbons, alcohols, acids and esters[13].The Sapindaceae family is known for its traditional medicinal uses as a diuretic, stimulant, expectorant, natural surfactant, sedative, vermifuge and against stomachache and dermatitis in many parts of the world. Chemical investigations of this family have led to the isolation of saponins, diterpenes and flavonoids, among other secondary metabolites. Several saponins and acyclic sesquiterpene and diterpene oligoglycosides have been isolated as main secondary metabolites of several Sapindaceae species used in traditional oriental medicine[14]. One such tree *Majidea zanquebarica J.Krikex Oliv* (Sapindaceae)Syn. *Harpullia zanquebarica* is a medicinal tree, *Harpullia* species are used as hair wash and excellent source of leech repellent, fish poison, as antirheumatic and to prevent leech bites[15]. However, there is no report regarding this plant. Therefore, the aim of the present work was to analysis the bioactive compound from seed hexane extract of *M. zanquebarica* by Gas chromatography and mass spectrum.

2. MATERIALS AND METHODS

Plant material

The healthy and matured seeds of *M. zanquebarica* were collected From Coimbatore district Tamil Nadu and identified by Botanical Survey of India, Tamil Nadu.

Extraction of plant material

Plant materials thoroughly washed and shade dried at room temperature after that grind into powder was packed with No.1 Whatman filter paper and placed in soxhlet apparatus along with hexane. The crude extract were collected and dried at room temperature, 30˚C after which yield was weighed and then performed.

Gas chromatography and mass spectrum analysis

Gas chromatography (GC) analysis was carried out at South Indian Textile Research Institute (SITRA), Coimbatore. It is one of the key techniques generally used for screening/ identification of many groups of plant phytochemicals. The high attainable separation power in combination with wide range of the detectors that are employed in various detection principles can be coupled. Gas chromatography is an important, often irreplaceable tool in the phytochemical analysis even at trace level of plant chemical compounds. Gas chromatography study includes the important optimization process such as i) introduction of sample extract onto the GC column, ii)separation of its components on an analytical column and iii) detection of target analysis by using mass spectrometric(MS) detector. The extracts were then subjected into GC-MS analysis. Chromatographic separation was carried out with CE GC 8000 top MSMD8000 Fyson instrument with Db 35 mr column (10 m x 0.5mm, 0.25 µm film thicknesses). Heating programs were executed from 100 - 250 ^{0}C at 3 minutes by using the helium gas as a carrier gas with a flow rate of 1ml/minute in the split mode (1:50). An aliquot (2 µl) of oil was injected into the column with the injector heater at 250^{0}C. Injection temperature at 250°C, interface temperature at200°C, quadruple temperature at 150°C and ion source temperature at 230°C were maintained. Injection was performed in split less mode. The mass spectra of compounds in samples were obtained by electron ionization(EI) at 70 eV and the detector operated in scan mode from 20 to 600 atomic mass units (amu). Identifications were based on the molecular structure, molecular mass and calculated fragmentations. Resolved spectra were identified for phytochemicals by using the standard mass spectral database of WILEY and NIST.

Identification of components

Identification was based on the molecular structure, molecular mass and calculated fragments. Interpretation on mass spectrum GC-MS was conducted using the database of National Institute Standard and Technology (NIST) having more than 62,000 patterns. The name, molecular weight and structure of the components of the test materials were ascertained. The relative percentage amount of each component was calculated by comparing its average peak area to the total areas. The spectrum of the unknown component was compared with the spectrum of the component stored in the NIST library version (2005), software, Turbomas 5.2.

This is done in order to determine whether this plant species contains any individual compound or group of compounds, which may substantiate its current commercial and traditional use as an herbal medicine. Further it helps to determine the most appropriate methods of extracting these compounds. These results will consequently be discussed in the light of their putative biological or therapeutic relevance.

RESULT

The gas chromatograms of seed hexane extract of *M. zanquebarica* confirmed the presence of various interesting compounds with different retention times as illustrated in Figures 1, 2, and 3. These compounds were identified through mass spectrometry attached with GC. The identified compounds and their retention time, molecular formula, molecular weight, peak area (%), structure, category of the compound, and activities related with medicinal uses are given in Tables 1. The compound prediction is based on Dr. Duke's Phytochemical and Ethnobotanical Databases. Eight compounds were detected in the methanolic leaf extract of *M. zanquebarica*. Among them, the most prevailing major compounds were 10- Undecanal, 2-Buten-1-ol,3-Methyl(cas) Prenol, 2-methyl-2, 2,6,10,15,19,23-Hexamethyl, 2,6,10,14,18,22-Tetracosa, Eicosane(cas) N-Eicosane, Nonadecane N-Nonadecane, 1-Tetradecanol-Alfol 14, Tetradecanol, 9,12-Octadecadienoic acid,Methylester, Hexadecanoic acid, ethylesters Ethylpalm.

DISCUSSION

The gas chromatogram shows that the relative concentrations of various compounds are getting eluted as a function of retention time. The height of the peaks indicates the relative concentrations of the compounds present in the plant. The mass spectrometer analyzes of the compounds eluted at different times to identify the nature and structure of the compounds. The conversion of larger compound fragments into smaller compounds gives rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. Generally, the reliability of medicinal plant for its usage is evaluated by correlating the phytochemical compounds with their biological activities [14]. In the present study, the GCMS analysis of the seed hexane extract of *Majidea zhanquebarica* altogether showed the presence of 8 compounds. 10-undecenal also posses antimicrobial, antifungal, anti-inflammatory and anticancer activity[16].

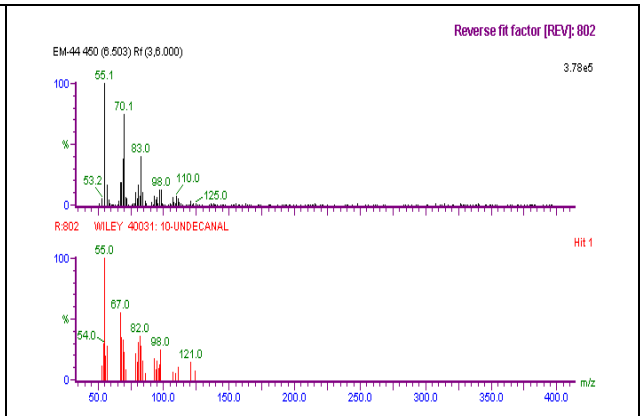
Octadecanoic acid which is regarded as linolic acid in nature, posses antioxidant, antimicrobial, anti-inflammentory, nematicide, insectifuge, hypocholesteromic, cancer preventive, hepatoprotective, antiacne, antihistaminic and antiarthritic[17].

The compounds identified possess many biological properties for instance, 9,12-Octadecadienoic acid (Z,Z) – Linolenic acid (R/T 20.19) is an essential fatty acid so called because they are necessary for health, and they cannot be produced within the human body. They must be acquired through diet[18] and 9-Octadecenoic acid (Z)-,methyl ester, a fatty acid ester (R/T 17.07) both possess Antiinflammatory, Nematicide, Insectifuge, Hypocholesterolemic, Cancer preventive, Hepatoprotective, Antihistaminic, Antiacne, Antiarthritic, Antieczemic, 5-Alpha reductase inhibitor, Antiandrogenic,

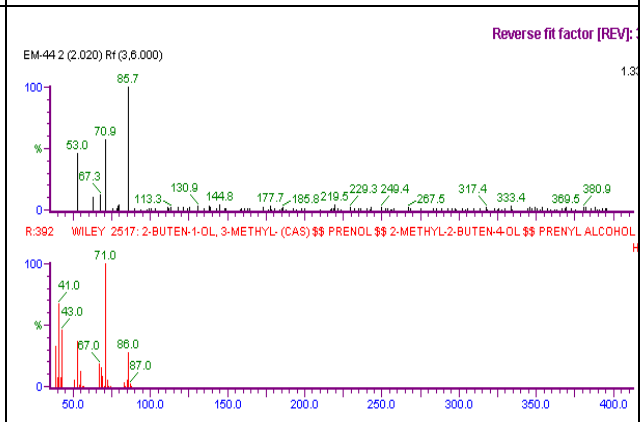
Anticoronary properties. n-Hexadecanoic acid – palmitic acid (R/T 15.83) can be an Antioxidant, Hypocholesterolemic, Nematicide, Pesticide, Lubricant, Antiandrogenic, Flavor, Hemolytic, 5-Alpha reductase inhibitors. n-Hexadecanoic acid or Palmitic acid is used to produce soaps, cosmetics, and release agents[19]. Hydrogenation of palmitic acid yields acetyl alcohol, which is used to produce detergents and cosmetics. Sodium palmitate is permitted as a natural additive in organic products[20]. Hexadenoic acid has earlier been reported as a component in alcohol extract of the leaves of *Kigelia pinnata*[21]. Octanoic acid tridec-2eny ester also called Caprylic acid. is used commercially in the production of perfumes and also in the manufacture of dyes[22].

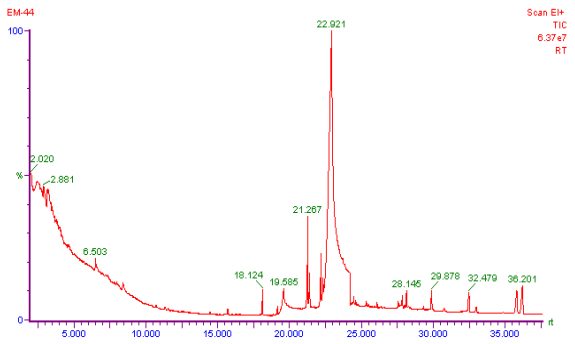
Table 1: GC-MS analysis revealed the presence of phytochemical components in hexane seed extract of *M. zanquebarica*

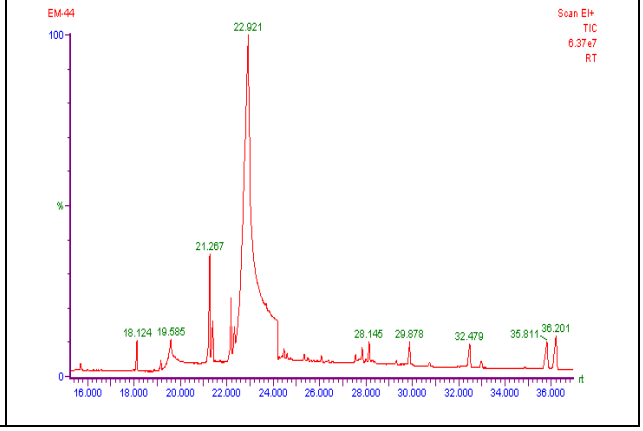
Hit	Compound Name	Formula	M.W.
1	10-UNDECANAL	C11H20O	168
2	1,2-EPOXY-4-VINYLCYCLODODECENE	C14H24O	208
3	7-METHYLBICYCLO[3.2.1]OCTANE-1-OL	C9H16O	140
4	1,2,3,5-TETRAMETHYLCYCLOHEXANE (1R,2T,3T,5C)	C10H20	140
5	DECANAL (CAS) $$ N-DECANAL $$ DECYL ALDEHYDE $$ DE	C10H20O	156
6	ETHYLIDENECYCLODODECANE	C14H26	194
7	1-PENTATRIACONTANOL	C35H72O	508
8	TRIDECANAL	C13H26O	198
9	.BETA.-CITRONELLOL $$ 6-OCTEN-1-OL, 3,7-DIMETHYL- (CA	C10H20O	156
10	Z,Z-6,28-HEPTATRIACTONTADIEN-2-ONE	C37H70O	530
11	(Z)-9-HYDROXY-4-METHYL-7-NONENOIC ACID LACTONE	C10H16O2	168
12	DECENAL	C10H18O	154
13	(R)-(-)-(Z)-14-METHYL-8-HEXADECEN-1-OL	C17H34O	254
14	3-METHYL-2-(2-OXOPROPYL)FURAN	C8H10O2	138
15	DODECANAL (CAS) $$ N-DODECANAL $$ 1-DODECANAL $$ L	C12H24O	184
16	1,2,3,5-TETRAMETHYLCYCLOHEXANE (1R,2T,3C,5T)	C10H20	140
17	2-OCTENE, 4-ETHYL-, (E)-	C10H20	140
18	13-TETRADECENAL	C14H26O	210
19	CYCLOPROPANE, 1-(1,2-DIMETHYLPROPYL)-1-METHYL-2-N	C18H36	252
20	N-(5-AZIDOPENTYL)-4-METHYL-4-VINYLAZETIDIN-2-ONE	C11H18ON4	222



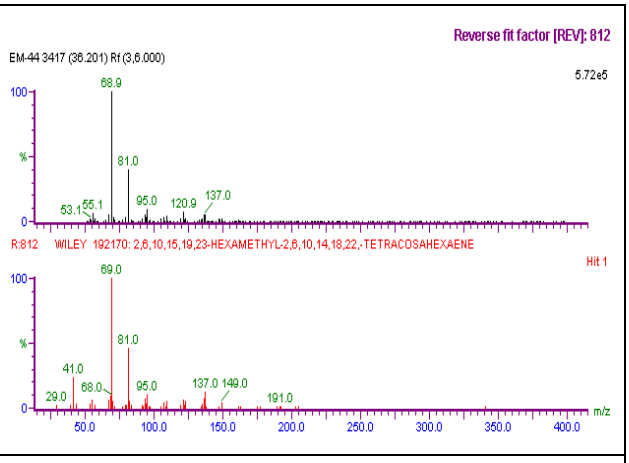
Hit	Compound Name	Formula	M.W.
1	GERMACRA-4E,1(10)E-DIENE-12,8-.BETA.-OLIDE	C14H22O2	222
2	2-BUTEN-1-OL, 2-METHYL- (CAS) $$ 2-METHYL-BUT-2-ENE-1-	C5H10O	86
3	1-BUTENE, 1-METHOXY-	C5H10O	86
4	2-BUTEN-1-OL, 2-METHYL- (CAS) $$ 2-METHYL-BUT-2-ENE-1-	C5H10O	86
5	2-BUTEN-1-OL, 2-METHYL-	C5H10O	86
6	2-BUTEN-1-OL, 3-METHYL- (CAS) $$ PRENOL $$ 2-METHYL-2	C5H10O	86
7	2-BUTEN-1-OL, 3-METHYL- (CAS) $$ PRENOL $$ 2-METHYL-2	C5H10O	86
8	1-PENTYN-3-ONE, 4-METHYL-	C6H8O	96
9	6-NITRO-7-ETHOXY-4,7-DIHYDRO-1,2,4-TRIAZOLO 5,1-C 1,2,	C6H8O3N6	212
10	5-HEPTEN-3-ONE, 5-ETHYL-2-METHYL-	C10H18O	154
11	PREGNAN-1-OL, 3-(METHYLAMINO)-, (1.ALPHA.,3.ALPHA.,5.A	C22H39ON	333
12	4 OR 5 METHYL 3 FURANTHIOL	C5H10OS	118
13	TYROSINE, N- N- N-(1-ADAMANTYLCARBONYL)-GLYCYL -L-LE	C29H41O6N3	527
14	3-PENTEN-2-OL	C5H10O	86
15	3-PENTEN-2-OL (CAS) $$ 2-PENTEN-4-OL $$ METHYL PROP	C5H10O	86
16	THIAZOLE, 4-ETHYL-2-METHYL-	C6H9NS	127
17	2-BUTENE, 1-METHOXY-, (E)-	C5H10O	86
18	2-HEXENE, 1-METHOXY-, (E)-	C7H14O	114
19	1,5,7-OCTATRIEN-3-OL, 3,7-DIMETHYL-	C10H16O	152
20	THIAZOLE, 2,4,5-TRIMETHYL-	C6H9NS	127





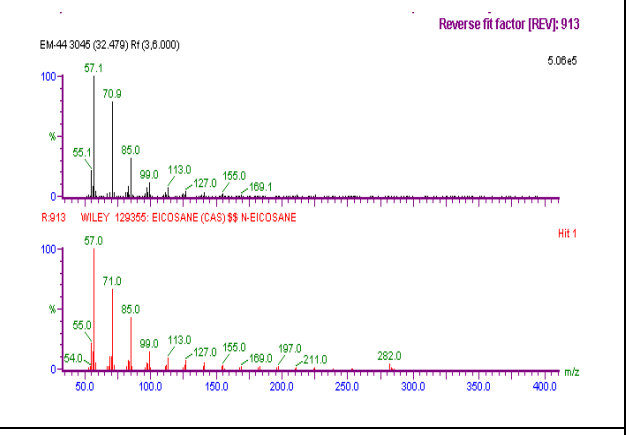


Hit	Compound Name	Formula	M.W.
1	2,6,10,15,19,23-HEXAMETHYL-2,6,10,14,18,22,-TETRACOSA	C30H50	410
2	2,6,10,14,18,22-TETRACOSAHEXAENE, 2,6,10,15,19,23-HEX	C30H50	410
3	LYCOPERSEN $$ .PSI.,.PSI.-CAROTENE, 7,7',8,8',11,11',12,1	C40H66	546
4	2,6,10,14,18,22-TETRACOSAHEXAENE, 2,6,10,15,19,23-HEX	C30H50	410
5	3,7,11-TRIDECATRIENENITRILE, 4,8,12-TRIMETHYL-	C16H25N	231
6	10-DEMETHYLSQUALENE $$ 2,6,10,14,18,22-TETRACOSAH	C29H48	396
7	3,7,11-TRIDECATRIENENITRILE, 4,8,12-TRIMETHYL- (CAS) $	C16H25N	231
8	2,6,10-DODECATRIEN-1-OL, 3,7,11-TRIMETHYL-, (E,E)-	C15H26O	222
9	FARNESOL 3	C15H26O	222
10	2,6,10,14,18,22,26,30-DOTRIACONTAOCTAEN-1-OL, 3,7,11,1	C40H66O	562
11	SQUALENE	C30H50	410
12	3,7,11-TRIDECATRIENOIC ACID, 4,8,12-TRIMETHYL-, METHY	C17H28O2	264
13	3,7,11-TRIDECATRIENOIC ACID, 4,8,12-TRIMETHYL-, METHY	C17H28O2	264
14	3,7,11-TRIDECATRIENOIC ACID, 4,8,12-TRIMETHYL-, METHY	C17H28O2	264
15	2,6,10-DODECATRIENOIC ACID, 3,7,11-TRIMETHYL-, METHY	C16H26O2	250
16	6,10,14-HEXADECATRIEN-1-OL, 3,7,11,15-TETRAMETHYL-,	C20H36O	292
17	METHYL (2E,6E)-3,7,11-TRIMETHYL-2,6,10-DODECATRIENO	C16H26O2	250
18	6,10,14-HEXADECATRIEN-1-OL, 3,7,11,15-TETRAMETHYL-, [	C20H36O	292
19	2-(FENCH-2-YL)FENCHANE	C20H34	274
20	6,10,14-HEXADECATRIENOIC ACID, 3,7,11,15-TETRAMETHY	C21H36O2	320

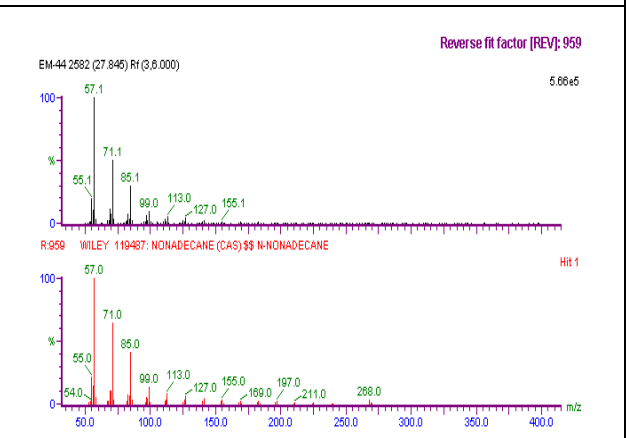


Sample ID: SEED EXTRACTION - HEXANE **Acquired at 15-May-200917:01:24**

Hit	Compound Name	Formula	M.W.
1	EICOSANE (CAS) $$ N-EICOSANE	C20H42	282
2	DOCOSANE (CAS) $$ N-DOCOSANE $$ C22H46 STANDARD	C22H46	310
3	HENEICOSANE (CAS) $$ N-HENEICOSANE	C21H44	296
4	NONADECANE (CAS) $$ N-NONADECANE	C19H40	268
5	DECANE, 2-METHYL- (CAS) $$ 2-METHYLDECANE $$ 2-MET	C11H24	156
6	TRIACONTANE (CAS) $$ N-TRIACONTANE	C30H62	422
7	HEXATRIACONTANE (CAS) $$ N-HEXATRIACONTANE	C36H74	506
8	NONACOSANE (CAS) $$ N-NONACOSANE $$ CELIDONIOL, D	C29H60	408
9	TRITETRACONTANE	C43H88	604
10	PENTACOSANE (CAS) $$ N-PENTACOSANE	C25H52	352
11	OCTACOSANE (CAS) $$ N-OCTACOSANE	C28H58	394
12	TRITETRACONTANE (CAS) $$ N-TRIATETRACONTANE	C43H88	604
13	HENTRIACONTANE (CAS) $$ UNTRIACONTANE $$ N-HENTRI	C31H64	436
14	HENTRIACONTANE (CAS) $$ UNTRIACONTANE $$ N-HENTRI	C31H64	436
15	NONACOSANE (CAS) $$ N-NONACOSANE	C29H60	408
16	HEXACOSANE (CAS) $$ N-HEXACOSANE	C26H54	366
17	TRITRIACONTANE (CAS) $$ N-TRITRIACONTANE	C33H68	464
18	TRICOSANE (CAS) $$ N-TRICOSANE	C23H48	324
19	HEPTADECANE, 2,6,10,15-TETRAMETHYL-	C21H44	296
20	HENEICOSANE (CAS) $$ N-HENEICOSANE	C21H44	296

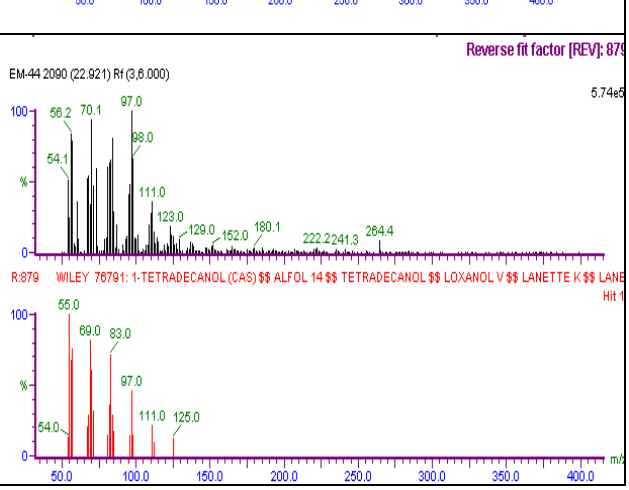


Hit	Compound Name	Formula	M.W.
1	NONADECANE (CAS) $$ N-NONADECANE	C19H40	268
2	EICOSANE (CAS) $$ N-EICOSANE	C20H42	282
3	HENEICOSANE (CAS) $$ N-HENEICOSANE	C21H44	296
4	DOCOSANE (CAS) $$ N-DOCOSANE $$ C22H46 STANDARD	C22H46	310
5	DECANE, 2-METHYL- (CAS) $$ 2-METHYLDECANE $$ 2-MET	C11H24	156
6	TRITETRACONTANE	C43H88	604
7	TRITETRACONTANE (CAS) $$ N-TRIATETRACONTANE	C43H88	604
8	NONACOSANE (CAS) $$ N-NONACOSANE $$ CELIDONIOL, D	C29H60	408
9	PENTACOSANE (CAS) $$ N-PENTACOSANE	C25H52	352
10	OCTACOSANE (CAS) $$ N-OCTACOSANE	C28H58	394
11	HENTRIACONTANE (CAS) $$ UNTRIACONTANE $$ N-HENTRI	C31H64	436
12	EICOSANE (CAS) $$ N-EICOSANE	C20H42	282
13	TRICOSANE (CAS) $$ N-TRICOSANE	C23H48	324
14	HENEICOSANE (CAS) $$ N-HENEICOSANE	C21H44	296
15	TRITRIACONTANE (CAS) $$ N-TRITRIACONTANE	C33H68	464
16	HEPTADECANE, 2,6,10,15-TETRAMETHYL-	C21H44	296
17	HEPTADECANE, 2,6,10,15-TETRAMETHYL- (CAS) $$ 2,6,10,1	C21H44	296
18	NONADECANE (CAS) $$ N-NONADECANE	C19H40	268
19	TETRATETRACONTANE (CAS) $$ N-TETRATETRACONTANE	C44H90	618
20	TETRATETRACONTANE	C44H90	618



Sample ID: SEED EXTRACTION - HEXANE **Acquired at 15-May-200917:01:24**

Hit	Compound Name	Formula	M.W.
1	1-TETRADECANOL (CAS) $$ ALFOL 14 $$ TETRADECANOL $	C14H30O	214
2	1-TRIDECANOL	C13H28O	200
3	(TRANS)-2-NONADECENE	C19H38	266
4	1-UNDECANOL (CAS) $$ N-UNDECANOL $$ 1-HENDECANOL $	C11H24O	172
5	1-DODECANOL (CAS) $$ N-DODECANOL $$ CO 12 $$ S 1298	C12H26O	186
6	1-ETHYL-2-METHYL CYCLODODECANE $$ CYCLODODECAN	C15H30	210
7	(CIS)-2-NONADECENE	C19H38	266
8	ACETIC ACID, DECYL ESTER (CAS) $$ DECYL ACETATE $$	C12H24O2	200
9	1-NONANOL (CAS) $$ N-NONYL ALCOHOL $$ N-NONANOL $$	C9H20O	144
10	1-TETRADECANOL, ACETATE (CAS) $$ TETRADECYL ACET	C16H32O2	256
11	1-DODECENE (CAS) $$ ADACENE 12 $$ N-DODEC-1-ENE $$.	C12H24	168
12	1-DECANOL (CAS) $$ DECYL ALCOHOL $$ T 148 $$ ALFOL 1	C10H22O	158
13	1-OCTANOL (CAS) $$ OCTILIN $$ ALFOL 8 $$ SIPOL L8 $$ N-	C8H18O	130
14	OCT-7-EN-4-ONE N,N-DIMETHYLHYDRAZONE	C10H20N2	168
15	1-HEXADECANOL (CAS) $$ CETAL $$ ETHAL $$ ETHOL $$ C	C16H34O	242
16	9-OCTADECENOIC ACID (Z)- (CAS) $$ OLEIC ACID $$ RED OI	C18H34O2	282
17	UNDECENAL (CAS) $$ UNDECENOIC ALDEHYDE $$ UNDECY	C11H20O	168
18	CYCLODODECANE (CAS)	C12H24	168
19	1-HENEICOSYL FORMATE	C22H44O2	340
20	6-TERT-BUTYL-2,3,4,5-TETRAHYDROPYRIDINE $$ PYRIDINE	C9H17N	139



Sample ID: SEED EXTRACTION - HEXANE Acquired at 15-May-200917:01:24

Hit	Compound Name	Formula	M.W.
1	1,11-CYCLOEICOSADIENE	C20H36	276
2	11-ACETOXY-2-UNDECENE	C13H24O2	212
3	9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER (CAS)	C19H34O2	294
4	(E)-4-TRIDECENYLACETATE	C15H28O2	240
5	9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER (CAS)	C19H34O2	294
6	LINOLEIC ACID ETHYL ESTER	C20H36O2	308
7	ETHYL LINOLEATE $$ LINOLEIC ACID, ETHYL ESTER $$ ET	C20H36O2	308
8	2-CHLOROETHYL LINOLEATE	C20H35O2Cl	342
9	2-CHLOROETHYL LINOLEATE	C20H35O2Cl	342
10	ETHYL LINOLEATE $$ LINOLEIC ACID, ETHYL ESTER $$ ET	C20H36O2	308
11	9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER (CAS)	C19H34O2	294
12	ETHYL LINOLEATE $$ LINOLEIC ACID, ETHYL ESTER $$ ET	C20H36O2	308
13	CYCLODECENE (CAS)	C10H18	138
14	9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER (CAS)	C19H34O2	294
15	9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER	C19H34O2	294
16	9,12-OCTADECADIENOIC ACID, METHYL ESTER, (E,E)- (CAS)	C19H34O2	294
17	9,12-OCTADECADIENOIC ACID (Z,Z)- (CAS) $$ LINOLEIC ACID	C18H32O2	280
18	8,11-OCTADECADIENOIC ACID, METHYL ESTER	C19H34O2	294
19	9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER (CAS)	C19H34O2	294
20	CIS-LINOLEIC ACID METHYL ESTER	C19H34O2	294

Hit	Compound Name	Formula	M.W.
1	TETRADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL MY	C16H32O2	256
2	HEXADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL PALM	C18H36O2	284
3	TETRADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL MY	C16H32O2	256
4	OCTADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL STEA	C20H40O2	312
5	HEPTADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL N-H	C19H38O2	298
6	DODECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL LAURAT	C14H28O2	228
7	HEXADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL PALM	C18H36O2	284
8	ETHYL TRIDECANOATE	C15H30O2	242
9	PENTADECANOIC ACID, ETHYL ESTER $$ ETHYL PENTADE	C17H34O2	270
10	TETRADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL MY	C16H32O2	256
11	HEXADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL PALM	C18H36O2	284
12	DODECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL LAURAT	C14H28O2	228
13	DECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL DECANOAT	C12H24O2	200
14	DODECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL LAURAT	C14H28O2	228
15	PENTADECANOIC ACID, ETHYL ESTER	C17H34O2	270
16	DODECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL LAURAT	C14H28O2	228
17	NONANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL NONANOA	C11H22O2	186
18	HEXADECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL PALM	C18H36O2	284
19	UNDECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL UNDECY	C13H26O2	214
20	DECANOIC ACID, ETHYL ESTER (CAS) $$ ETHYL DECANOAT	C12H24O2	200

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