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GCMS ANALYSIS OF VAYAHSTHAPANA KHANDA

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Abstract: Ayurveda pharmaceutics deals with preparation of medicines. There are five basic preparations mentioned termed as *Panchavidha Kashaya kalpana* meant for instant use. A*valeha Kalpana*, *khanda kalpana* are prepared from these five basic formulations as a base or liquid media. *Khanda kalpana* is accepted by all age group people because of its palatability and higher shelf-life. *Vayahsthapana khanda* was prepared from *Vayahsthapana* gana *kashaya* to increase the palatability and shelf life and it was subjected for analysis. To overcome issue of genuine analytical methods HPTLC, TLC, GC, GCMS are utilised. In this work GCMS analysis of *Vayahsthapana khanda* is carried to set standards for the formulation**.**

I. INTRODUCTION

Ayurveda is an ancient Indian science which focuses on curing the ailment of diseased person and improving the health of the healthy individual[1]. It has eight branches; *jara-chikitsa* or *Rasayana-chikitsa* is one among them. It is considered as the science which restores the youthful vigour, alleviates diseases and bestows longevity[2]. *Acharya Charaka* has mentioned the group of ten drugs under *vayahsthapana gana* which are said to possess longevity effect[3]. *Bhaishajyakalpana* is a specialized branch which deals with the preparation of medicines. *Panchavidha Kashaya kalpana* are the primary dosage forms which are meant for instant use. Further, the secondary preparations like *avaleha Kalpana (confectionary), khanda kalpana (preparations in granules form), sneha kalpana* (oleaginous preparations) are prepared from the five basic formulations[4]. *Khanda kalpana* is one such dosage form which is accepted by all age group people because of its palatability andhigher shelf-life.Herbal medications are recognised as essential therapeutic agents for the treatment of a wide range of ailments. The development of genuine analytical methods which is capable of consistently profiling the phytochemical composition, including quantitative studies of marker/bioactive chemicals and other important ingredients is an issue for current period[5]. To overcome this, the chromatographic methods such as high-performance liquid chromatography (HPLC), gas chromatography (GC), gas chromatography - mass spectrometry (GC-MS) and thin layer chromatography (TLC) were utilised extensively and is available in numerous publications.GC-MS is a combination of two different

analytical techniques namely Gas Chromatography (GC) and Mass Spectrometry (MS). It is used to analyse complex organic and biochemical mixtures. GC can separate volatile and semi-volatile compounds with great resolution. MS can provide detailed structural information on most compounds such that they can be exactly identified and quantified[6]. In the present work an attempt was made to analyse the results obtained from GC-MS of prepared *Vayahsthapana khanda*.

Vayahsthapana gana dravya were taken and were made into granular form by following the general method of *khanda* preparation as mentioned by *Acharya Sharangadhara*. It was subjected to GC-MS analysis to know the components[7].

RESEARCH METHODOLOGY

GC-MS analysis of *Vayahsthapana Khanda* was done at Chromatogen Analytical solutions Mysuru.

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 × 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:

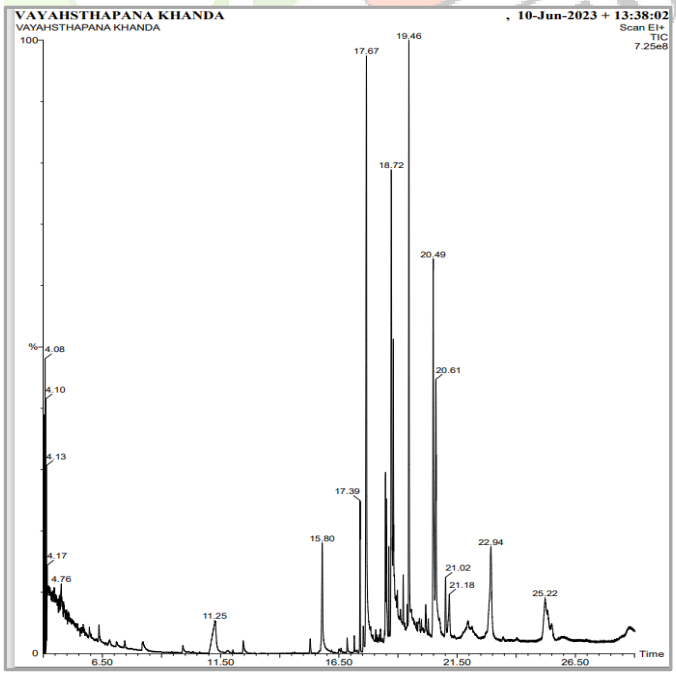


Figure 1: GC-MS plot of *Vayahsthapana Khanda* (TIC)

RESULTS AND DISCUSSION

Table 1: GC-MS of *Vayahsthapana Khanda* at RT= 22.9

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	Glycidyloleate	$C_{21}H_{38}O_3$	717	-	4.91
2	9,12-Octadecadienoyl chloride, (Z,Z)-	$C_{18}H_{31}ClO$	714	7459-33-8	4.34%
3	17-Octadecynoic acid	$C_{18}H_{32}O_2$	713	34450-18-5	4.17%
4	9-Octadecenal	$C_{18}H_{34}O$	712	5090-41-5	4.01%
5	13-Octadecenal, (Z)-	$C_{18}H_{34}O$	709	58594-45-9	3.54%
6	8-Hexadecenal, 14-methyl-, (Z)-	$C_{17}H_{32}O$	705	60609-53-2	2.99%
7	cis-11-Hexadecenal	$C_{16}H_{30}O$	703	53939-28-9	2.76%
8	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	702	60-33-3	2.65%
9	cis-9-Hexadecenal	$C_{16}H_{30}O$	700	56219-04-6	2.45%
10	Pentanoic acid, 10-undecenyl ester	$C_{16}H_{30}O_2$	697	-	2.16%

Table 2: GC-MS of *Vayahsthapana Khanda* at RT= 20.4

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	17-Octadecynoic acid	$C_{18}H_{32}O_2$	721	34450-18-5	5.24%
2	9,12-Octadecadienoyl chloride (Z,Z)-	$C_{18}H_{31}ClO$	712	7459-33-8	3.80%
3	Glycidyloleate	$C_{21}H_{38}O_3$	711	-	3.65%
4	13-Octadecenal, (Z)-	$C_{18}H_{34}O$	708	58594-45-9	3.23%
5	9-Octadecenal	$C_{18}H_{34}O$	706	5090-41-5	2.98%
6	Undec-10-ynoic acid, undec-2-en-1-yl ester	$C_{22}H_{38}O_2$	702	-	2.51%
7	E-10-Pentadecenol	$C_{15}H_{30}O$	701	-	2.42%
8	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	700	60-33-3	2.32%
9	8-Hexadecenal, 14-methyl-, (Z)-	$C_{17}H_{32}O$	699	60609-53-2	2.23%
10	9-Eicosyne	$C_{20}H_{38}$	696	71899-38-2	1.97%

Table 3: GC-MS of *Vayahsthapana Khanda* at RT= 19.4

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	Glycidylpalmitate	$C_{19}H_{36}O_3$	767	-	58.0%
2	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$C_{19}H_{38}O_4$	657	23470-00-0	3.71%
3	Undecanoyl chloride	$C_{11}H_{21}ClO$	645	17746-05-3	2.47%
4	Octadecanoic acid	$C_{18}H_{36}O_2$	634	57-11-4	1.69%
5	15-Hydroxypentadecanoic acid	$C_{15}H_{30}O_3$	634	4617-33-8	1.69%
6	Cyclohexanecarboxylic acid, hexyl ester	$C_{13}H_{24}O_2$	627	27948-10-3	1.29%
7	Myristoyl chloride	$C_{14}H_{27}ClO$	622	112-64-1	1.04%
8	1-Tetradecyl acetate	$C_{16}H_{32}O_2$	622	638-59-5	1.04%
9	2-Dodecylcyclobutanone	$C_{16}H_{30}O$	621	35493-46-0	1.00%
10	Glycerol 1-palmitate	$C_{19}H_{38}O_4$	621	542-44-9	1.00%

Table 4: GC-MS of *Vayahsthapana Khanda* at RT= 18.7

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	11-Octadecenoic acid, (Z)-	$C_{18}H_{34}O_2$	837	506-17-2	6.70%
2	9-Octadecenoic acid, (E)-	$C_{18}H_{34}O_2$	833	112-79-8	5.66%
3	Hexadecenoic acid, Z-11-	$C_{16}H_{30}O_2$	832	2416-20-8	5.44%
4	trans-13-Octadecenoic acid	$C_{18}H_{34}O_2$	832	693-71-0	5.44%
5	cis-13-Octadecenoic acid	$C_{18}H_{34}O_2$	831	13126-39-1	5.23%
6	9-Eicosenoic acid, (Z)-	$C_{20}H_{38}O_2$	830	29204-02-2	5.02%
7	9-Hexadecenoic acid, (Z)-	$C_{16}H_{30}O_2$	828	373-49-9	4.63%
8	Oleic Acid	$C_{18}H_{34}O_2$	828	112-80-1	4.63%
9	Oleic Acid	$C_{18}H_{34}O_2$	826	112-80-1	4.63%
10	Palmitoleic acid	$C_{16}H_{30}O_2$	823	373-49-9	4.63%

Table 5: GC-MS of *Vayahsthapana Khanda* at RT= 17.6

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	852	57-10-3	56.5%
2	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	836	57-10-3	56.5%
3	Pentadecanoic acid	$C_{15}H_{30}O_2$	808	1002-84-2	12.2%
4	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	800	57-10-3	56.5%
5	Tetradecanoic acid	$C_{14}H_{28}O_2$	799	544-63-8	8.88%
6	Undecanoic acid	$C_{11}H_{22}O_2$	791	112-37-8	6.62%
7	Tetradecanoic acid	$C_{14}H_{28}O_2$	790	544-63-8	8.88%
8	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	785	57-10-3	56.5%
9	Dodecanoic acid	$C_{12}H_{24}O_2$	779	143-07-7	4.41%
10	Tridecanoic acid	$C_{13}H_{26}O_2$	777	638-53-9	4.07%

Table 6: GC-MS of *Vayahsthapana Khanda* at RT= 17.3

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	836	112-39-0	37.4%
2	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	825	112-39-0	37.4%
3	Methyl 2,2'-dibenzoate(ester)	$C_{16}H_{14}O_4$	822	-	23.4%
4	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	818	112-39-0	37.4%
5	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	812	112-39-0	37.4%
6	[1,1'-Biphenyl]-4,4'-dicarboxylic acid, dimethyl ester	$C_{16}H_{14}O_4$	805	792-74-5	12.8%
7	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	792	112-39-0	37.4%
8	Phthalic acid, 3-methylphenyl 2-nitrophenyl ester	$C_{21}H_{15}NO_6$	787	-	6.58%
9	Tridecanoic acid, 4,8,12-trimethyl-, methyl ester	$C_{17}H_{34}O_2$	785	10339-74-9	6.07%
10	Diethylmalonic acid, propyl 1,1,1-trifluoroprop-2-yl ester	$C_{13}H_{21}F_3O_4$	775	-	4.28%

Table 7: GC-MS of *Vayahsthapana Khanda* at RT= 15.8

Peak	Compound name	Formula	Match factor	CAS#	Prob %
1	Undecanoic acid	$C_{11}H_{22}O_2$	772	112-37-8	24.0%
2	Tetradecanoic acid	$C_{14}H_{28}O_2$	770	544-63-8	22.1%
3	Tridecanoic acid	$C_{13}H_{26}O_2$	768	638-53-9	20.4%
4	Tetradecanoic acid	$C_{14}H_{28}O_2$	757	544-63-8	22.1%
5	Tetradecanoic acid	$C_{14}H_{28}O_2$	747	544-63-8	22.1%
6	Tetradecanoic acid	$C_{14}H_{28}O_2$	747	544-63-8	22.1%
7	n-Decanoic acid	$C_{10}H_{20}O_2$	746	334-48-5	8.05%
8	n-Decanoic acid	$C_{10}H_{20}O_2$	746	334-48-5	8.05%
9	Tridecanoic acid	$C_{13}H_{26}O_2$	744	638-53-9	20.4%
10	Dodecanoic acid	$C_{12}H_{24}O_2$	743	143-07-7	7.12%

Discussion:

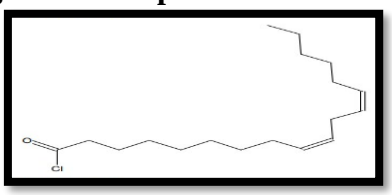
Vayahsthapana Khanda was analysed using Gas Chromatography-Mass Spectrometry (GC-MS) at varied retention times (RTs), which produced a diverse array of bioactive chemicals. Glycidyloleate, Octadecadienoyl chloride, 17-Octadecynoic acid, 9-Octadecenal and 13-Octadecenal were among the significant substances at RT=22.9. The 17-Octadecynoic acid, Octadecadienoyl chloride, glycidyloleate and 13-Octadecenal were among the substances visible at RT=20.4. Compounds including Glycidyl palmitate, derivatives of hexadecanoic acid and undecanoyl chloride were present in RT=19.4. Different fatty acid isomers such as cis-Vaccenic acid, 9-Octadecenoic acid and trans-13-Octadecenoic acid were present in RT=18.7. The fatty acid compounds Hexadecanoic acid methyl ester and Methyl dibenzoate were identified by RT=17.6. The variety of detected chemicals and their varying relative abundances over various RTs point to the *Vayahsthapana Khanda's* complicated chemical makeup. The components like 17-Octadecynoic acid, dodecynoic acid, Tetradecanoic acid, Hexadecanoic acid-methyl ester, n-Hexadecanoic acid and Pentadecanoic acid possess antioxidant property. Further,9-Octadecenamide, 9,12-Octadecadienoic acid, cis-Vaccenic acid act as anti-inflammatory[8,9]. Also,GCMSsuggests the existence of fatty acids, esters and other derivatives, which help to explain other therapeutic properties of the sample. *Vayahsthapana Khanda* contains a complex combination of compounds, which is highlighted by the changes in compound probabilities and match factors. This GC-MS analysis offers important insights into the molecular structure of *Vayahsthapana Khanda*, assisting in its characterisation for therapeutic application and fostering a better knowledge of its possible pharmacological actions.

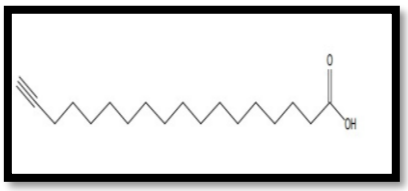
CONCLUSION:

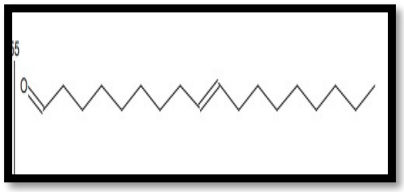
In the present work prepared *vayahsthapana khanda* was subjected for GC-MS analysis and the obtained results were tabulated and discussed with respect to its properties.Seventy constituents were found with seven different Retention Times. It helps to predict the formula andstructure of bio-molecules which can be used as drugs. The GC-MS results found in *Vayahsthapana Khanda* can be considered as the preliminary standards for further study.

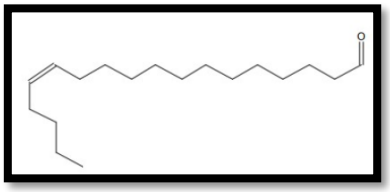
Figure 2: Compounds at different RT

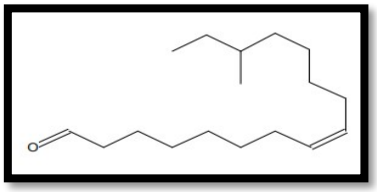

Glycidyloleate

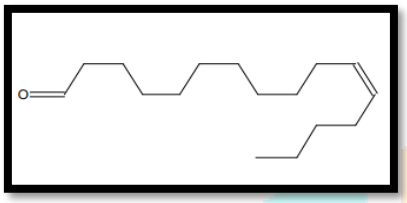

9,12-Octadecadienoyl chloride, (Z,Z)-


17-Octadecynoic acid

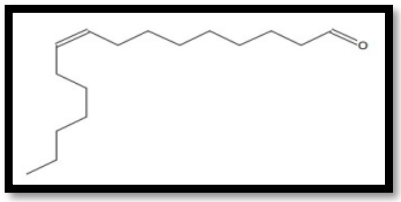

9-Octadecenal

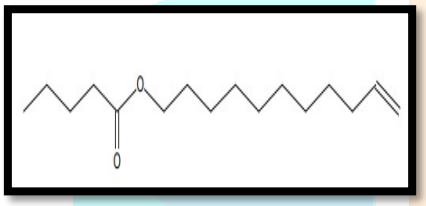

13-Octadecenal, (Z)-

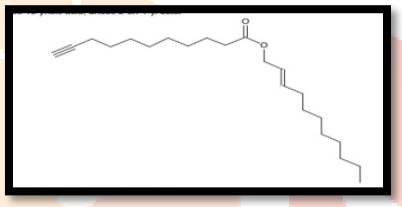

8-Hexadecenal, 14-methyl-, (Z)-

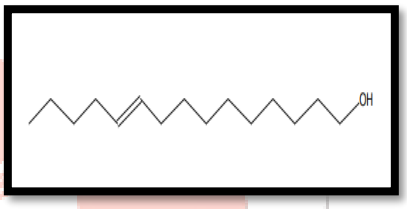

cis-11-Hexadecenal

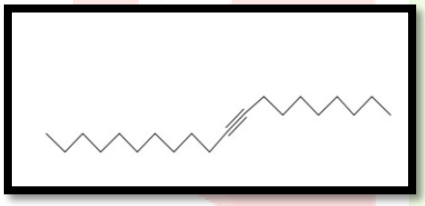

9,12-Octadecadienoic acid (Z,Z)-

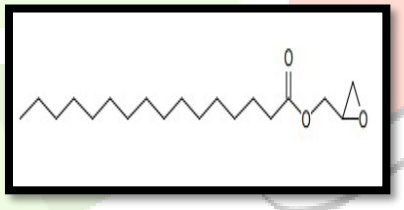

cis-9-Hexadecenal

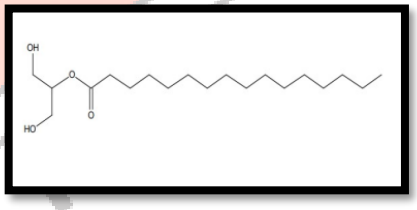

Pentanoic acid, 10-undecenyl ester

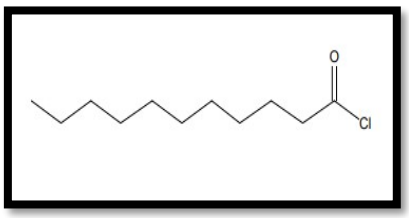

Undec-10-ynoic acid, undec-2-en-1-yl ester

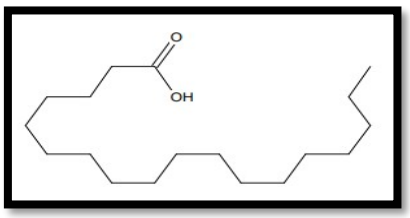

E-10-Pentadecenol

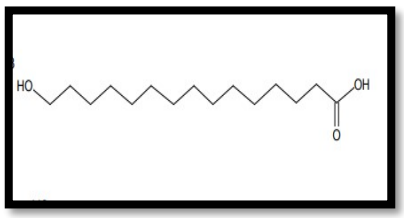

9-Eicosyne

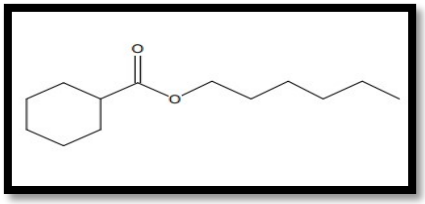

Glycidyl palmitate

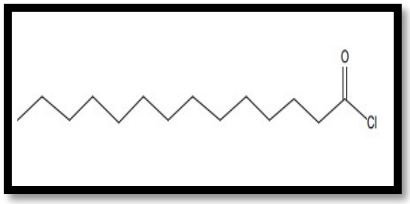

Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester


Undecanoyl chloride


Octadecanoic acid


15-Hydroxypentadecanoic acid


Cyclohexane carboxylic acid, hexyl ester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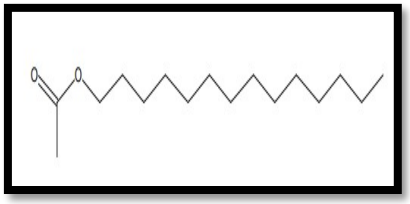
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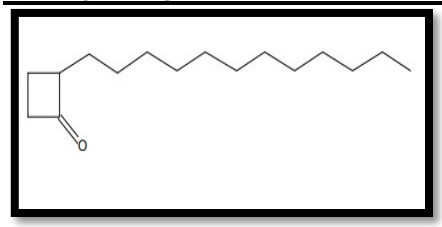
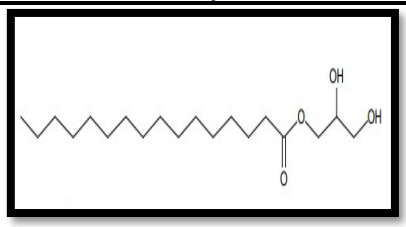
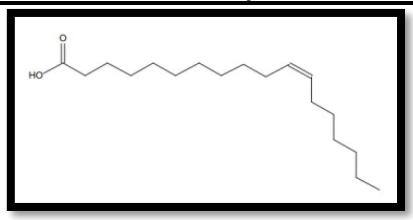
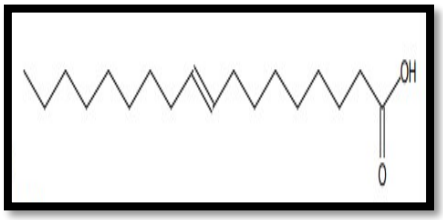
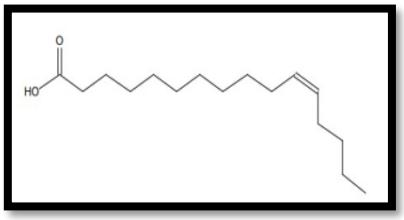
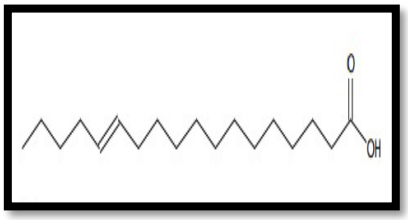

2-Dodecylcyclobutanone

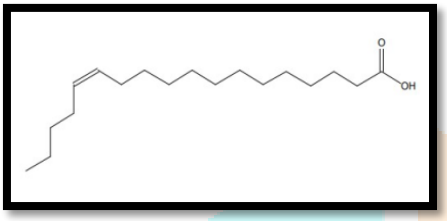

Glycerol 1-palmitate

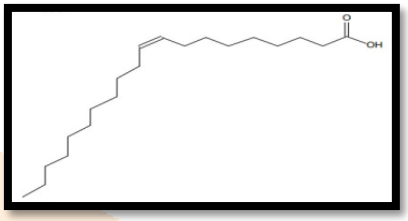

11-Octadecenoic acid, (Z)-

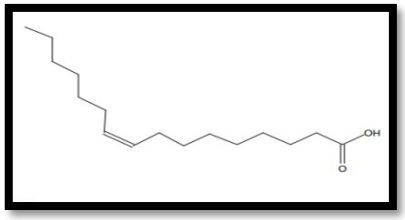

9-Octadecenoic acid, (E)

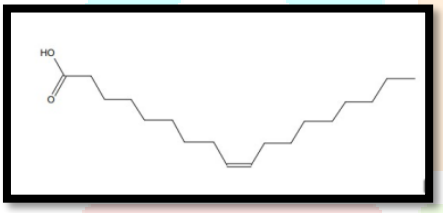

Hexadecenoic acid, Z-11-

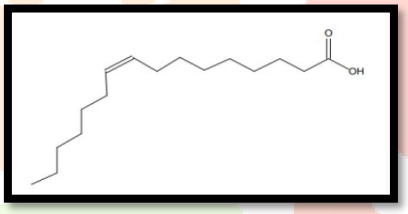

trans-13-Octadecenoic acid


cis-13-Octadecenoic acid

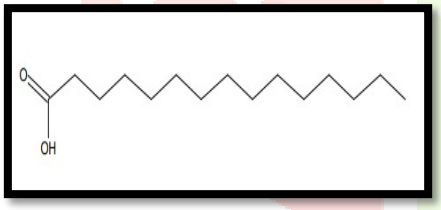

9-Eicosenoic acid, (Z)

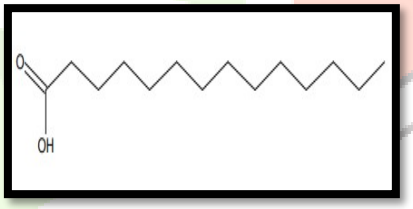

9-Hexadecenoic acid, (Z)-

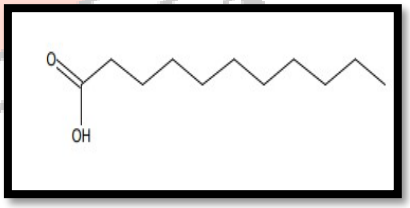

Oleic Acid

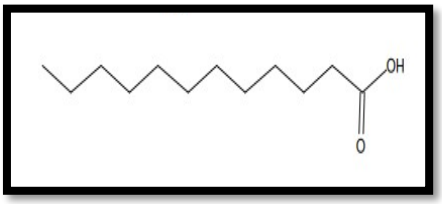

Palmitoleic acid

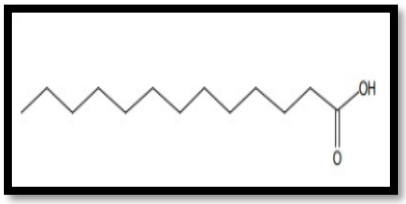

n-Hexadecanoic acid

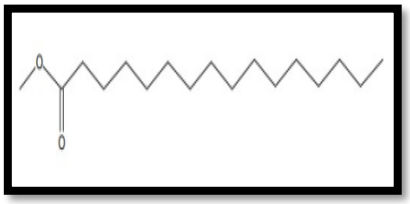

Pentadecanoic acid

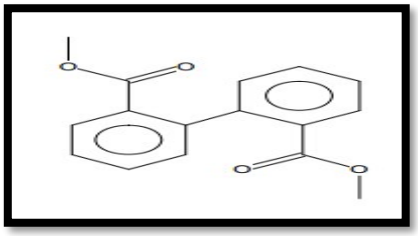

Tetradecanoic acid

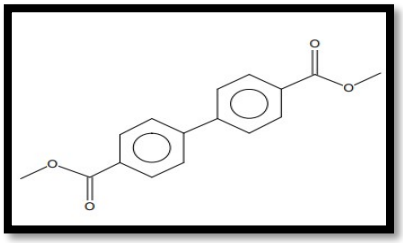

Undecanoic acid

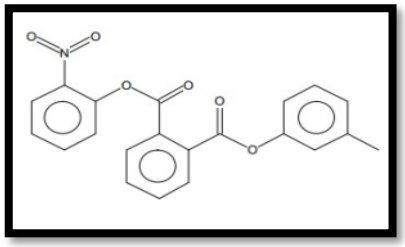

Dodecanoic acid

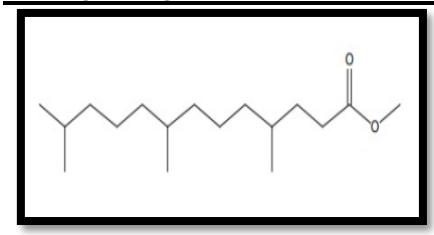

Tridecanoic acid


Hexadecanoic acid, methyl ester

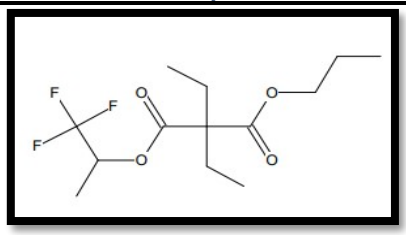

Methyl 2,2'-dibenzoate(ester)


[1,1'-Biphenyl]-4,4'-dicarboxylic acid, dimethyl ester

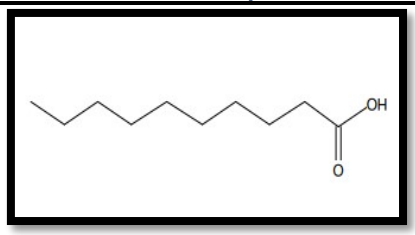

Phthalic acid, 3-methylphenyl 2-nitrophenyl ester



Tridecanoic acid, 4,8,12-trimethyl-, methyl ester



Diethylmalonic acid, propyl 1,1,1-trifluoroprop-2-yl ester



n-Decanoic acid

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