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Original

A comparative study on the chemical constituent's fatty acids and lignans from sesame seeds and flaxseeds by Gas Chromatography/Mass Spectrometry

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Abstract

Background *Sesamum indicum* (sesame) and *Linum usitatissimum* (flaxseed) seeds are rich in fatty acids and lignans which have been stated to be the reason for their wide range of activities. *Sesamum indicum* seeds have been shown to possess cholesterol lowering activity, neuroprotective, anti-carcinogenic and coronary protective effect and *Linum usitatissimum* seeds health benefits include reducing cardiovascular diseases, decrease the risk of cancer, anti-inflammatory activity, laxative effect, osteoporosis and alleviation of menopausal symptoms.

Experimental *Sesamum indicum* and *Linum usitatissimum* seeds were coarsely grounded for oil extraction and for sample preparation by methyl esterification for the GC-MS instrument. Another amount of the seeds was taken and the methanol extraction followed by n-hexane method was carried out, then injected into the GC/MS instrument. From the results of GC/MS, the fatty acid and lignan composition were determined and a comparison was made.

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Results The major constituents in sesame seeds fixed oil were linoleic acid, methyl ester (34.80%), oleic acid, methyl ester (30.89%), palmitic acid, methyl ester (15.41%) and methyl stearate (13.89%).The major constituents in flaxseeds fixed oil were alpha-linolenic , methyl ester (53.05%), linoleic acid, methyl ester (18.83%), palmitic acid, methyl ester (12.86%), methyl stearate (11.94%).The major constituents in sesame seeds extract were linoleic methyl ester (22.52%), vitamin E (25.18%), oleic acid, methyl ester (13.44%), and palmitic acid, methyl ester (11.66%).The major constituents in flaxseeds extract were isobutylglycerol-nitro (13.16%), D-sesamin (22.89%) and episesamin (40.49%).

Conclusion Both *Sesamum indicum* and *Linum usitatissimum* seeds are a rich source of fatty acids and dietary lignans.

Keywords: Chemical constituents, fatty acids, lignans, sesame seeds, flaxseed, GC/MS,Sudan.

Introduction:

Fatty acids are saturated or unsaturated monocarboxylic acids naturally occurring in the form of esters in fats and fatty oils. There are two groups of polyunsaturated Omega-fatty acids, omega-3-fatty acids and omega-6-fatty acids [1]. Flaxseed and sesame are rich in fatty acids particularly linoleic acid.

Lignans are diphenolic compounds of higher plants formed by the coupling of two coniferyl alcohol residues that are present in the plant cell wall [2]. They are becoming increasingly important for their variety of biological properties that can be applied in pharmacy and nutrition. Secoisolariciresinol (SECO) and its conjugated form secoisolariciresinol diglycoside (SDG) is the major lignan present in flaxseed which is the richest dietary source of plant based SDG and it can be metabolized to the mammalian lignans, enterodiol and enterolactone by human intestinal microflora. The main lignans in sesame oil are sesamin, sesamolin and sesamol. In biological systems, these molecules may protect the cell membrane from oxidative damage, thus acting as membrane stabilizers. Published studies also indicated that tocopherol and lignan possess cholesterol lowering activity, neuroprotective, anti-carcinogenic and coronary protective effect [3]-[4].

The aim of this study was to compare the chemical constituents of fatty acids and lignans from sesame seeds and flaxseeds by GC/MS.

Experimental:

Plant material

Linum ustitatisimum and *Sesamum indicum* seeds were purchased from the local drug store in Bahri, Khartoum North. The seeds of *Linum ustitatisimum* and *Sesamum indicum* were coarsely grounded for oil extraction and for sample preparation for the GC-MS instrument.

GC/MS condition and technique:

The fatty acid and lignin profile of plant seeds oil was determined using gas chromatography as described by Christie [5]. The qualitative and quantitative analysis of the sample was carried out by using GC/MS technique model (GC/MS-QP2010-Ultra) from Japans Simadzu Company, with serial number 020525101565SA and capillary column

(Rtx-5ms-30m × 0.25mm × 0.25µm). The sample was injected using split mode, helium as the carrier gas passed with flow rate 1.61 ml/minute, the temperature program was started from 60˚C with rate 10˚C/minute to 300˚C as final temperature degree with 3 minutes hold time, the injection port temperature was 300˚C, the ion source temperature was 200˚C and the interface temperature was 250˚C.The sample was analyzed by using scan mode in the range of m/z 40-500 charges to ratio and the total run time was 26 minutes. Identification of the components for the sample was achieved by comparing their retention times and the mass fragmentation patents with those available in the library, The National Institute of Standards and Technology (NIST).

Extraction of oil

The finely powered seeds (20 gram) were placed into the soxhlet thimble. Then the thimble was placed in the soxhlet apparatus. The extraction was done for 7 hours using n-hexane as a solvent. The n-hexane was then evaporated by rotary evaporator and remaining oil was weighed [6] .

Fatty acid composition [6]

The extracted oil was prepared for fatty acid determination by methylation of the esters[7]. Where 2 ml from the oil was placed into a test tube, it was followed by 7 ml of alcoholic NaOH that was prepared by dissolving 2 gram sodium hydroxide in 100 ml methanol. Then 7 ml of alcoholic H_2SO_4 1% that was prepared by mixing 1 ml concentrated H_2SO_4 with 99 ml of methanol. This was shaken by vortex for 3 minutes and the contents were left overnight. 2 ml from supersaturated NaCl and 2ml normal hexane was added and shaken for three minutes then the hexane layer was collected. From the hexane layer 5 µl was collected and diluted it with 5 ml diethyl ether. Then 1 gram was added from sodium sulphate as a drying agent and it was filtered through a syringe filter 0.45 µm. The filtrate was transferred to the GC-MS vial and injected directly to the GC-MS instrument.

Lignan composition (sequential extraction) [3]

10 grams of powdered seeds was taken and placed in a beaker then 20 ml of methanol was added. The beaker was transferred to the Ultra-sound bath and placed there for

an hour. Then the extract was transferred to a separatory funnel where it was washed with three quantities of 20 ml n-hexane(defatting). The sample was concentrated by evaporation and injected into GC-MC instrument.

Results and discussion:

Chemical investigation of sesame seed oil (fatty acid profile):

The chemical composition of seed oil obtained from sesamum indicum L. (pedaliaceae) Sudanese variety was analyzed by GC/MS. The 13 constituents were identified. The major constituents were 9,12-Octadecadienoic acid (Z,Z)-, methyl ester (34.80%), 9-Octadecenoic acid (Z)-, methyl ester (30.89%), Hexadecanoic acid, methyl ester (15.41%) and methyl stearate (13.89%).

The present study revealed that the seed oil of S.indicum is rich in fatty acids (99.90%).

The chemical compositions of the investigated fixed oil obtained from S. indicum seeds are shown in Figure 1 and Table 1.

Figure 1. GC/MS chromatogram of fatty acids in the fixed oil of *Sesamum indicum*

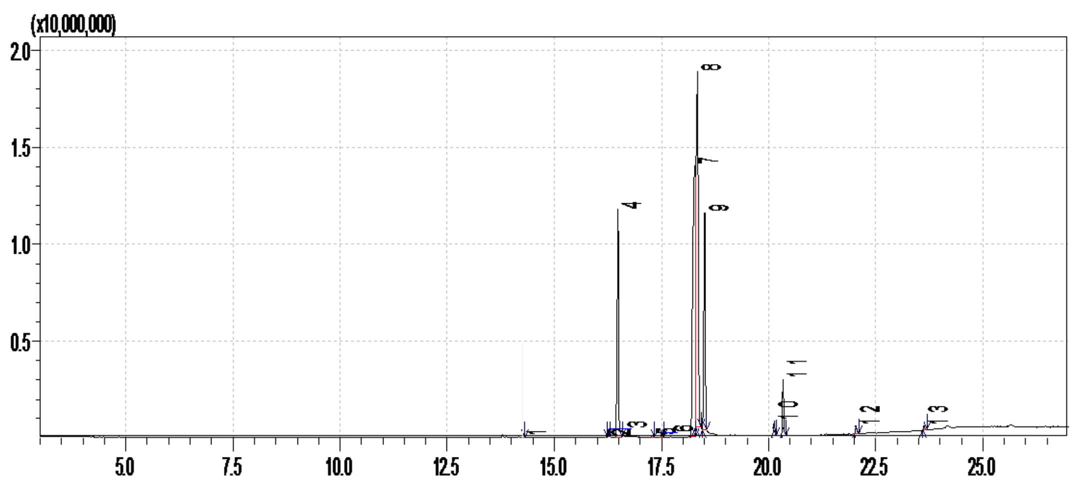

Table 1. Seed fixed oil composition of *Sesamum indicum*

Peak number	Compound	Other names	Molecular weight	Formula	Area%
1	Methyl tetradecanoate	Methyl myristate; myristic acid methyl ester	242.39	$C_{15}H_{30}O_2$	0.03
2	7-Hexadecenoic acid, methyl ester, (Z)-	Methyl-7-hexadecenoate	268.441	$C_{17}H_{32}O_2$	0.07
3	9-Hexadecenoic acid, methyl ester, (Z)-	Methyl palmitoleate ; palmitoleic acid methyl ester	268.441	$C_{17}H_{32}O_2$	0.36
4	Hexadecanoic acid, methyl ester	Methyl palmitate; palmitic acid methyl ester	270.45	$C_{17}H_{34}O_2$	15.41
5	cis-10-Heptadecenoic acid, methyl ester	-	282	$C_{18}H_{34}O_2$	0.10
6	Heptadecanoic acid, methyl ester	Margaric acid methyl ester; Methyl margarate	284.484	$C_{18}H_{36}O_2$	0.20
7	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	Linoleic acid methyl ester; methyl linoleate	294.479	$C_{19}H_{34}O_2$	34.80
8	9-Octadecenoic acid (Z)-, methyl ester	Oleic acid methyl ester; methyl oleate	296.49	$C_{19}H_{36}O_2$	30.89

9	Methyl stearate	Stearic acid methyl ester; methyl stearic	298.51	$C_{19}H_{38}O_2$	13.35
10	cis-11-Eicosenoic acid, methyl ester		324.54	$C_{21}H_{40}O_2$	0.86
11	Eicosanoic acid, methyl ester	Arachidic acid methyl ester; methyl arachidate	326.54	$C_{21}H_{42}O_2$	3.05
12	Docosanoic acid, methyl ester	Behenic acid methyl ester; methyl behenate	354.61	$C_{23}H_{46}O_2$	0.54
13	Tetracosanoic acid, methyl ester	Lignoceric acid methyl ester	382.67	$C_{25}H_{50}O_2$	0.24

Chemical investigation of flaxseed oil (fatty acid profile):

The chemical composition of seed oil from *L.usitatissimum* L. (Linaceae) sold in local market was analyzed by GC/MS. The 14 constituents were identified. The major constituents were 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z) (53.05%), 9,12-Octadecadienoic acid (Z,Z)-, methyl ester (18.83%), Hexadecanoic acid, methyl ester (12.86%), methyl stearate (11.94%).

The present study revealed that the seed oil of *L.usitatissimum* is rich in fatty acids (100%).

The chemical composition of the investigated fixed oil obtained from *L.usitatissimum* seeds is shown in Figure 2 and Table 2.

Figure 2. GC/MS chromatogram of fatty acids in the fixed oil *Linum usitatissimum*:

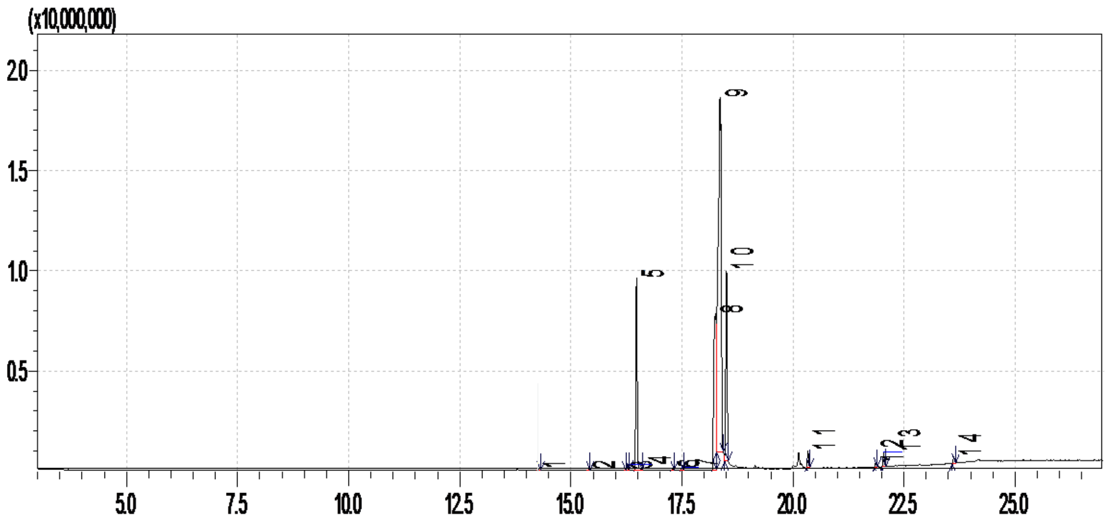

Table 2. Seed fixed oil composition of *Linum usitatissimum*:

Peak number	Compound	Other names	Molecular weight	Formula	Area%
1	Methyl tetradecanoate	Methyl myristate; myristic acid methyl ester	242.39	$C_{15}H_{30}O_2$	0.13
2	Pentadecanoic acid, methyl ester		256.43	$C_{16}H_{32}O_2$	0.07
3	7-Hexadecenoic acid, methyl ester, (Z)-	Methyl-7-hexadecenoate	268.43	$C_{17}H_{32}O_2$	0.06
4	9-Hexadecenoic acid, methyl ester, (Z)-	Methyl palmitoleate ; palmitoleic acid methyl ester	268.44	$C_{17}H_{32}O_2$	0.27

5	Hexadecanoic acid, methyl ester	Methyl palmitate; palmitic acid methyl ester	270.45	$C_{17}H_{34}O_2$	12.86
6	cis-9-Hexadecenal	-	238	$C_{16}H_{30}O$	0.10
7	Heptadecanoic acid, methyl ester	Margaric acid methyl ester; Methyl margarate	284.48	$C_{18}H_{36}O_2$	0.18
8	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	Linoleic acid methyl ester; methyl linoleate	294.47	$C_{19}H_{34}O_2$	18.83
9	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	Alpha- linolenic acid methyl ester	292.46	$C_{19}H_{32}O_2$	53.05
10	Methyl stearate	Stearic acid methyl ester; methyl stearic	298.51	$C_{19}H_{38}O_2$	11.94
11	Eicosanoic acid, methyl ester	Arachidic acid methyl ester; methyl arachidate	326.61	$C_{21}H_{42}O_2$	0.89
12	cis-10-Nonadecenoic acid, methyl ester	-	310.51	$C_{20}H_{38}O2$	0.29
13	Docosanoic acid, methyl ester	Behenic acid methyl ester; methyl behenate	354.61	$C_{23}H_{46}O2$	0.90
14	Tetracosanoic acid, methyl ester	Lignoceric acid methyl ester	382.67	$C_{25}H_{50}O2$	0.42

Chemical investigation of sesame seed extract (lignan profile):

The chemical composition of seed extract obtained from *sesamum indicum* L. (Pedaliaceae) Sudanese variety was analyzed by GC/MS. The 17 constituents were identified. The major constituents were 9,12-Octadecadienoic acid (Z)-, methyl ester (22.52%), vitamin E

(25.18%), 9-Octadecenoic acid, (E)- (13.44%), and n-Hexadecanoic acid, methyl ester (11.66%).

The chemical compositions of the investigated extract obtained from *S. indicum* seeds is shown in Figure 3 and Table 3.

Figure 3. GC/MS chromatogram of lignan in the extract of *Sesamum indicum*

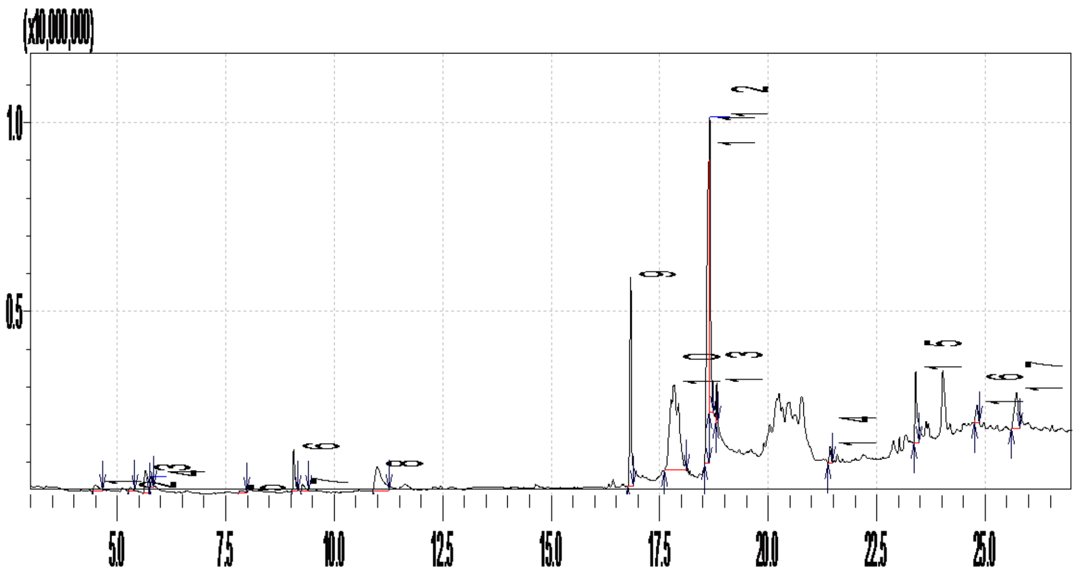

Table 3. Seed extract composition of *Sesamum indicum*

Peak number	Compound	Other names	Molecular weight	formula	Area%
1	2-Hydroxy-gamma-butyrolactone	3-hydroxydihydro-2(3H)-furanone	102.08	C4H6O3	0.90
2	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	Furaneol; Alleton	128.12	C6H803	0.33

3	Thymine	2,4-dihydroxy-5-methyl pyrimidine; 5-methyl uracil	126.11	C5H6N2O2	2.70
4	Phenol, 2-methoxy-	Guaiacol; Anastil	124.13	C7H8O2	0.60
5	Benzofuran, 2,3-dihydro-	Coumaran	120.15	C8H8O	0.41
6	2-Methoxy-4-vinylphenol	p-vinyl guaiacol	150.17	C9H10O2	2.45
7	1,3-Benzodioxol-5-ol	Sesamol	138.12	C7H6O3	0.75
8	1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-	Isobutylglycerol, nitro	151	C4H9NO5	5.53
9	n-Hexadecanoic acid	Palmitic acid methyl ester	256.43	C16H32O2	11.66
10	Vitamin E	Alpha-tocopherol	430	C29H50O2	25.18
11	9,12-Octadecadienoic acid (Z,Z)-	Linoleic acid	280.45	C18H3202	22.52
12	9-Octadecenoic acid, (E)-	Oleic acid	282.46	C18H3402	13.44
13	Octadecanoic acid	Stearic acid	284.48	C18H36O2	1.38
14	3-Cyclopentylpropionic acid, 2-dimethylaminoethyl ester	-	213	C12H23NO2	0.99
15	E,E,Z-1,3,12-Nonadecatriene-5,14-diol	-	294.47	C19H34O2	5.06
16	.beta.-Amyrin	Olean-12-en-3-beta-ol	426.72	C30H50O	1.40
17	Lup-20(29)-en-3-ol, acetate, (3.beta.)-	Lupeol acetate; lupenyl acetate	468.76	C32H52O2	4.71

Chemical investigation of flaxseed extract (lignan profile):

The chemical composition of seed extract from *L.usitatissimum* L. (Linaceae) sold in local market was analyzed by GC/MS. The 15 constituents were identified. The major constituents were 1,3-Propanediol, 2-(hydroxymethyl)-2-nitro- (13.16%), 2,6-Bis(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo(3.3.0)octane (22.89%) and 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.)] (40.49%).

The chemical composition of the investigated extract obtained from *L.usitatissimum* seeds is shown in Figure 4 and Table 4.

Figure 4. GC/MS chromatogram of lignans in the extract of *Linum usitatissimum*

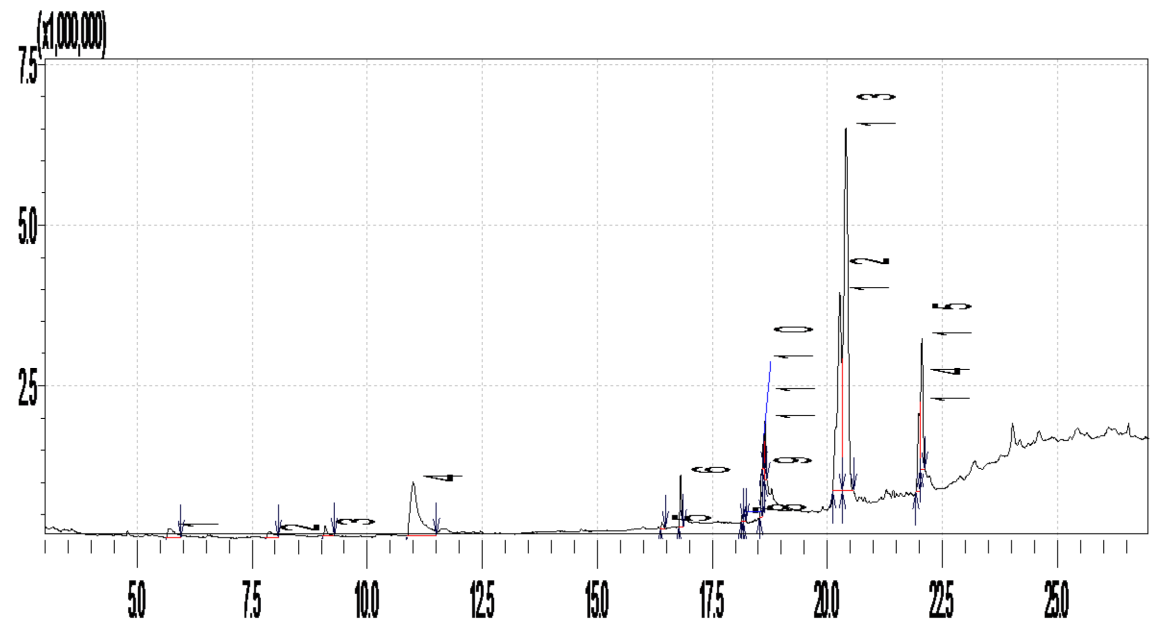

Table 4. Seed extract composition of *Linum usitatissimum*:

Peak number	Compound	Other names	Molecular weight	formula	Area %
1	Thymine	2,4-dihydroxy-5-methyl pyrimidine; 5-methyl uracil	126.11	C5H6N2O2	1.76
2	Benzofuran, 2,3-dihydro-	Coumaran	120.15	C8H8O	0.93
3	2-Methoxy-4-vinylphenol	p-vinyl guaiacol	150.17	C9H10O2	0.83
4	1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-	Isobutylglycerol, nitro	151	C4H9NO5	13.16
5	Hexadecanoic acid, methyl ester	Palmitic acid methyl ester	270.45	C17H34O2	0.34
6	n-Hexadecanoic acid	Palmitic acid	256.43	C16H32O2	2.28
7	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	Linoleic acid	280.45	C18H32O2	0.17
8	9-Octadecenoic acid (Z)-, methyl ester	Oleic acid methyl ester	296	C19H36O2	0.27
9	Linoleic acid ethyl ester	Ethyl linoleate	308.50	C20H36O2	1.84
10	Oleic Acid	Elaidoic acid	282.46	C18H34O2	0.90
11	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	Alpha- linolenic acid	278.43	C18H30O2	1.75

12	2,6-Bis(3,4-methylenedioxyphenyl)-3,7-dioxabicyclo(3.3.0)octane	D-sesamin; Asarinin; pseudo.cubebin	354.358	C20H18O6	22.89
13	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.)]-	Episesamin	354.353	C20H18O6	40.49
14	3-Amino-4-piperonyl-5-pyrazolone	-	233.22	C11H11N3O3	4.98
15	Pyrrolidine-2,5-dione, 1-(adamantan-1-yl)methyl-3-(4-chlorobenzyl)-	-	371	C22H26CLNO2	7.43

Comparison of the seed oil composition from different geographical origins shared some qualitative and quantitative variation in their fixed oil constituents. Linoleic acid and oleic acid were found to be the major components identified in higher concentration in sesame oil of India, Sudan, Iraq, and Korea origin. Arachidic acid (3.05%) in sesame Sudanese (Sudanese variety) have not been previously reported among other samples.

Table 5. Comparison of constituents (%) of *Sesamum indicum* from different origins

Fatty acid profile	Present study (Sudan)	India [6]	Pakistan [7]	Korea [8]	Iraq [9]
Palmitic acid(16:0)	15.41	10.15	19.3	8.5	5.6
Stearic acid(18:0)	13.35	5.61	13.9	5.7	5.3
Arachidic acid(20:0)	3.05	-	-	-	-
Oleic acid (18:1)	30.89	39.88	10.2	39.3	40.3
Linoleic acid (18:2)	34.80	41.73	12.5	43.4	46.1
Linolenic acid(18:3)	-	0.32	11.6	0.4	0.4

Table 6. Comparison of some constituents (%) of *Linium usitatissium* L. from different origins

Fatty acid profile	Present study (Sudan)	Turkey [10]	Gergia [11]	Romania [12]	India [13]	Brazil [14]
Palmitic acid(16:0)	12.86	5.33	-	6.58	5.51	6

Stearic acid(18:0)	11.94	6.11	-	4.43	4.87	1.56
Arachidic acid(20:0)	0.89	0.21	-	-	-	0.18
Oleic acid (18:1)	-	25.79	-	18.51	19.00	19.78
Linoleic acid (18:2)	18.83	12.38	31.3	17.25	15.91	12.75
Linolenic acid(18:3)	53.05	50.04	40.2	53.21	54.82	39.66

Conclusion:

Based on this study, it was concluded that sesame seeds and flax seeds are rich in fatty acids where the major constituents with high concentration are linoleic acid, oleic acid, palmitic acid and stearic acid (especially linoleic acid and oleic acid) for *Sesamum indicum* and palmitic acid, linoleic acid , alpha- linolenic acid and stearic acid (especially alpha linoleic acid) for *Linium usitatissium.*

Sesame seeds were found to be rich in Alpha-tocopherol and have a small amount the lignan sesamol. While the flax seeds are rich in the lignans D-sesamin and Episesamin.

Recommendations:

A different method should be conducted for the extraction of lignans from Sesamum *indicum* and *Linium usitatissium* for more accurate quantitative determination.

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