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ORIGINAL ARTICLE

Assessment of variability in lignan and fatty acid content in the germplasm of *Sesamum indicum* L.

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Abstract Information on the variability available in lignan and fatty acid content in the oilseed crop of *Sesamum indicum* has been limited. This article presents and discusses the composition, quantity, and variability available for the two traits in the sesame germplasm that are grown in diverse agro climatic regions of India. HPLC and GC analysis of sesame seeds harvested over a period of three crop seasons revealed a considerable amount of variability in lignan and fatty acids. The antioxidant lignans sesamol, sesamin and sesamolin were observed to be in the range of 0.16–3.24, 2.10–5.98 and 1.52–3.76 mg/g of seed, respectively. Similarly oleic and linoleic acids, respectively, have ranged from 34.71 to 45.61% and 38.49 to 49.60%. The black sesame seeds were found rich in sesamin, sesamolin, total lignan content and oleic acid and are thus identified nutritionally and pharmaceutically more important than white and brown seeds. Pearson statistics showed a strong correlation between the components within a particular trait and also some correlation was found between the traits. The study revealed promising cultivars for use in sesame breeding aimed at improving lignan and fatty acid contents, and can be thus directly used in human foods, nutrition, health and welfare.

Keywords *Sesamum indicum* L. · Seed coat colour · Lignans · Fatty acids · HPLC · GC · Pearson correlation

Introduction

Sesamum indicum L. commonly known as Gingelley, is the world's most ancient oilseed crop (Bedigian 2004). Sesame is characterized by its high oil content containing up to 60% oil, 25% protein, 13.5% carbohydrates and about 1% as minerals (Dar et al. 2015). The bio chemical composition of sesame seed differs with variety, origin, colour and size. The crop is the major source of medicinally important lignans namely, sesamin and sesamolin that are known for their anti-proliferative, antihypertensive and neuroprotective properties (Cooney et al. 2001; Cheng et al. 2006; Yokota et al. 2007; Visavadiya and Narasimhacharya 2008; Dar and Arumugam 2013). Sesame oil is the most stable of all edible oils, due to the presence of the antioxidant lignans thus inciting a proposition to incorporate sesame lignans in other edible oils for improving their shelf life (Suja et al. 2004). Oleic acid and linoleic acid are the two major fatty acids of sesame oil constituting about 85% of the total fatty acids.

Despite being ancient and with high pharmacological significance and nutritional values, the crop remains neglected. There are hardly a few reports that describe genetic diversity of the crop for fatty acid composition and lignan content (Hemalatha and Ghafoorunissa 2004; Uzun et al. 2008; Rangkadilok et al. 2010; Mondal et al. 2010; Bhunia et al. 2015). Since lignans and unsaturated fatty acids are responsible for several pharmacological properties, information on the available variability for these compounds is essential, especially for identifying superior sesame genotypes for use as food ingredients. Such

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genotypes would also be highly useful in breeding programmes aimed at enhancing the content of the two metabolites (Uzun et al. 2008; Williamson et al. 2008; Rangkadilok et al. 2010). Understanding the variation in the content of such physiologically active constituents is desirable for their incorporation in functional foods. Therefore, the aim of this study was to determine the extent of variability for lignans and fatty acid contents in the sesame germplasm grown widely in India, and to find out the correlation between the two traits.

Materials and methods

Plant material

Forty-three different accessions of *S. indicum* used in this study were obtained from National Bureau of Plant Genetic Resources, New Delhi, is presented in Table 1. The germplasm was maintained by raising it once every year in the experimental garden of our Department at School of Life Sciences, Pondicherry University, India.

Reagents and chemicals

Solvents used for extraction of lignans and fatty acyl methyl esters (FAME's) were of analytical grade and HPLC grade, procured from Merck and Himedia, India. Reference standard of sesamin (Cat. No. S9314), sesamol (Cat. No. S8518), and naringenin (the internal standard—Cat. No. N5893) were procured from Sigma, USA. Pure sesamolin was isolated in-house from sesame oil, authenticated by NMR, and used as reference standard for quantification of sesamolin in the germplasm.

Lignan analysis

Extraction of lignans from seeds

Isolation of lignans from seeds of different sesame varieties was performed by following methodology described in Wang et al. (2012). 100 mg of sesame seed was homogenized in 5 ml of 80% ethanol using a pestle and mortar. The whole content was transferred into 30-ml Oakridge tube and centrifuged at 8000 rpm for 10 min at room temperature. The supernatant was transferred to a fresh tube and the residue was subjected to one more round of extraction. Ethanol was evaporated by rotary evaporation. To the residue, 1 ml of 80% methanol was added and filtered through 0.45 µm nylon membrane. The sample thus prepared was used for HPLC analysis.

Table 1 Variation in lignan content in seeds of different accessions of *Sesamum indicum* germplasm studied over a period of 3 years

Variety	Seed colour	Lignan content (mg/g)			
		Sesamol	Sesamin	Sesamolin	Total
AKT64	White	0.62	3.99	2.39	7.00
Amrit	Brown	0.32	4.56	1.85	6.73
Chandana	Brown	0.46	2.10	1.58	4.14
DS1	White	0.63	4.39	2.41	7.43
E8	White	1.08	5.75	2.68	9.51
FFAT0822	White	3.24	4.19	2.64	10.07
GT1	White	2.27	3.32	2.46	8.05
GT2	White	1.82	2.98	2.10	6.90
JLT1	Black	0.74	3.33	2.91	6.98
JLT7	White	0.81	5.33	2.57	8.71
JLT26	White	0.98	4.10	1.72	6.80
JT7	White	0.48	3.11	2.81	6.40
JTS8	White	0.85	2.82	2.06	5.73
Kallika	Brown	0.23	3.93	2.95	7.11
Krishna	Black	0.42	4.49	3.76	8.67
N8	Brown	0.17	4.36	2.18	6.71
N32	White	0.68	3.51	2.07	6.26
Nirmala	Brown	0.63	3.44	1.74	5.81
Phuletil	White	1.21	5.51	2.85	9.57
Prachi	Black	0.43	4.97	2.95	8.35
Praghti	White	1.43	3.46	2.82	7.71
Rajeswari	White	0.35	4.99	3.47	8.81
RT103	White	0.49	2.93	3.06	6.48
RT125	White	0.52	4.38	3.52	8.42
RT127	White	0.83	3.39	3.12	7.34
SVPR1	White	0.63	5.86	3.37	9.86
T12	White	1.50	4.62	2.93	9.05
T13	White	2.30	3.26	2.31	7.87
T78	White	1.69	3.32	1.96	6.97
Tarun	White	1.80	2.25	1.69	5.74
TC25	White	1.02	4.57	2.78	8.37
TC289	White	0.87	3.10	1.77	5.74
TKG22	White	0.80	3.33	2.44	6.57
TKG55	White	0.35	3.31	2.80	6.46
TMV3	Black	0.30	4.89	3.08	8.27
TMV4	Brown	0.25	4.97	2.90	8.12
TMV5	Brown	0.24	5.73	3.43	9.40
TMV6	Brown	0.28	4.87	3.24	8.39
Uma	Brown	0.16	3.91	1.52	5.59
Vinayak	Brown	0.47	4.00	3.28	7.75
VRI1	Brown	0.29	5.98	3.31	9.58
XLM19	Brown	0.22	3.92	3.02	7.16
YLM17	Brown	0.46	3.90	2.75	7.11
Mean	–	0.82	4.07	2.63	7.53
SD	–	0.67	0.97	0.59	1.35

Table 1 continued

Variety	Seed colour	Lignan content (mg/g)			
		Sesamol	Sesamin	Sesamolin	Total
CV	–	81.67	23.76	22.43	17.89
Minimum	–	0.16	2.10	1.52	4.14
Maximum	–	3.24	5.98	3.76	10.07

Preparation of lignan standards and calculation of response factor (Rf)

A 0.0001 M stock solution of each of naringenin, sesamol, sesamin and sesamolin standards were prepared in HPLC grade methanol and filtered through 0.45 µm nylon membrane. Initially the lignan standards were analysed individually by HPLC to determine their specific RT (retention time). The response factor (Rf) of each of the compound, which is required for their quantification in the methanol extract, was determined by analysing a mixture of known concentration of the reference standards along with naringenin as internal standard by HPLC (Kupiec 2004). Calculation of Rf and estimation of lignans in the methanol extract of seeds were carried out by following Dar et al. (2015). Each sample was analysed thrice to ensure reproducibility.

Instrumentation and chromatographic conditions for HPLC of lignans

A Shimadzu-make HPLC (model LCATVP) equipped with a reverse phase C18 column (250 mm × 4.6 mm i.d) and UV detector (model SPD-10AVP) was used and the analysis was performed at 24 °C and 55% humidity. The mobile phase was isocratic and consisted of methanol and water (70:30), run at a flow rate of 0.7 ml/min and the peaks were detected at 290 nm.

Fatty acid analysis

Preparation of fatty acid methyl esters

Fatty acid methyl esters for GC analysis were prepared following the procedure described in Thies (1971). About 500 mg of dry clean seeds of each accession was made into a powder in a pestle and mortar and 200 mg of the powder was transferred into 12 × 75 mm size polystyrene tubes. About 1 ml of 0.5 M sodium methylate was then added and mixed using a vortex before it was left for incubation at room temperature. After 20 min, 100 µl of 5% aqueous $NaHSO_4$ was added and mixed properly. Isooctane (300 µl) was added and left undisturbed for 20 min, thereby, allowing the diffusion of fatty acid methyl esters into the upper clear organic phase. The upper clear phase was taken out gently with the help of sterile syringe and transferred to 200 µl GC vial. The analysis was performed in a Perkin Elmer GC by following the procedure of Velasco et al. (1997).

Gas chromatograph conditions for fatty acid analysis

Perkin Elmer gas chromatograph (Model Autosystem XLGC, USA) equipped with a split liner (split ratio 15:1) injector and flame ionization detector (FID) was used. Analytical separation was achieved using capillary column (30 m × 0.25 mm i.d) with 0.25 µm film thickness. The detector and injector temperatures were maintained at 280 °C and 250 °C, respectively. The oven temperature was increased from 180 to 196 °C at the rate of 4 °C/min and kept at 196 °C for 1.5 min. Temperature was further ramped from 196 to 202 °C at the rate of 4 °C/min and kept at 202 °C for 1 min. Oven temperature was again increased from 202 to 230 °C at the rate of 6 °C/min and kept at 230 °C for 1.3 min. Nitrogen was used as carrier gas, whereas hydrogen and zero air were supplied to FID to maintain 280 °C during the analysis. Carrier flow rate of 2 ml/min, hydrogen flow rate of 40 ml/min and zero air flow rate of 400 ml/min were maintained during the analysis. A sample volume of 2 µl was injected for quantitation of different fatty acid in a sample. The FAME's peaks in samples were identified by comparison with retention time of standard methyl esters (oil reference standard supplied by Sigma Aldrich) under identical GC conditions. The quantitative determination was performed by calculating the peak areas using Turbochrome Software. The peak areas were expressed as percentage of total fatty acids in a sample. Each sample was analysed thrice to ensure reproducibility.

Calculation of fatty acid desaturation ratios and oxidizing potential of the oil

Total saturated and unsaturated fatty acid content was directly read from the GC chromatogram as percentages of respective fatty acids. The GC data was used to compute oleic desaturation ratio (ODR), linoleic desaturation ratio (LDR) and oxidazibility potential (COX) of the oil by following Pleines and Friedt (1988) and Fatemi and Hammond (1980). The equations used were as follows:

(a) SFA = (%Myristic acid + %Palmitic acid + % Stearic acid + %Arachidic acid)

(b) MUFA = (%Oleic acid + %Gadoleic acid)

(c) PUFA = (%Linoleic acid + %Linolenic acid)

(d) $$\text{ODR} = \frac{(\%\text{Linoleic acid} + \%\text{Linolenic acid})}{(\%\text{Oleicacid} + \%\text{Linoleic acid} + \%\text{Linolenic acid})}$$

(e) $\text{LDR} = \frac{(\%\text{Linolenic acid})}{(\%\text{Linoleic acid}+\%\text{Linolenic acid})}$

(f) $\text{COX} = \frac{[1(18:1)+10.3(18:2)+21.6(18:3)]}{100}$

Statistical data analysis

For statistical analysis, Microsoft Excel 2007 and SPSS statistical package version 16.0.2 were used. Pearson correlation coefficient ($p < 0.01$, $p < 0.05$) was calculated by using SPSS.

Results and discussion

Lignan analysis

HPLC of reference and internal standards of lignans

Independent HPLC of the reference standards of sesamin, sesamolin and sesamol revealed their retention time (RT) in the order of 23.7, 32.0 and 6.5 min, respectively. Similarly, for the internal standard naringenin, the RT was 7.5 min. This result was reproduced when a mixture of the four standards was run in the HPLC for the calculation of Rf (Fig. 1a). Response factor for sesamin, seamolin and sesamol with respect to the naringenin was found to be 0.11, 0.09 and 0.08, respectively, which were subsequently used for the quantification of the lignans in the germplasm.

Quantification of major lignans in seeds

HPLC of ethanol extracts of sesame seeds under study revealed that sesamin and sesamolin are the major lignans present in sesame (Fig. 1b). In addition, there were up to eight other distinct peaks observed and one of them was identified as sesamol. Using TLC, it was reported earlier that there are about 15 different lignans present in sesame (Kamal-Eldin et al. 1994). Computation of lignan contents in the crude extracts of the accessions harvested over three consecutive crop seasons is presented in Table 1. An analysis of the table shows that there is considerable variation in lignan contents among the accessions tested indicating presence of divergence for the trait in the germplasm. Sesamol content on an average ranged from 0.16 to 3.24 mg/g of seed with minimum and maximum contents, respectively, in Uma and FFAT0822. Sesamin was in the range of 2.10–5.98 mg/g of seed with minimum and maximum contents, respectively, in Chandana and VRI1. Sesamolin came next to sesamin with an amount ranging from 1.52 to 3.76 mg/g seed with minimum content in Uma and maximum in Krishna. The coefficient of variation (CV) for total lignan content was 17.89%. Even though FFAT0822 ranked first in terms of total lignan content and considering sesamol as degradation product of sesamin, VRI1 remains the candidate of choice for highest sesamin content. One way ANOVA for lignan content revealed that sesamin content remained unchanged across the years but a significant seasonal variation was observed in case of the other two lignans (data not shown). Differences in secondary metabolite content among accessions with years may be attributed to micro environmental variation with respect to daily sunshine, temperature, rainfall and humidity as it has been reported in crops like soybean and also in sesame (Were et al. 2006; Cho et al. 2013; Kim et al. 2014).

While the total lignan content (for the Indian germplasm) reported here is higher than those reported for germplasm from Thailand (Rangkadilok et al. 2010), it agrees with those reported for certain exotic germplasm (Moazzami et al. 2007; Williamson et al. 2008; Bhunia et al. 2015). Our results also agree with an earlier study that showed sesamin followed by sesamolin as the major antioxidant lignans in sesame seeds (Moazzami et al. 2007; Bhunia et al. 2015). The covariance (CV) for sesamin and sesamolin were 23.76% and 22.43% respectively. Though sesamol showed highest variability, the mean sesamol content was the least among the three lignans. The difference in our observation on total lignan content from the recent report on Indian sesame could be due to exclusion of the variety VRI1 in their study (Bhunia et al. 2015). Moazzami and Kamal-Eldin (2006) reported sesamin in the range of 0.07–7.12 and sesamolin in the range of 0.21–2.9 mg/g in the 65 different sesame accessions maintained by Sesaco Corporation, USA. In European accessions, sesamin and sesamolin ranged from 1.67 to 8.0 mg and 0.5 to 2.8 mg, respectively, per gram of seed (Moazzami et al. 2007).

A comparison of seed color with respect to mean lignan content revealed that black seeded varieties contain highest sesamin, sesamolin and total lignan content, while white seeded varieties contain high sesamol content (Table S1). Similar observation was reported by Shi et al. (2017), where black sesame seeds were found rich in these types of lignans. But the results were contradictory with the report on Korean sesame in which white seeds were shown to have higher lignan content (Kim et al. 2014). The CV for total lignan content was found highest for white seeds followed by brown and black seed varieties (Table S1). The black Indian sesame with its higher lignan content could be considered nutrition rich and thus may be recommended for incorporation in human health foods and as supplements in nutraceuticals. A distribution plot of population size verses sesamol content showed skewness towards left side with majority of the accessions falling in the class range 0–1 mg/g of seed (Fig. 2a). In case of sesamin, the

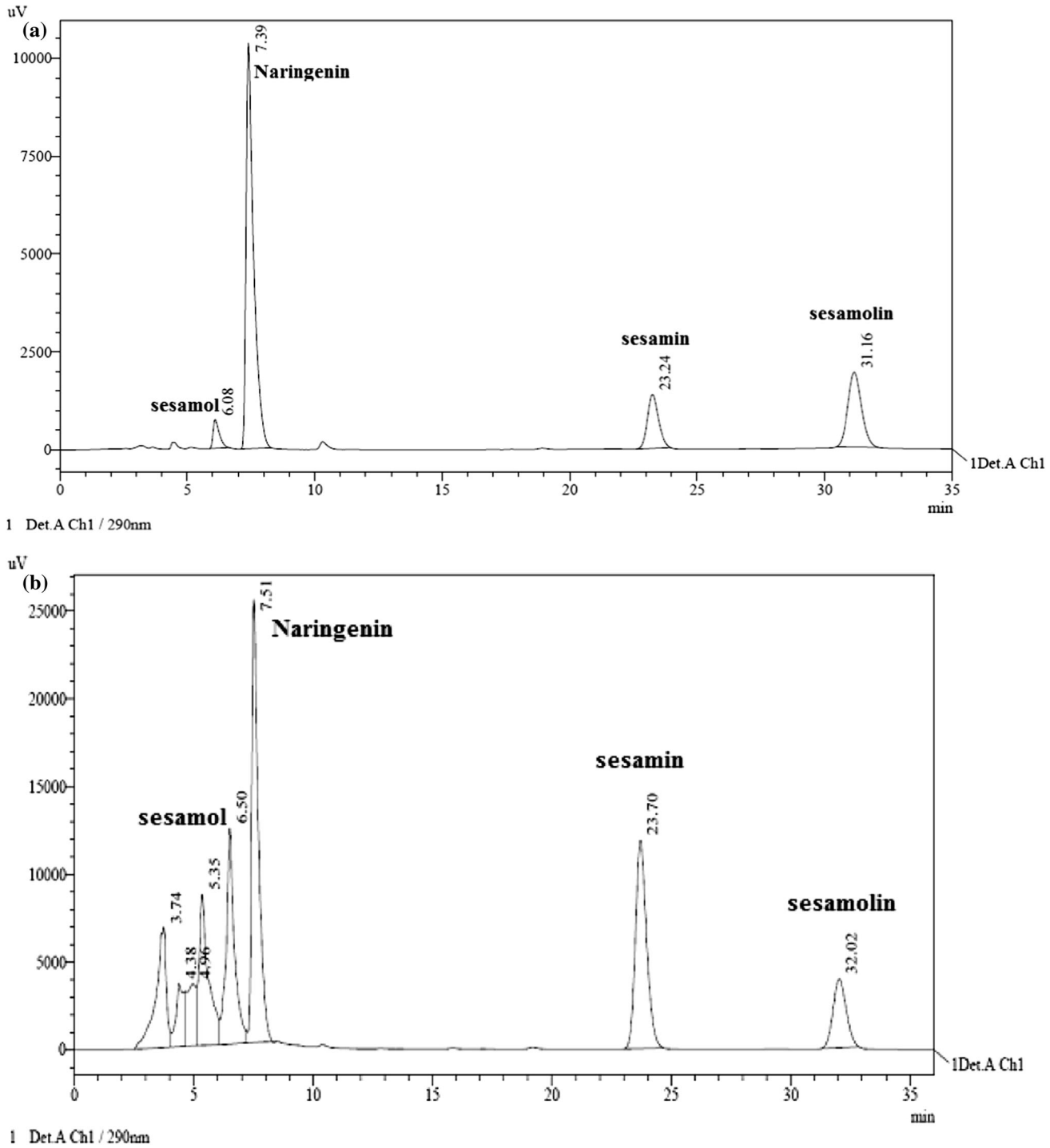

Fig. 1 HPLC of lignans of *Sesamum indicum* L. **a** A picture of detector response to HPLC of a mixture of reference standards sesamol, naringenin (internal standard), sesamin and sesamolin showing peaks at their corresponding retention times. **b** HPLC profile of ethanol extract of seeds of *S. indicum* var. T78 showing prominent peaks corresponding to major sesame lignans and the internal standard shown in **a** above indicating their presence in the extract

plot turned out to be Gaussian type with accessions having 3–4 mg/g of seed constituting the highest frequency class. The four frequency classes recognised here gives an impression that there could be multiple genes controlling this trait (Fig. 2b). Similar is the case for sesamolin where the population resolved into five major classes (Fig. 2c).

Fatty acid analysis

Fatty acid profiling by gas chromatography

A picture of the chromatograph showing fatty acid profile of sesame seeds of variety Chandana by GC is presented in Fig. 3. It shows two major peaks for the unsaturated fatty acids, oleate (18:1) and linoleate (18:2). In addition, there are two distinct but smaller peaks representing saturated palmitate (16:0) and stearate (18:0). Mean percent fraction of such fatty acids in different accessions of *S. indicum* studied over a period of 3 years is presented in Table 2. Analysis of the data given in the table clearly shows that oleate and linoleate are the main fatty acid constituents of sesame seed, together constituting about 84% of the total fatty acids. Palmitate and stearate are the abundant saturated fatty acids constituting about 15% of total fatty acids.

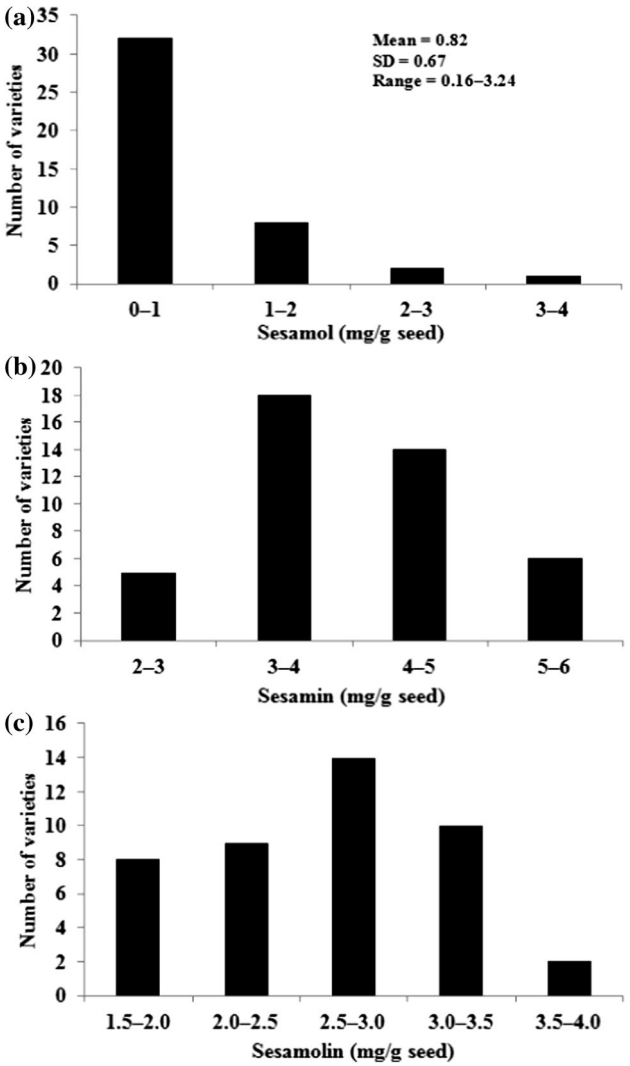

Fig. 2 Frequency distribution of the accessions of *Sesamum indicum* L. for the seed lignan content. **a** sesamol, **b** sesamin and **c** sesamolin

Linoleneate (18:3), arachidate (20:0) and gadoleate (20:1) were the other prominent FAs but were found in trace amounts in the germplasm. Palmitate ranged from 8.94 to 11.02% with minimum in Prachi and maximum in T12. Stearate ranged from 4.05 to 5.89% with lowest in AKT64 and highest in Prachi. The percentage of oleate was found minimum (34.71%) in DS1 but maximum (45.61%) in Prachi. However, linoleate was least (38.49%) in Prachi but highest (49.60%) in DS1. Unlike lignans, that showed considerable variation among the accessions, the fatty acid fractions did not change much and remained almost stable across the years. The results were consistent with the earlier reports on exotic and other germplasm (Were et al. 2006), but were contradictory with the report of Bhunia et al. (2015) where T12, DS1 showed a different percentages for FA content. The difference may be attributed to environmental or soil conditions in which the crops were raised. Yermanos et al. (1972) in an earlier report indicated that the sesame is characterised by 39.6% oleate, 46% linoleate, 9.5% palmitate and 4.4% stearate. Similarly Were et al. (2006) observed linoleate as the major component of fatty acids in East African sesame accessions. Similar results were also reported in Turkish germplasm as well (Uzun et al. 2008). From the studies outlined above, including the present study, it is evident that the linoleate is the major component of the total fatty acids in the sesame seeds. Mondal et al. (2010) and Bhunia et al. (2015) however found oleate to be the major fatty acid in certain Indian varieties of sesame. As far as variability is concerned, a maximum variability of 4% could be observed for both oleate and linoleate, indicating a possibility of marginal improvement that can be achieved for this trait by breeding.

As far as seed coat colour is concerned, oleic acid was found little higher in black seeds followed by white and brown seeds (Table S2). The distribution plot of major fatty acids showed that the highest frequency class for palmitic and stearic acids fell in the region of 9–11% and 4.5–5.0%, respectively (Fig. S1A and S1B). Highest frequency class for oleic and linoleic acids, fell in the region of 40–43% and 41–43%, respectively (Fig. S1C and S1D). The total saturated fatty acid content (SFA) ranged from 14.29 to 16.19% with maximum percentage in T12 and minimum in XLM19. Total saturated fatty acid content in sesame is in the levels that are recommended for human consumption. Polyunsaturated fatty acid (PUFA) and monounsaturated fatty acid (MUFA) contents are the attributes that determine the suitability of edible oil in human nutrition. The MUFA content was highest in Prachi (45.69%) and lowest in DS1 (35.03%). The high MUFA level is responsible for maintenance of oil quality and shelf life. As far as PUFA is concerned, it is maximum in DS1 (49.95%) and minimum

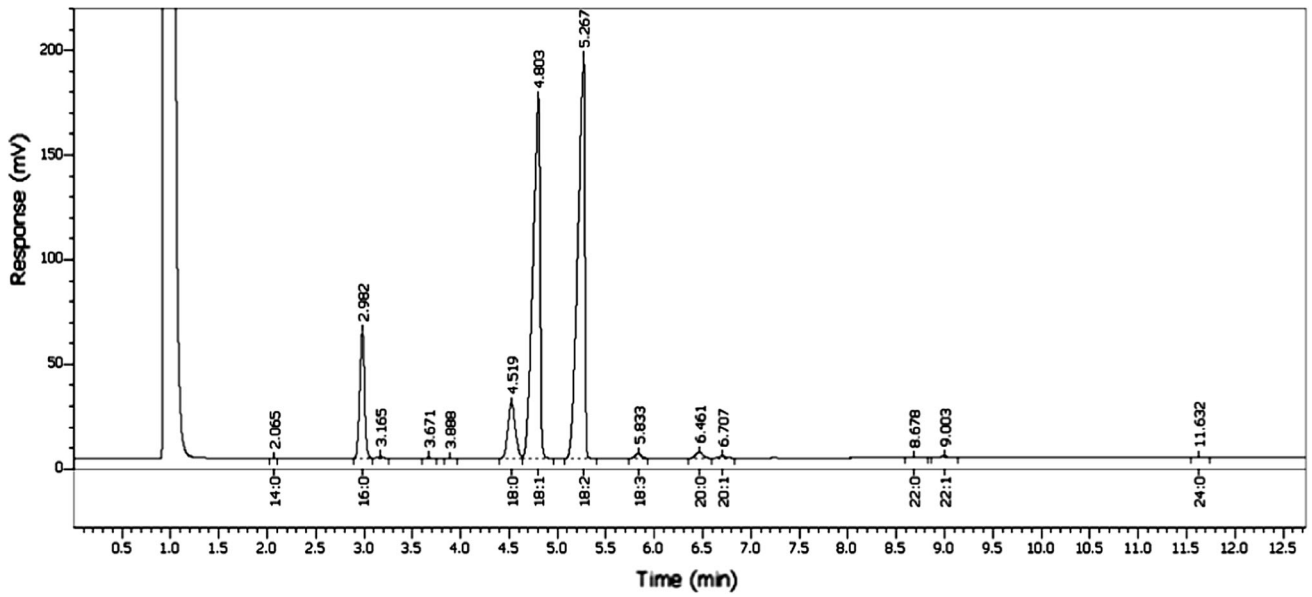

Fig. 3 GC of fatty acid methyl esters (FAME) prepared from seeds of *Sesamum indicum* L. The picture presents detector response to GC of the preparation from seeds of the sesame variety Chandana showing peaks corresponding to 12 different fractions of fatty acids (FA). Details of the prominent FA fraction are explained in the text

in Prachi (38.89%). For stability of oil, a low level of PUFA is preferred (Table 2).

Desaturation efficiency and oxidizing potential of the oil

An estimate of relative efficiency of desaturation pathway operating in the crop is an important attribute to be considered before designing breeding programmes. The estimated oleic and linoleic acid desaturation efficiencies for sesame is presented in Table 2. The mean ODR estimated for sesame germplasm was 0.515 with a minimum ODR value of 0.460 found in Prachi and a maximum value of 0.590 in DS1. A high ODR indicates considerably higher conversion of oleic acid to linoleic acid and thereby implying that this conversion being efficient (Velasco et al. 1997; Mondal et al. 2010). However, the LDR was found to be very insignificant with the mean value of 0.008 implying that the linoleic desaturation pathway is lacking in the crop. Therefore, we conclude that the pathway converting oleic acid to linoleic is only operative in *S. indicum*.

An estimation of oxidizability (COX) helps to infer the capacity of the oil to resist oxidation and thereby its stability (Coni et al. 2004). In this regard, DS1 exhibited maximum oxidizability value of 5.532, while Prachi had the minimum value of 4.508 (Table 2). Oils with higher oxidizability value have higher tendency to undergo auto oxidation. The seed colour appeared to be non-influential on fatty acid content in the present germplasm (Table S2).

Correlation between lignans and fatty acids

Pearson analysis revealed a positive correlation of 0.55 ($p < 0.01$) between sesamin and sesamolin, and a negative correlation value for these two with that of sesamol (Table 3). Similar correlation was reported earlier in Indian sesame by Bhunia et al. (2015). Since, fatty acids are synthesized from FAS complex in a sequential manner, a correlation study would enable better understanding of the relationship in their biosynthesis. The data on Pearson analysis of correlation coefficient for the major fatty acids is presented in Table 3. Computation for the oleic and linoleic acid content revealed a strong negative correlation of -0.960 ($p < 0.01$), as has been reported earlier in sesame (Were et al. 2006) and soybean (Patil et al. 2007). A negative correlation was also observed between palmitic and stearic acid (-0.440, $p < 0.01$), palmitic and arachidic acid (-0.396, $p < 0.01$), arachidic and gadoleic acid (-0.459, $p < 0.01$). Such inverse relationships have been attributed to the combined influence of environment and the constituent genotype (Uzun et al. 2008). A positive correlation, however, was found between stearic and arachidic acid (0.531, $p < 0.01$). The elongation of 16-carbon acyl chains followed by desaturation plays a vital role in regulation of the relative amounts of palmitic acid and the other fatty acids derived from it (Carlsson et al. 2000). A deficiency in this step has lead to the reduction in the amounts of 18-carbon fatty acids and increase in the palmitic acid content of plant tissues. This has been considered as the cause observed in the correlations (Were et al. 2006).

Table 2 Mean data of fatty acid attributes estimated over a period of 3 years by GC in the germplasm of *Sesamum indicum* L.

Variety name	Saturated fatty acid (%)				Unsaturated fatty acid (%)			SFA (%)	MUFA (%)	PUFA (%)	ODR	LDR	COX
	Palmitate	Stearate	Arachidate	Oleate	Linoleate	Linolinate	Gadoleate						
AKT64	10.50	4.05	0.34	39.93	44.56	0.33	0.30	14.893	40.236	44.890	0.529	0.007	5.061
Amrit	10.08	5.19	0.70	39.21	44.45	0.38	0.09	15.966	39.299	44.823	0.533	0.008	5.052
Chandana	9.63	5.55	0.52	38.86	44.46	0.44	0.36	15.692	39.220	44.893	0.536	0.010	5.062
DS1	9.58	4.86	0.42	34.71	49.60	0.35	0.33	14.862	35.033	49.951	0.590	0.007	5.532
E8	9.55	5.06	0.43	39.31	44.81	0.34	0.37	15.042	39.677	45.142	0.535	0.007	5.081
FFAT0822	10.39	4.25	0.50	41.83	42.35	0.39	0.19	15.144	42.021	42.744	0.505	0.009	4.865
GT1	9.73	4.72	0.42	41.78	42.49	0.34	0.35	14.874	42.133	42.833	0.506	0.008	4.868
GT2	9.81	4.61	0.53	40.54	44.32	0.43	0.23	14.952	40.776	44.749	0.525	0.010	5.063
JLT1	10.81	4.73	0.48	40.48	42.93	0.31	0.29	16.016	40.769	43.232	0.516	0.007	4.892
JLT7	10.43	4.61	0.50	39.88	43.97	0.39	0.19	15.536	40.073	44.363	0.527	0.009	5.013
JLT26	10.62	4.50	0.39	41.71	42.50	0.36	0.34	15.516	42.052	42.863	0.507	0.008	4.873
JT7	10.26	4.68	0.41	41.74	42.09	0.40	0.33	15.348	42.069	42.493	0.504	0.009	4.839
JTS8	10.26	4.50	0.41	42.11	42.48	0.37	0.21	15.180	42.318	42.850	0.504	0.009	4.876
Kallika	9.42	4.84	0.40	40.51	44.36	0.35	0.24	14.663	40.743	44.704	0.525	0.008	5.049
Krishna	10.07	4.79	0.52	41.55	42.13	0.39	0.40	15.381	41.941	42.523	0.506	0.009	4.840
N8	10.24	4.19	0.51	36.46	48.10	0.46	0.22	14.950	36.683	48.553	0.571	0.009	5.417
N32	10.09	4.71	0.42	41.68	43.06	0.22	0.07	15.220	41.746	43.279	0.509	0.005	4.899
Nirmala	10.36	4.88	0.73	38.46	45.00	0.36	0.06	15.972	38.524	45.364	0.541	0.008	5.098
Phuletil	10.55	4.92	0.39	41.57	42.19	0.34	0.24	15.863	41.810	42.527	0.506	0.008	4.834
Prachi	8.94	5.89	0.91	45.61	38.49	0.41	0.08	15.733	45.688	38.893	0.460	0.010	4.508
Praghti	10.65	4.43	0.39	42.14	41.93	0.32	0.14	15.468	42.288	42.248	0.501	0.008	4.809
Rajeswari	10.30	4.53	0.37	40.89	43.26	0.44	0.18	15.196	41.068	43.701	0.517	0.010	4.960
RT103	10.41	4.48	0.60	41.70	42.56	0.38	0.20	15.487	41.902	42.933	0.507	0.009	4.882
RT125	9.33	5.01	0.61	40.57	43.95	0.38	0.24	14.953	40.802	44.327	0.522	0.009	5.014
RT127	10.18	4.66	0.44	42.22	42.19	0.25	0.35	15.283	42.577	42.437	0.501	0.006	4.822
SVPR1	9.99	5.14	0.50	41.17	42.90	0.36	0.23	15.629	41.404	43.256	0.512	0.008	4.908
T12	11.02	4.78	0.39	40.73	42.61	0.35	0.22	16.192	40.954	42.963	0.513	0.008	4.872
T13	10.57	4.80	0.44	40.68	43.57	0.33	0.12	15.803	40.800	43.899	0.519	0.007	4.965
T78	9.98	4.40	0.57	40.15	44.57	0.28	0.21	14.947	40.364	44.856	0.528	0.006	5.054
Tarun	10.10	4.40	0.55	40.61	43.96	0.36	0.19	15.050	40.799	44.320	0.522	0.008	5.012
TC25	9.61	4.41	0.37	42.99	42.29	0.36	0.22	14.388	43.201	42.644	0.498	0.008	4.863
TC289	9.95	4.15	0.41	42.16	43.28	0.39	0.34	14.510	42.492	43.669	0.509	0.009	4.964

Table 2 continued

Variety name	Saturated fatty acid (%)				Unsaturated fatty acid (%)			SFA (%)	MUFA (%)	PUFA (%)	ODR	LDR	COX
	Palmitate	Stearate	Arachidate	Oleate	Linoleate	Linolinate	Gadoleate						
TKG22	9.73	4.57	0.58	41.80	42.90	0.39	0.22	14.883	42.020	43.282	0.509	0.009	4.920
TKG55	9.96	4.67	0.47	42.43	41.84	0.40	0.36	15.098	42.783	42.238	0.499	0.009	4.820
TMV3	9.77	4.89	0.61	42.33	41.71	0.39	0.20	15.262	42.530	42.093	0.499	0.009	4.803
TMV4	9.56	5.01	0.53	42.95	42.24	0.33	0.29	15.094	43.233	42.569	0.498	0.008	4.851
TMV5	9.80	5.03	0.52	42.91	41.67	0.38	0.33	15.357	43.234	42.049	0.495	0.009	4.803
TMV6	9.88	4.72	0.55	42.34	42.38	0.27	0.20	15.146	42.543	42.653	0.502	0.006	4.847
Uma	10.02	4.92	0.62	38.35	45.34	0.41	0.18	15.556	38.526	45.751	0.544	0.009	5.142
Vinayak	9.57	4.58	0.45	41.13	43.54	0.25	0.37	14.600	41.501	43.791	0.516	0.006	4.950
VRI1	9.45	5.14	0.62	42.45	41.66	0.37	0.22	15.206	42.671	42.030	0.497	0.009	4.796
XLM19	9.60	4.27	0.42	43.09	42.09	0.36	0.25	14.288	43.343	42.444	0.496	0.008	4.843
YLM17	9.76	4.44	0.65	41.76	42.76	0.24	0.21	14.850	41.976	43.009	0.507	0.006	4.875
Mean	10.01	4.72	0.50	41.06	43.24	0.36	0.24	15.234	41.298	43.601	0.515	0.008	4.942
SD	0.44	0.36	0.11	1.85	1.77	0.05	0.09	0.446	1.849	1.772	0.021	0.001	0.166
CV	4.39	7.59	22.74	4.51	4.08	15.12	36.35	2.928	4.477	4.064	4.116	15.174	3.354
Minimum	8.94	4.05	0.34	34.71	38.49	0.22	0.06	14.288	35.033	38.893	0.460	0.005	4.508
Maximum	11.02	5.89	0.91	45.61	49.60	0.46	0.40	16.192	45.688	49.951	0.590	0.010	5.532

SFA saturated fatty acid, *MUFA* monounsaturated fatty acid, *PUFA* polyunsaturated fatty acid, *ODR* oleic desaturation ratio, *LDR* linoleic desaturation ratio, *COX* oxidizability value

Table 3 Pearson correlation between different lignan and fatty acid components of the oilseed crop *Sesamum indicu*m L.

	Palmitic acid	Stearic acid	Oleic acid	Linoleic acid	Linolenic acid	Arachidic acid	Gadoleic acid	Sesamol	Sesamin
Stearic acid	− 0.440*								
Oleic acid	− 0.182	0.073							
Linoleic acid	0.064	− 0.209	− **0.960***						
Linolenic acid	− 0.063	0.160	− 0.161	0.106					
Arachidic acid	− 0.396*	0.531*	0.096	− 0.164	0.166				
Gadoleic acid	− 0.133	− 0.101	− 0.037	0.064	0.017	− 0.459*			
Sesamol	0.336**	− 0.278	− 0.028	− 0.033	− 0.094	− 0.227	− 0.102		
Sesamin	− 0.192	0.336**	0.105	− 0.133	0.033	0.093	− 0.027	− 0.268**	
Sesamolin	− 0.188	0.145	0.426*	− 0.438*	− 0.121	− 0.052	0.219	− 0.256**	**0.550***

Bold values indicate the Pearson values for the highly correlating components

*Correlation is significant at the 0.01 level, **correlation is significant at the 0.05 level

Biosynthesis of lignans and fatty acids follows entirely different pathways but finally they are targeted towards the seeds. Therefore it would be worthwhile to analyse the data obtained to find if there is any relationship in the production and distribution of the two metabolites. Analysis of the results showed presence of some positive correlation between oleic acid and sesamolin (0.426, $p < 0.01$), palmitic acid and sesamol (0.336, $p < 0.05$), stearic acid and sesamin (0.336, $p < 0.05$). A negative correlation was observed for linoleic acid and sesamolin content (−0.438, $p < 0.01$). However, further studies are required to find out if there is any definite link between the two biosynthetic pathways. Modern plant breeding relies on integration of techniques such as classical breeding, induced mutations and transgenic technology for genetic enhancement of qualitative and quantitative traits in plants (Zhao et al. 2009). Crops like Safflower and soybean have been earlier improved through mutation breeding (Sahu et al. 1980; Rahman et al. 1996). Mutagenesis has also been reported in sesame with an improvement in the seed oil content and fatty acid composition (Savant and Kothekar 2011). Recent report on sesame genome sequencing has opened up a new face for researchers to study this orphan crop thoroughly for genetic improvement (Zhang et al. 2013). It is our endeavour that researches on lignan and fatty acid biosynthetic mechanisms in sesame would definitely lead to altering of genes for improvement of nutritional quality of edible oil.

Conclusion

The lignan and fatty acid profile of different varieties of *S. indicum* L. cultivated in diverse agroclimatic regions of India is reported. The data from the present study revealed presence of considerable variability among the accessions for lignan and fatty acid contents. A positive correlation found between lignans and fatty acids indicates possibility of a link between the lignan and fatty acid biosynthetic pathways. However, further study is required to establish this relationship between the two traits. Due to rich source of antioxidant lignans and unsaturated fatty acids, sesame seeds can be effectively used as nutraceuticals and as functional foods. The study has led to identification of varieties with desirable nutritional composition that can be recommended for nutraceuticals and medical applications. Such varieties include VRI1, SVPR1 and E8 for sesamin; Krishna, RT125 and Rajeswari for sesamolin; FFAT0822, SVPR1 and Phule til for total lignan content; Prachi and XLM19 for oleic acid; and DS1 and N8 for linoleic acid. These varieties may be considered as superior lines for the traits cited. The black seeded sesame being rich in sesamin, sesamolin, total lignan content and oleic acid have been identified to be nutritionally and pharmaceutically more important than white and brown sesame. The variability reported in this study would serve as base line for transferring favourable genes into desirable varieties by breeding to enhance the nutritional value and quality of the crop.

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Compliance with ethical standards

Conflict of interest The authors declare that there is no conflict of interest.

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