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To cite this article: Fahmidha Halaldeen, Izfah Zahir, Savani Ulpathakumbura, Lalith Jayasinghe, Nazrim Marikkar, Muneeb M. Musthafa, Mohammed Arshad, Abdul Aziz Al Kheraif, Fohad Mabood Husain & Mohd Adil (2024) Characterization of oils and defatted residues of *Terminalia catappa* L. seed kernels of two varieties, International Journal of Food Properties, 27:1, 30-43, DOI: [10.1080/10942912.2024.2426666](https://doi.org/10.1080/10942912.2024.2426666)

To link to this article: <https://doi.org/10.1080/10942912.2024.2426666>



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Published online: 11 Nov 2024.



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## Characterization of oils and defatted residues of *Terminalia catappa* L. seed kernels of two varieties

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### ABSTRACT

The seed kernel of *Terminalia catappa* Linn (*T. catappa*) is an underutilized plant food with promising potential. This study investigated the physico-chemical properties, fatty acid composition, thermal behavior, and Fourier transform infrared (FTIR) spectral characteristics of oils extracted from kernels of yellow and purple cultivars of *T. catappa* and proximate compositions of their defatted residues. The oils extracted through a cold press micro-exPELLER, differed in color, with yellow oil being lighter than purple oil. Both cultivars demonstrated high iodine values and lower saponification values. Thermal profiles displayed major exothermic and endothermic peaks associated with the crystallization and melting of triacylglycerols (TAGs). Both oils were rich in unsaturated fatty acids (USFAs), particularly oleic and linoleic acids, with palmitic acid being the predominant saturated fatty acid (SFA). FTIR spectra indicated the presence of functional groups such as methyl, methylene and esters representing the complex composition of the oils. Proximate composition analysis revealed that whole kernels were high in fat, while defatted residues were richer in protein and minerals. These findings suggest that *T. catappa* kernels from both cultivars were good sources of plant oils with potential for high-fat products, and defatted residues could be used in protein-rich supplements, offering diverse industrial applications.

### ARTICLE HISTORY

Received 2 September 2024  
Revised 23 October 2024  
Accepted 1 November 2024

### KEYWORDS

Fatty acid composition;  
Food; FTIR; Protein; Thermal  
profile

## Introduction

*Terminalia catappa* Linn (*T. catappa*) (Family: Combretaceae) is a plant species found across many tropical and subtropical zones of the Indian and Pacific Oceans. It is planted extensively as an ornamental tree<sup>[1]</sup> and is widely known for its medicinal properties. Various species of this genus have documented uses for traditional drug development in both East and West African countries.<sup>[2]</sup> Several parts of *T. catappa* have already been used for treatment of skin conditions such as scabies, gonorrhoea, and diarrhoea.<sup>[3]</sup> Some previous research suggested that dysentery can be treated with any part of this tree, including the bark, fruits, and leaves.<sup>[4]</sup> According to Untwal and Kondawar,<sup>[5]</sup> the fruits might have the potential for treatment of leprosy, headaches,

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and travel sickness. Its leaf, bark, and fruits are exploited in India, Indonesia, and the Philippines for antidiarrheic, antipyretic, and hemostatic purposes.<sup>[6]</sup> In the reproductive health, the seed kernel of *T. catappa* has been recognized as a potent component as it was identified to have sexual stimulant properties, that might help to treat premature ejaculation.<sup>[3]</sup> Other than these, different parts of this plant were also found to exhibit several other pharmacological effects.

*T. catappa* tree produces edible fruits having a seed with hard shell.<sup>[7]</sup> The fruits are sessile, laterally compressed, smoothly skinned, and have ovoid to ovate-shaped drupes.<sup>[8]</sup> The hard nut contains an edible kernel, which is similar in shape, size and taste to almond seeds. The kernel consists of two delicate cotyledons protected by a pale brown seed coat. There is limited information on inter-varietal comparison of nutritional composition, utilization and physicochemical properties of the *T. catappa* oil and defatted residues. By comparing the nutrient composition of oil and defatted residues, they can be utilized as base materials for human diets as well as for medicinal uses. The seed kernels of *T. catappa* contain about 60% oil,<sup>[9]</sup> which is extracted either through machine pressing or using solvents as extraction media.<sup>[10,11]</sup> According to previous studies, oil is reported to have contained more than 50% of USFA, with high proportions of oleic and linoleic,<sup>[12]</sup> making it beneficial for cardiovascular health. In recent times, the seed kernel of *T. catappa* received considerable interest due to its health benefits such as ability to lower low-density lipoprotein (LDL) cholesterol, while maintaining high-density lipoprotein (HDL) cholesterol.<sup>[13]</sup> Based on the fatty acid (FA) composition of the seed kernel oil reported from other parts of the world, it could be an alternative food ingredient for unsaturated vegetable oil.<sup>[14]</sup> Although there has been considerable amount of research studies on the medicinal properties of the stem-bark, roots, fruits, and leaves of *T. catappa*, studies strictly focused on the inter-varietal differences of cold-pressed oils extracted from its yellow and purple cultivars and their defatted residues are scanty. Hence, the aim of this research was to characterize the oils by evaluating its physicochemical characteristics, fatty acid profile, thermal behavior, FTIR spectral characteristics and proximate compositions of their defatted residues.

## Materials and methods

### Sampling

Fruit seeds from the yellow and purple cultivars of *T. catappa* were collected in Sri Lanka's Central Province between February and April 2023. Fruit seeds were initially dried at 55°C for 8 h using blower-assisted drying oven (Biobase, model – BOV-V230F, China). Once dried, the seeds were cracked open to separate out the kernels. The kernels were refrigerated until further testing. Analytical grade chemicals and reagents were used in the assays unless stated otherwise.

### Micro-expeller extraction

Prior oil extraction, dried kernels of individual cultivars were placed in a blower-assisted drying oven (Biobase, model – BOV-V230F, China) at 70°C for 8 h. Following drying, the kernels were cold pressed using a micro-oil expeller (Komet DD85 machine, Germany) to extract the oil. After extraction, the crude oil from each cultivar was purified through gravitational filtration and kept under refrigerated conditions until further analysis.

### Physicochemical characteristics of the oil

**Color:** The oil color was determined using a Lovibond Tintometer (PFX-I UK) and reported in terms of red (R) and yellow (Y) units (Y +5 R) according to AOCS Method Cc 13b-45.<sup>[15]</sup>

**Iodine Value:** The iodine value of the oil sample was measured using the AOCS Method Cd 1d-92.<sup>[16]</sup> Initially, 10.0 mL of chloroform was added to an iodine flask containing 0.5 g of the oil sample. Then, 25.0 mL of iodine solution was introduced, and the flask was kept in darkness for 1 h. After that, 10.0 mL of 10% potassium iodide solution was added, and the mixture was shaken thoroughly. Next, 75.0 mL of distilled water was added. Then, the mixture was titrated with 0.1N sodium thiosulfate until it turned nearly colorless. Finally, 1% starch solution was added, and titration was carried out until the blue color vanished.

$$\text{Iodine Value} = (B - S) \times N \times 100 / \text{Weight of oil sample}$$

where:

$B$  - Volume of  $\text{Na}_2\text{S}_2\text{O}_3$  used for the blank  $S$  - Volume of  $\text{Na}_2\text{S}_2\text{O}_3$  used for the oil sample

$N$  - Normality of  $\text{Na}_2\text{S}_2\text{O}_3$  solution

**Saponification Value:** The saponification value of the oil was measured following the AOCS method Cd 3-25.<sup>[15]</sup> Initially, 5 g of oil sample was dissolved in 50.0 mL of 4% ethanolic KOH in a round bottom flask. The flask was then refluxed for 30 min to achieve complete saponification of the sample. After cooling, a few drops of phenolphthalein were added to the mixture. It was then titrated with 0.5 N HCl until the pink color disappeared completely.

$$\text{Saponification Value} = (V_B - V_S) \times 28.05 / \text{Weight of oil sample}$$

where:  $V_B$  - Volume required for the blank,  $V_S$  - Volume required for the oil sample

### Fatty acid analysis

Analysis of FA was conducted following the procedure described by Gunarathne *et al.*<sup>[17]</sup> with minor adjustments. An oil sample (0.4 g) was placed into screw-capped glass tubes, to which 4.0 mL of methanol and 0.1 mL of methanolic KOH were added. The mixture was heated to 60°C in a water bath for 10 min, then allowed to cool. Next, 2.0 mL of hexane and 4.0 mL of distilled water were added. The contents were vortexed at 2500 rpm for 10 min. Once the layers separated, the upper layer was injected into a gas chromatograph (Agilent 7890B, China) fitted with a flame ionization detector (FID). The analysis utilized a polar capillary column (100 m × 250 μm × 0.2 μm, CP-Sil 88 for FAME) with a column pressure of 39.512 psi. The oven temperature was programmed as follows: an initial temperature 100°C for 5 min, increased from 100 to 180°C at 8 °C/min, from 180 to 230°C at 1 °C/min and held at 230°C for 15 min. The injector and detector temperatures were set to 260°C. Nitrogen was used as the carrier gas at a flow rate of 1.2863 mL/min, and the injector was operated with a split ratio of 50:1. FAs were identified by comparing their retention times to those of standard fatty acid methyl esters, their percentages were calculated based on the peak area relative to the total peak areas for all FAs.

### Thermal analysis of oil by DSC

Differential scanning calorimetric (DSC) analysis was carried out following the method outlined by Gunarathne *et al.*<sup>[17]</sup> with some adjustments. The Q200 differential scanning calorimeter (TA Instruments, USA) was employed for the analysis, using an aluminum T zero pan with a T zero hermetic lid. Nitrogen gas with a purity of 99.9% was used as the purge gas at a flow rate of 50.00 mL/min. Approximately 10–12 mg of the sample (in liquid form) was loaded into a standard DSC aluminum pan and sealed hermetically. An empty hermetically sealed aluminum pan was served as a reference. The thermal analysis was conducted using the following temperature program: an isotherm at -40°C for 1 min, followed by heating at 5 °C/min to 40°C, an isotherm at 40°C for 1 min, and then cooling at 5 °C/min back to -40°C.

### FTIR measurements

The oil samples were subjected to FTIR measurements using the method outlined by Gunarathne *et al.*<sup>[18]</sup> with few amendments. In each measurement, a 100 mg portion of KBr (FT-IR grade, 99% trace metals basis, Sigma Aldrich) was combined with approximately 1.0 mg of oil to create a pallet. The mid-infrared spectra, covering the range of 4000–500  $\text{cm}^{-1}$ , were recorded using a FTIR Nicolet iS50 spectrometer (Thermo Nicolet, Madison, WI) equipped with a deuterated triglycine sulfate (DTGS) detector and KBr beam splitter. The spectra were collected by co-adding 64 scans with a resolution of 8  $\text{cm}^{-1}$ . Each spectrum was compared to a background spectrum of pure KBr, and absorbance values were recorded in four duplicates.

### Proximate analysis

The proximate compositional analysis of whole kernels and defatted residues from different cultivars was conducted to assess moisture, crude fat, total ash, and protein contents, following the procedures outlined in the AOAC International (2019) manual.<sup>[19]</sup> Moisture content was measured using an oven (Biobase, model – BOV-V230F, China) by drying samples at 105°C for 3 hours until constant weight was achieved (AOAC Official Method 934.06). Crude fat content was determined through Soxhlet extraction with hexane (40–60°C) as the solvent (AOAC Official Method 948.22). The ash content was measured using the dry ashing method (AOAC Official Method 942.05), while crude protein was assessed using the micro Kjeldahl method (AOAC Official Method 970.02). The total carbohydrate content was calculated with the formula: Total Carbohydrate content (%) = 100 – % (Moisture + ash + protein + fat).

### Spectral analysis

Spectral pre-processing and qualitative analysis were carried out using the manufacturer's software (OMNIC, version 7.0 Thermo Nicolet). Baseline correction and scale normalization processes were applied to the raw spectra of the purple and yellow cultivars.

### Statistical analysis

In this study, chemical measurements were performed in triplicate ( $n = 3$ ), and results were reported as mean  $\pm$  standard deviation (SD). Statistical analysis was conducted using one-way analysis of variance (ANOVA) with Tukey's Test, utilizing the Minitab 17 software package.

## Results

### Physicochemical characteristics of *T. catappa* oil

The color, iodine value, and saponification value of the oils from the two cultivars are given in Table 1. Based on the overt observation, the colors of the oil samples of the *T. catappa* were a little lighter and

**Table 1.** Color, iodine value and saponification value of oil from purple and yellow cultivars of *T. catappa* seed kernel.

Parameter	Yellow cultivar	Purple cultivar
Color	Y +5 R = 12.0	Y +5 R = 13.0
IV (g I <sub>2</sub> /100 g)	90.20 <sup>a</sup> $\pm$ 0.85	91.81 <sup>a</sup> $\pm$ 2.46
SV (mg KOH/g)	174.15 <sup>a</sup> $\pm$ 0.02	179.80 <sup>b</sup> $\pm$ 0.14

Each value in the table represents the mean of three replicates  $\pm$  standard deviation. The means within each row bearing different superscripts are significantly ( $p < .05$ ) different. Abbreviations: IV, iodine value; SV, saponification value.

compatible with the individual color values obtained from the Lovi-bond tintometer. As presented in Table 1, the color of *T. catappa* yellow cultivar was lighter than that of *T. catappa* purple cultivar. As shown in Table 1, iodine values of oils obtained from *T. catappa* purple and yellow cultivars were 91.81 and 90.20, respectively. Apparently, no significant ( $p > .05$ ) differences were found between the two cultivars in terms of their degree of unsaturation. It is clear from Table 1 that the saponification value (SV) of *T. catappa* purple and yellow were 179.80 and 174.15, respectively. Based on statistical analysis, remarkable ( $p < .05$ ) differences were noticed between them.

### Fatty acid profile of *T. catappa* oil

The FA profiles for the oils from the two cultivars of *T. catappa* are given in Table 2. The major FAs in both cultivars were palmitic, followed by oleic and linoleic acid. It is quite clear that the FA profile of the oils was remarkably different from those of coconut and palm kernel oils as they were lauric dominant oils. As shown in Table 2, the oils from both purple and yellow cultivars predominantly contained USFAs, with totals of 57.16% and 57.40%, respectively. The total SFA in the oils of purple and yellow cultivars were 42.84% and 42.60%, respectively. In *T. catappa* oils, palmitic acid was identified as the most dominant SFA, making up 36.06% in the purple cultivar and 33.28% in the yellow cultivar. Other SFAs, including butyric, lauric, myristic, stearic, arachidic and lignoceric acids were present in low amounts. Remarkable ( $p < .05$ ) differences were found between the two cultivars with regard to all SFAs except stearic and arachidic acids. According to Table 2, the most predominant USFAs in both cultivars were oleic and linoleic acids. The proportions of oleic acid in the purple and yellow cultivars were 28.34% and 30.09%, respectively. Likewise, linoleic acid proportions of purple and yellow cultivars were  $27.45 \pm 0.14\%$  and  $25.16 \pm 0.05\%$ , respectively. Polyunsaturated fatty acids (PUFA) such as Eicosapentaenoic acid (EPA) and Docosahexaenoic acid (DHA) were present in lesser amounts. Between the two cultivars, remarkable differences ( $p < .05$ ) were found only in the oleic, linoleic, and DHA contents.

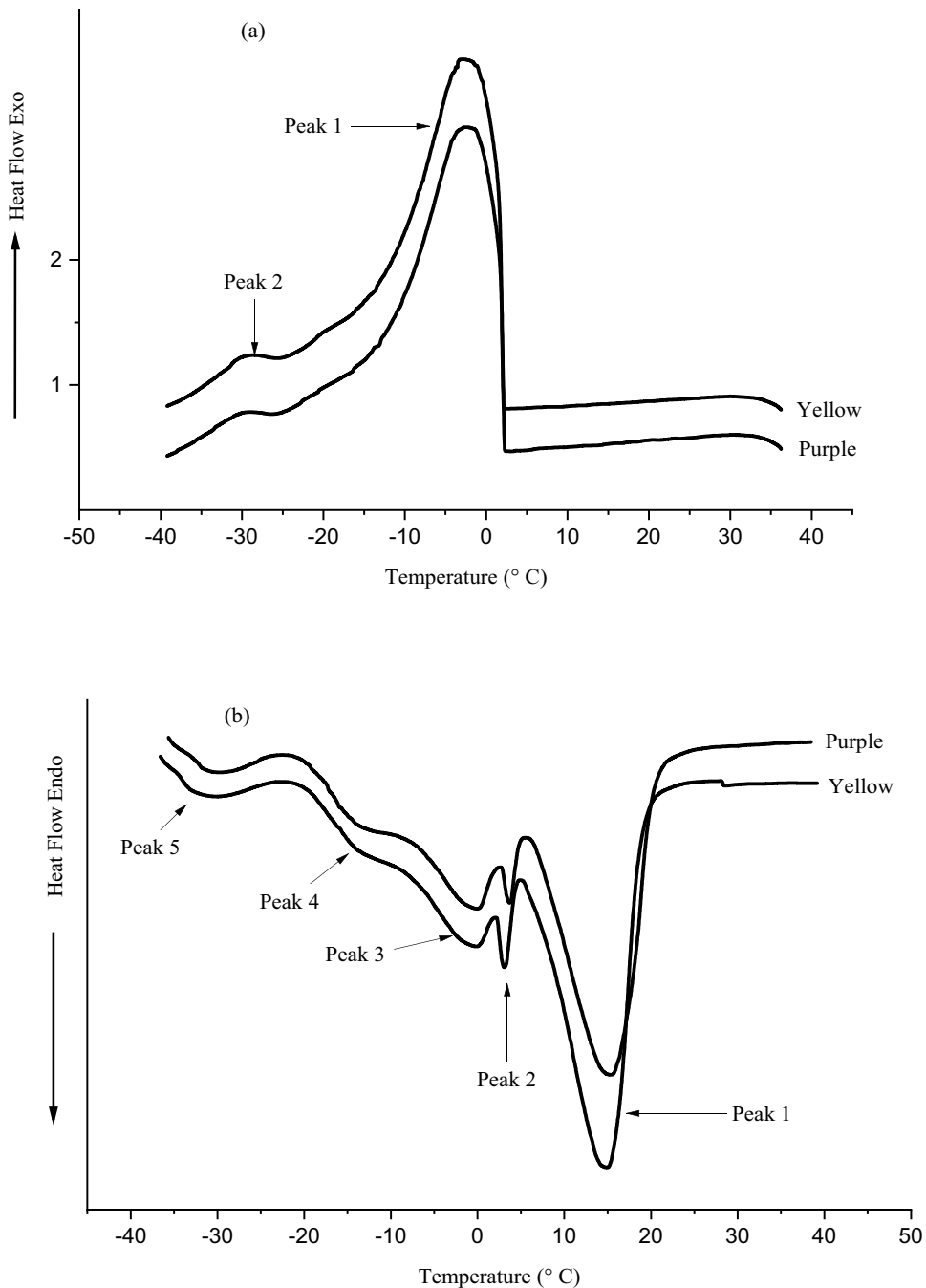
### DSC thermal profiles of *T. catappa* oil

Thermal curves of the cooling and heating process are given in Figs. 1a, b, respectively. As shown in Fig. 1a, the profile of the cooling curve of the oils consisted of one major exothermic peak (peak-1) in the upper-temperature region with a minor exothermic peak (peak-2) in the low-temperature region.

**Table 2.** Varietal differences in fatty acid compositions of oil from purple and yellow cultivars of *T. catappa* seed kernel.

Component FA	Purple	Yellow
Butyric acid (C4:0)	$0.99^a \pm 0.01$	$1.09^b \pm 0.01$
Lauric acid (C12:0)	$0.19^a \pm 0.02$	$0.76^b \pm 0.04$
Myristic acid (C14:0)	$0.17^a \pm 0.07$	$0.61^b \pm 0.07$
Palmitic acid (C16:0)	$36.06^b \pm 0.04$	$33.28^a \pm 0.02$
Palmitoleic acid (C16:1)	$0.36^a \pm 0.14$	$0.27^a \pm 0.04$
Stearic acid (C18:0)	$4.30^a \pm 0.70$	$4.69^a \pm 0.08$
Oleic acid (C18:1 <i>cis</i> $\omega$ -9)	$28.34^a \pm 0.01$	$30.09^b \pm 0.01$
Linoleic acid (C18:2 <i>cis</i> $\omega$ -6)	$27.45^b \pm 0.14$	$25.16^a \pm 0.05$
Linolelaidic acid (C18:2 <i>trans</i> $\omega$ -6)	$0.41^a \pm 0.09$	$0.51^a \pm 0.07$
Arachidic acid (C20:0)	$0.14^a \pm 0.07$	$0.06^a \pm 0.02$
Lignoceric acid (C24:0)	$0.99^a \pm 0.15$	$2.11^b \pm 0.09$
Eicosapentaenoic acid (EPA) (C20:5 $\omega$ -3)	$0.28^a \pm 0.02$	$0.34^a \pm 0.01$
Nervonic acid (C24:1)	ND	$0.18 \pm 0.02$
Docosahexaenoic acid (DHA) (C22:6 $\omega$ -3)	$0.32^a \pm 0.08$	$0.85^b \pm 0.04$
Saturated Fatty Acids ( $\Sigma$ SFA)	42.84	42.60
Unsaturated Fatty acids ( $\Sigma$ USFA)	57.16	57.40

Each value in the table represents the mean of three replicates. Means within each row bearing different superscripts are significantly ( $p < .05$ ) different. Abbreviations: ND, not detected.



**Figure 1.** DSC cooling curves (a) and heating curves (b) of oils from purple and yellow cultivars of *T. catappa* seed kernel.

The peak-1 might correspond to the crystallization of high-melting TAG groups while peak-2 might be due to crystallization of minor low-melting TAG groups in the oils. Based on overt observations, the cooling curves of the two cultivars were roughly similar, yet remarkable ( $p < .05$ ) differences were noticed in certain DSC parameters corresponding to peak-1 and peak-2. For peak-1, the peak maxima of peak-1 of *T. catappa* purple and yellow were at  $-2.08^{\circ}\text{C}$  and  $-2.45^{\circ}\text{C}$ , respectively. The peak areas of

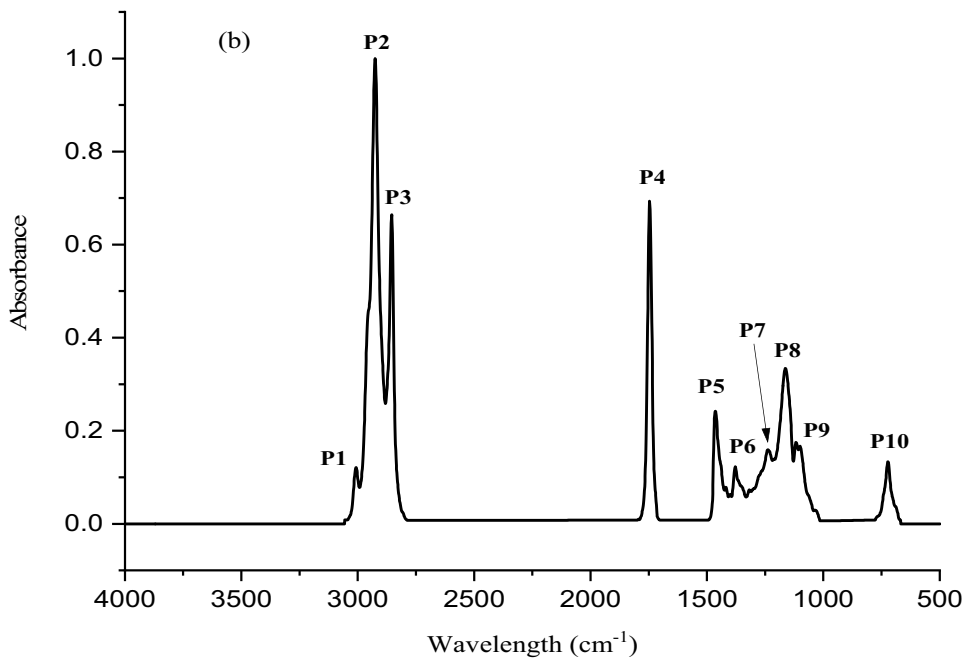
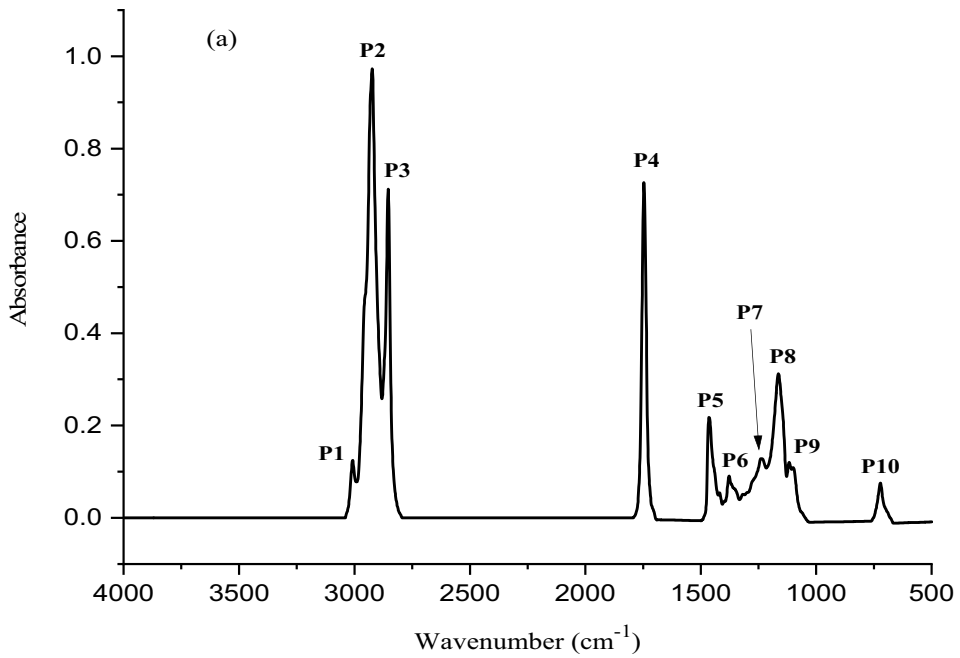
the major thermal transitions corresponding to *T. catappa* purple and yellow were 28.80 and 29.58 J/g, respectively, but no remarkable ( $p > .05$ ) differences noticed between them. Nevertheless, remarkable ( $p < .05$ ) differences were observed between purple and yellow cultivars of *T. catappa* with regard to the onset temperature. DSC cooling curve might bring forth several pieces of information, including cloud points of oils. The cloud point refers to the temperature at which the oil sample begins to form a cloud, indicating the initial stage of crystallization. Based on the onset temperature, the cloud point of *T. catappa* purple oil and yellow oil could be around 2.39°C and 2.10°C, respectively. Furthermore, the end-set temperature of both *T. catappa* purple and yellow showed similar ( $p > .05$ ) values. When considering peak 2, the peak maxima of purple and yellow cultivars of *T. catappa* were at -29.96°C and -30.35°C, respectively. Likewise, the onset temperatures of *T. catappa* purple and yellow were at -26.12°C and -25.71°C, respectively. The peak area values of purple and yellow cultivars of *T. catappa* were at 0.36 J/g and 0.53 J/g, respectively. Between the two cultivars, remarkable ( $p < .05$ ) differences were detected only in peak-maxima and onset-temperature. Nevertheless, both cultivars displayed similar values ( $p > .05$ ) with regard to the peak area and end-set temperature.

The DSC heating curves of the oils from the two cultivars are shown in Fig. 1b. In fact, DSC heating curves might bring forth several pieces of information, including melting point of oils. DSC melting point is an alternative way for the tedious method employed for determination of slip melting point of oils. In contrast to the cooling curves, the profile of the heating curves exhibited multiple thermal transitions, indicating polymorphic phase changes taking place due to the distribution of TAG groups of varying melting points. During the heating process, *T. catappa* purple and yellow showed melting profiles with a major peak (peak 1) at 15.62°C and 15.11°C, respectively, and a minor sharp peak (peak 2) at 3.68°C and 3.15°C, respectively. Based on these results, the melting point of *T. catappa* purple oil and yellow oil could be around 15.62°C and 15.11°C, respectively. Apart from these, a broad thermal transition (peak 3) corresponding to *T. catappa* purple and yellow were found at -0.44°C and -1.29°C, respectively. This broad thermal transition was found to consist of a shoulder peak (peak 4) at -14.31°C and -14.10°C, respectively. In addition, minor thermal transitions (peak 5) corresponding to *T. catappa* purple and yellow cultivars appeared at -31.62°C and -30.87°C, respectively.

### FTIR characterization of *T. catappa* oil

Figures 2a, b illustrate the FTIR spectra of *T. catappa* oils of two cultivars. Since the analysis is done for oils of *T. catappa*, the FTIR characteristic peaks would be reflective of the common triacylglycerol molecules. According to Figs. 2a, b, the characteristic features of the FTIR spectral patterns of the two cultivars were quite similar. Although the precise wavenumbers of the peaks varied only within a limited range, the peak intensities of several spectral bands of purple and yellow cultivars were found to vary within the fingerprint region (1500–950  $\text{cm}^{-1}$ ). According to Nandiyanto *et al.*,<sup>[20]</sup> peak 1 (P1) at  $\sim 3009 \text{ cm}^{-1}$  was attributed by the terminal (vinyl) C-H stretching of alkenes, while peaks 2 (P2) and 3 (P3) at  $\sim 2925 \text{ cm}^{-1}$  and  $\sim 2855 \text{ cm}^{-1}$  were caused by the asymmetrical and symmetrical C-H stretching of methylene groups, respectively. In fact, triacylglycerols being the constituents of lipids would have a significant number of aliphatic chains connected to them, which are usually responsible for these bands. The C=O stretching vibration of the saturated aliphatic ester moieties linked to lipid biomolecules was indicated by a distinctive strong peak 4 (P4) at  $\sim 1746 \text{ cm}^{-1}$ . The peak 6 (P6) found at  $\sim 1377 \text{ cm}^{-1}$  was attributed to the symmetric C-H bending of methyl groups,<sup>[21]</sup> while the P5 at  $\sim 1463 \text{ cm}^{-1}$  was caused by the asymmetric C-H bending of hydrocarbons,<sup>[20]</sup> confirming the presence of alkanes ( $\text{CH}_3$ ) in the oil sample. The aryl—O stretching vibrations corresponding to aromatic ethers occurred at  $\sim 1243 \text{ cm}^{-1}$  (P7).<sup>[20]</sup> Furthermore, the peaks 8 (P8) and 9 (P9) appearing at  $\sim 1163 \text{ cm}^{-1}$  and  $\sim 1116 \text{ cm}^{-1}$ , respectively, were attributed to C—O stretching vibrations corresponding to ether linkage.<sup>[20,21]</sup> The peak 10 (P10) at  $\sim 722 \text{ cm}^{-1}$  was due to  $(\text{CH}_2)_n$  bending vibration of hydrocarbon chains.<sup>[20]</sup>





**Figure 2.** FTIR spectral overlay of oils from purple (a) and yellow (b) cultivars of *T. catappa* seed kernel.

### **Proximate composition of defatted residues**

Proximate composition of defatted residue and whole kernel from two cultivars is given in Table 3. The overall data indicated that, except for protein content, all components in whole kernel were differed significantly ( $p < .05$ ). Similarly, in defatted residue, all components except

**Table 3.** Varietal differences in proximate composition of *T. catappa* whole kernel and defatted residue of two cultivars.

Parameters	Defatted residue		Whole kernel	
	Purple	Yellow	Purple	Yellow
Moisture (%)	4.10 <sup>a</sup> ± 0.07	4.96 <sup>b</sup> ± 0.08	2.44 <sup>A</sup> ± 0.14	2.88 <sup>B</sup> ± 0.20
Fat (%)	6.13 <sup>a</sup> ± 0.29	6.82 <sup>a</sup> ± 0.05	60.36 <sup>A</sup> ± 0.77	66.25 <sup>B</sup> ± 0.28
Protein (%)	62.10 <sup>a</sup> ± 0.56	70.00 <sup>b</sup> ± 0.42	25.95 <sup>A</sup> ± 0.09	25.22 <sup>A</sup> ± 0.92
Ash (%)	10.17 <sup>b</sup> ± 0.12	9.33 <sup>a</sup> ± 0.40	4.30 <sup>B</sup> ± 0.05	4.03 <sup>A</sup> ± 0.28
Carbohydrate (%)	17.50 <sup>b</sup> ± 0.14	8.89 <sup>a</sup> ± 0.14	6.95 <sup>B</sup> ± 0.62	1.62 <sup>A</sup> ± 1.26

Each value in the table represents the mean of three replicates ± standard deviation. Means that do not share a similar simple superscription letter in the same row in defatted residue and similar capital superscription letter in the same row in whole kernel are significantly ( $p < .05$ ) different.

fat content showed significant ( $p < .05$ ) differences. Among the macronutrients, fat was the most predominant component in the whole kernel; however, after oil extraction, protein became the most dominant nutrient in the defatted residue. The defatted residue exhibited higher moisture content, ranging from 4.10 to 4.96%, compared to the whole kernel, which had moisture content ranging from 2.44 to 2.88%. The fat content of the whole kernel was more than ten times higher, ranging from 60.36 to 66.25%, compared to the defatted residue, which ranged from 6.13 to 6.82%. Conversely, the protein content in the defatted residue (62.10 to 70.00%) was more than twice that of the whole kernel (25.22 to 25.95%). The ash content of the whole kernel was lower (4.03 to 4.30%) when compared to that of the defatted residue (9.33 to 10.17%). Similarly, the carbohydrate content of the whole kernel (1.62 to 6.95%) was lower than that of the defatted residue (8.89 to 17.50%).

## Discussion

### *Physicochemical characteristics of T. catappa oil*

Crude plant oils generally used to have relatively intense colors due to occurrence of pigments. For instance, crude palm oil is appeared to be orange in color due to the presence of carotenoids. Likewise, a light greenish color is a unique feature of unrefined olive oil. Animal fats apparently look pale white in color due to lack of pigments. The color values displayed by the oils of the two *T. catappa* cultivars were deeper than 5 in contrast to that of coconut oil.<sup>[22]</sup>

Iodine value (IV) of oils denotes the degree of unsaturation of the FAs present in TAG molecules of oils. This important oil index would measure the quantity of double bonds in the oils. The IVs of the two oils in this study were higher than those of coconut oil (8–10), palm oil (50–55), and olive oil (75–95).<sup>[14]</sup> According to Knothe<sup>[23]</sup> and Kyriakidis and Katsiloulis,<sup>[24]</sup> IV is also an indicator of the susceptibility of the oil to oxidative deterioration. As these two oils of *T. catappa* are highly unsaturated, precautionary measures are necessary to protect them from auto-oxidation and photo-oxidation leading to rancidity. Nevertheless, greater IVs shown by them might also have other benefits such as the occurrence of more omega-3 fatty acids; a micronutrient required to gain optimal health.

SV of oils and fats are inversely correlated with the mean molecular weight of FAs occurring in them. Kyari<sup>[25]</sup> previously stated that the SV of palm oil, groundnut oil, and coconut oil were 200 (mg KOH/g sample), 193 (mg KOH/g sample), and 257 (mg KOH/g sample), respectively. As SV of *T. catappa* of both cultivars were considerably lower than that of coconut oil, it may be useful to authenticate against adulterations by lauric oils.<sup>[26]</sup> It follows that oils displaying high SV might have a higher fraction of shorter fatty acid chains and vice versa. Generally, oils with high SV would have combination of normal triglycerides and may be useful in the production of liquid soap and shampoos.<sup>[27]</sup> From this perspective, the oils of the two cultivars of *T. catappa* may be useful as raw materials in the preparation of nutrient supplements rather than using in applications such as liquid soap and shampoos.

### **Fatty acid profile of *T. catappa* oil**

The FA composition of *T. catappa* cultivars employed in this study roughly agreed with the data from previous literature reported from elsewhere. Menkiti *et al.*<sup>[28]</sup> reported a similar FA profile with high contents of palmitic (~36.01%), oleic (~33.25%), and linoleic acids (~22.26%). According to Santos *et al.*,<sup>[29]</sup> oleic (~36.4%) was the most predominant FA, followed by palmitic (~32.2%), and linoleic (~24.4%) acids. When comparing the results of the two studies, a small difference in the order of dominance was quite clear. The fatty acid distribution pattern of *T. catappa* oil was considerably different from those of other edible oils extracted from major commercial seeds. For instance, Kostik *et al.*<sup>[30]</sup> reported that soybean oil has higher proportions of oleic (28.5%) and linoleic acids (49.5%), but a lower proportion of palmitic acid (9%) when compared to those of *T. catappa* oil. According to studies on peanut oil by Zambiasi *et al.*,<sup>[31]</sup> palmitic acid was the dominant SFA while oleic acid was the dominant USFA. As an important feature, the proportion of linoleic acid content of peanut oil was comparatively higher than those present in *T. catappa* oils. The high concentration of linoleic acid in *T. catappa* oils is beneficial for health, potentially reducing risk related to vascular diseases as several previous studies indicated the high consumption of monounsaturated fatty acids (MUFA) might provide better protection against coronary heart disease.<sup>[32]</sup>

### **DSC thermal profile of *T. catappa* oil**

Melting and crystallization are two key processes used to study the thermal behavior of oils and fats. As these two processes involve the absorption or release of heat, they can be very useful tools for measuring thermodynamic properties of oils and fats.<sup>[33]</sup> When looking at the melting curves of oil samples, we often see complicated patterns that are hard to understand, like small peaks overlapping to form into larger ones. These patterns result due to the complex nature of TAG molecules in oils. In contrast, the DSC crystallization curve is simpler than the melting curve because the crystallization process is primarily influenced by the chemical composition of the sample. For comparison of the results of this study, there is hardly any information on the thermal profiles of yellow and purple cultivars of *T. catappa* in the literature.

*T. catappa* kernel oils provide insightful information on its thermal behavior, highlighting distinct thermal transitions that can be compared with other edible oils. The results of this study indicated that the DSC cloud point of the two oils were relatively lower than those of coconut and palm kernel oil.<sup>[34]</sup> This is because coconut and palm kernel oils are abundant in SFAs like lauric acid whereas *T. catappa* oils contain a higher amount of USFAs. According to Tan and Che Man,<sup>[33]</sup> cooling curves of coconut oil had two distinct exothermic peaks, indicating simpler crystallization behavior compared to *T. catappa* oil. In contrast, other edible oils like corn, peanut, sesame, and soybean oil were reported to show three or more exothermic peaks corresponding to different TAG groups, indicating more complex crystallization patterns. Canola and olive oils also displayed three exothermic peaks, but with a different crystallization pattern indicated by the sharpest, tallest peak at the lowest temperature. On the other hand, *T. catappa* kernel oils exhibited two main exothermic peaks, reflecting a simpler crystallization behavior when compared to the three-peak patterns displayed by other oils. This difference is attributed to their unique TAG compositions and phase transition behavior. Specifically, the purple and yellow cultivars of *T. catappa* showed similar cooling curves but differed in their onset temperatures and peak maxima of the first exothermic peak, with the purple cultivar having higher values. This could be probably due to a higher proportion of high-melting TAGs in the purple cultivar.

The DSC melting point values of the two *T. catappa* oils were relatively lower than those of coconut and palm kernel oil.<sup>[34]</sup> It is because of the fact that, both of coconut and palm kernel oils are lauric acid dominating plant oils. In contrast to this, oils of *T. catappa* consisted of more palmitic, oleic and linoleic as FAs. According to Tan and Che Man,<sup>[33]</sup> DSC melting profile of palm oil consisted of two separate endo-thermic peaks representing high melting and low melting TAG molecules. This kind of thermal

behavior was not found with *T. catappa* oil. The heating curves of *T. catappa* oil and coconut oil were also drastically different as coconut oil showing a major endo-thermic peak with additional shoulder peak, indicating complex melting behavior.<sup>[33]</sup> As reported by Tan and Che Man,<sup>[33]</sup> corn, peanut, sesame, and soybean oils exhibited two distinct endothermic regions, while canola and olive oils showed a distinct tall endothermic peak with merging shoulder peaks. Though this was a complex melting behavior similar to *T. catappa* oil, but with different peak temperatures and patterns. *T. catappa* kernel oil displayed a detailed and complex thermal profile due to its unique TAG composition and polymorphic nature. Both purple and yellow *T. catappa* cultivars had a major melting peak around 15°C, attributed to TAGs rich in USFAs like oleic and linoleic acids. Minor peaks at lower temperatures indicated the melting of TAGs with lower melting points, influenced by other unsaturated and minor SFAs. The broad thermal transition and minor peaks suggested polymorphic phase changes due to diverse TAG composition. The high proportions of USFAs (57.16% in purple and 57.40% in yellow) contributed to the complex melting behavior observed in the DSC curves.

### **FTIR characterization of *T. catappa* oil**

FTIR spectroscopy has become an increasingly popular technique for studying edible oils and fats due to advancements in its instrumentation.<sup>[35]</sup> This technique is highly valued for its ability to provide detailed information about molecular structures, allowing for the identification of specific functional groups through their characteristic absorption bands. These features make FTIR spectroscopy particularly effective in analyzing the complex compositions of fats and oils.<sup>[36]</sup> In this study, FTIR was used to analyze the oil samples of the purple and yellow cultivars of *T. catappa*. This showed distinct patterns in their spectra, providing insights into their chemical compositions.

When the spectra were examined in exclusive of the fingerprint region ( $1500\text{ cm}^{-1} - 950\text{ cm}^{-1}$ ), the P1 to P4 peaks were the most preponderant within this range. On a comparative basis, the intensity of peak P4 was relatively higher for purple cultivar than yellow cultivar. This would lead to the deduction that more ester groups were present in the oil of purple cultivar than in yellow cultivar. Peaks appearing in the fingerprint region are primarily suggestive of the presence of hydrocarbons and esters present in the oils. The intensity of peak P5 was higher for purple than yellow which may be suggestive of the existence of more hydrocarbons and esters in the oil of the purple cultivar than yellow cultivar, while P10 showed higher intensity in the yellow cultivar.

The absence of a broad-blunt band within the range of  $3600-3400\text{ cm}^{-1}$  in *T. catappa* oil could be due to the absence of free hydroxyl groups ( $-\text{OH}$ ) associated with phenolic compounds or other hydrophilic constituents. In this study, *T. catappa* oil showed a weak sharp peak (P1) at  $\sim 3009\text{ cm}^{-1}$ , suggesting a higher degree of unsaturation when compared to coconut oil. Rohman *et al.*<sup>[36]</sup> previously indicated that the occurrence of very weak peak near  $3008\text{ cm}^{-1}$  in the spectra of coconut oil was due to low level of USFAs. Similar to *T. catappa* oil, both palm oil and olive oil also had displayed sharp weak peaks around  $3005\text{ cm}^{-1}$ , indicating the presence of more USFAs. Similar to several other edible oils, *T. catappa* oil also displayed strong bands corresponding to asymmetrical and symmetrical C-H stretching of methylene groups and C=O stretching of ester groups. According to many previous reports, the C=O stretching vibration peak (P4) is usually found to appear distinctively in majority of the fats and oils since they are composed of about 98% TAG molecules.<sup>[37]</sup> Another distinctive feature of the FTIR spectrum of *T. catappa* oil is the absence of the  $-\text{HC}=\text{CH}-$  (trans-) bending vibration within the range of  $962-967\text{ cm}^{-1}$ . On the contrary, coconut oil exhibited a peak at  $962\text{ cm}^{-1}$  indicating the occurrence of double bond.<sup>[37]</sup> These findings provide valuable insights into the chemical composition of *T. catappa* kernel oil from different cultivars. The higher unsaturation levels observed in *T. catappa* oil compared to coconut oil suggested its potential health benefits, as unsaturated oils are generally considered to be healthier than saturated animal fats. Moreover, the presence of specific functional groups such as esters and methylene groups further enhance its potential applications in the food industry.

### **Proximate composition of whole kernels and defatted residues**

The whole kernels were characterized by high fat content, which aligns with the high oil content typically found in such kernels. Ladele *et al.*<sup>[12]</sup> reported a similar fat content of 61.76% for *T. catappa* seed kernels from Benin, which was consistent with our findings. This high fat content contributes to their nutrition and caloric density. The relatively low moisture content in the whole kernel suggests that they are stable, and less hygroscopic in nature, which might enhance their shelf life. The modest protein content of the whole kernel reflects its secondary role when compared to fat. The lower ash content indicates a reduced mineral content of the whole kernel, consistent with Oduro *et al.*<sup>[38]</sup> The carbohydrate content of the whole kernel was also low, as expected given the high fat content.

After oil extraction, the defatted residues exhibited a markedly different composition (Table 3). In order to compare the results of the present study, the availability of literature on the proximate composition of defatted residues from *T. catappa* cultivars is very scanty. The moisture content of the defatted residues was relatively higher than that of the whole kernels, potentially affecting handling and storage but also influencing their functionality. The increased ash content seen in the defatted residues reflects a higher mineral concentration, which consistent with post-extraction concentration effects. As anticipated, the fat content was significantly reduced. The most significant change was the increased protein content, resulting due to the removal of fat. This would make the defatted residues a valuable protein source for various food and feed applications. Additionally, the higher carbohydrate content of the defatted residues likely reflects the relative enrichment of carbohydrates after the fat removal. Edible seeds low in starches but high in proteins are potentially useful for those with diabetes.<sup>[39]</sup> The high protein content of *T. catappa* defatted residues presents an opportunity for addressing global protein deficiency. Overall, the results underscore the nutritional transformation from whole kernels to defatted residues and illustrate the distinct potential uses of both forms.

### **Conclusion**

The study examined the physicochemical characteristics, fatty acid compositions, thermal profiles, and FTIR spectra of oils from purple and yellow cultivars of *T. catappa* and proximate compositions of their defatted residues. The compositional differences between whole kernels and defatted residues highlight substantial changes occurring during oil extraction. Whole kernels were found to be rich in fat, making them suitable for high-fat applications. Defatted residues contained more protein and minerals, making them useful for dietary supplements and functional foods. They can help with protein malnutrition and provide various other nutritional benefits. The yellow oil was lighter in color than the purple, and both were darker than coconut oil. Lower saponification values suggested fewer short-chain fatty acids, making the oils better suited as nutrient supplements rather than for soap production. High iodine values indicated a high degree of unsaturation, making the oils prone to oxidation but rich in beneficial omega-3 fatty acids. The oils were rich in USFAs, primarily palmitic, oleic, and linoleic acids, beneficial for heart health. These results highlight the potential health benefits of *T. catappa* oils and suggest they could be used in food and dietary supplement products. Based on an overt observation, the cooling and heating curves of the two cultivars were roughly similar, yet remarkable ( $p < .05$ ) differences were noticed in certain DSC parameters. FTIR spectral analysis of *T. catappa* kernel oil from purple and yellow cultivars revealed the presence of several functional groups, including alkene, alkane, ester, and hydrocarbon groups. Regardless of the cultivar differences, the FTIR spectra pattern revealed similarities in functional groups in both oils. Moreover, this outcome can serve a very good option for food and feed production under sustainability developmental goals (SDG).

## Acknowledgments

The authors extend their sincere appreciation to Researchers Supporting Project number: RSPD2024R729, King Saud University, Riyadh, Saudi Arabia. This study was partly funded by the National Institute of Fundamental Studies, Hanthana Road, Kandy, Sri Lanka.

## Disclosure statement

No potential conflict of interest was reported by the author(s).

## Data availability statement

The data that support the findings of this study are available from the corresponding author upon request.

## Author's contributions

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