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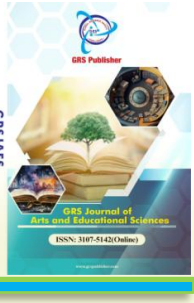

Physicochemical Properties, Phytochemical Composition, Fatty Acid Profile, and FT-IR Characterization of Neocarya macrophylla Seed Oil for Industrial Applications

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Abstract: This study investigated the physicochemical properties, phytochemical composition, fatty acid profile, FT-IR functional group characterization, and cyanogenic glycoside content of Neocarya macrophylla (gingerbread plum) seed oil sourced from Kebbi State, north-western Nigeria. Oil was extracted by Soxhlet method with n-hexane and analyzed using AOCS/AOAC standard methods, qualitative phytochemical tests, Fourier-transform infrared spectroscopy (FT-IR), and gas chromatography-mass spectrometry (GC-MS). Physicochemical analysis yielded a saponification value of 153.33 mgKOH/g, iodine value of 33.07 gI2/100g, peroxide value of 45.5 meq/kg, free fatty acid content of 3.72%, and acid value of 13.41 mgKOH/g, classifying the oil as a non-drying oil suitable for soap and cosmetic manufacture. FT-IR spectroscopy confirmed key functional groups: O–H carboxylic acid stretching at 3475.84 cm^{-1}, ester carbonyl C=O at 1740.81 cm^{-1}, and C–O triacylglycerol vibrations at 721.4 cm^{-1}, consistent with a triacylglycerol-rich oil composition. Qualitative phytochemical screening confirmed alkaloids, tannins, flavonoids, saponins, steroids, and terpenoids; cardiac and cyanogenic glycosides were absent. GC-MS fatty acid profiling identified eleven fatty acids; oleic acid was predominant at 42.46%, followed by icosatetraenoate/arachidonic acid (17.67%) and eicosatrienoic acid, palmitic, stearic, and erucic acids. The MUFA/PUFA ratio of ~1.31 indicates favourable oxidative stability. Collectively, these results confirm the multi-sector industrial potential of *N. macrophylla* seed oil for soap, cosmetics, pharmaceuticals, and nutraceutical applications.

Keywords: *Neocarya macrophylla; gingerbread plum; seed oil; physicochemical properties; FT-IR; GC-MS; fatty acid profile; phytochemical screening; cyanogenic glycosides.*

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Introduction

Vegetable oils occupy a central place in the global chemical and food economy, with worldwide demand exceeding 145 million metric tonnes and continuing to grow in response to population growth and the expanding oleochemical industry (Amza et al., 2013; Metzger et al., 2023). Despite the dominance of a small number of commodity oils palm, soybean, sunflower, and rapeseed there remains considerable scientific and industrial interest in underutilised botanical oil sources, particularly those native to sub-Saharan Africa (Anwar et al., 2014; Alcock et al., 2021).

Neocarya macrophylla (Sabine) Prance ex F. White (syn. Parinari macrophylla Sabine), locally known as gingerbread plum or 'gawasa' in Hausa, belongs to the family Chrysobalanaceae. It is widely distributed across the Sudano-Sahelian belt of West Africa, including Nigeria, Niger, Guinea, and Senegal (National Research Council, 2008; Bala et al., 2023). Its oil-rich kernel has been investigated for nutritional, antioxidant, and oleochemical applications. Previous studies report a substantial oil yield and a fatty acid profile dominated by oleic acid, together with linoleic and arachidonic acids (Amza et al., 2010; Yadav et al., 2022; El Harkaoui et al., 2024). The oil has also been investigated as a feedstock for biodiesel production (Mukhtar & Dabai, 2016; Ruatpuia et al., 2024). Previous investigations of *N. macrophylla* seed and kernel oils have established their physicochemical characteristics, fatty acid composition, antioxidant constituents, sterol profile, and tocopherol composition (Amza et al., 2010; Diaby et al., 2016; Fakai et al., 2024).

In the present study, FT-IR spectroscopy was used as an experimental tool to identify the principal functional groups in the extracted oil, while reported studies were used as comparative evidence for the physicochemical and fatty acid characteristics. This paper reports a comprehensive characterization of the physicochemical indices, FT-IR spectrum, phytochemical

screening, GC-MS fatty acid profile, and cyanogenic glycoside content of *N. macrophylla* seed oil sourced from Kebbi State, Nigeria, with a view to establishing its suitability for soap, cosmetic, pharmaceutical, and biodiesel applications.

Materials and Methods

Plant material collection and authentication

Mature *N. macrophylla* seeds were collected from indigenous trees in Birnin Kebbi, Kebbi State, Nigeria, in August. The plant was authenticated at the Herbarium of the Department of Biological Sciences, Bayero University, Kano (voucher No. 175). Seeds were cleaned, de-shelled, dried, and pulverised prior to extraction.

Oil extraction

Approximately 35 g of pulverised seed material was extracted using a Soxhlet apparatus with n-hexane (b.p. 40–60 °C) for six hours. Solvent was removed by evaporation at reduced temperature and pressure (reflux at 70 °C, followed by heating mantle), and the oil was stored at −2 °C. Oil yield (%) was calculated gravimetrically.

Physicochemical analysis

Physicochemical parameters were determined according to AOCS and AOAC standard methods: free fatty acid (AOCS Ca 5a-40), iodine value (AOCS Cd 1-25, Wijs method), saponification value (AOCS Cd 3-25), peroxide value (AOCS Cd 8-53), and acid value (AOAC 940.28). All determinations were performed in triplicate.

FT-IR spectroscopy

FT-IR spectra were obtained using a Nicolet 8400S Fourier-transform infrared spectrometer equipped with a deuterated triglycine sulphate (DTGS) detector and OMNIC software (version 7.0, Thermo Nicolet). A KBr disc was used to contact the oil sample; spectra were collected across 4500–400 cm^{-1} by co-adding 32 scans at a resolution of 4 cm^{-1}. Triplicate recordings were made and results expressed as absorbance.

GC-MS analysis

Fatty acid characterisation was performed on a Shimadzu QP2010 series gas chromatograph coupled with a Shimadzu QP2010 Plus mass spectrometry detector. The temperature programme ranged from 70 °C to 280 °C; helium was used as carrier gas; injection volume was 2 µL at an injection temperature of 250 °C; column flow was 1.80 mL/min. Data were acquired in scan mode over a range of 30–700 amu at 1478 rps, and mass spectra were matched against the NIST05 mass spectral library.

Qualitative phytochemical screening

Screening was performed by standard methods: alkaloids (Mayer's and Wagner's tests), tannins (ferric chloride test), flavonoids (Shinoda test), saponins (frothing test), steroids and terpenoids (Liebermann–Burchard test), and cardiac glycosides (Keller–Killiani test). Results were recorded as present (+) or absent (−).

Cyanogenic glycoside test

The picric acid paper test was used: oil extract was placed in a test tube with 1.5 mL distilled water and six drops of chloroform; a picric acid–sodium carbonate paper was suspended from the stopper and the assembly incubated for two hours at ambient temperature. A yellow-to-brick-red colour change indicates a positive result.

Results

Oil yield and physicochemical properties

Soxhlet extraction yielded 56.0 ± 1.2% crude oil (w/w, dry basis). Physicochemical results are summarised in Table 1.

Table 1: Physicochemical properties of Neocarya macrophylla seed oil

Parameter	Value (mean ± SD)	Comparable reference
Oil yield (%)	56.0 ± 1.2	50–67% (Diaby et al., 2017)
Free fatty acid (%)	3.72 ± 0.14	≤4% (edible-grade threshold)
Acid value (mgKOH/g)	13.41 ± 0.31	13.41 (Diaby et al., 2016)
Saponification value (mgKOH/g)	153.33 ± 1.87	153.33 (Diaby et al., 2016)
Iodine value (gI2/100g)	33.07 ± 0.65	16.10–45.0 (literature range)
Peroxide value (meq/kg)	45.5 ± 1.12	Typical of crude, unrefined oil

(mean ± SD, n = 3).

The saponification value of 153.33 mgKOH/g indicates an oil composed predominantly of higher-molecular-weight fatty acids (C18+). The low iodine value (33.07 gI2/100g) classifies the oil as a non-drying oil. The acid value of 13.41 mgKOH/g corresponds to an FFA of 3.72%, within acceptable quality bounds for soap-grade oil. The peroxide value of 45.5 meq/kg is characteristic of unrefined crude oil and is substantially reducible by standard refining.

FT-IR spectroscopic characterization

The FT-IR spectrum of *N. macrophylla* seed oil obtained in the present study is summarized in Table 2, which lists the principal band assignments across the 4500–400 cm^{-1} range.

Table 2: FT-IR band assignments for Neocarya macrophylla seed oil obtained in the present study

Wavenumber (cm^{-1})	Intensity	Functional group assignment
4259.93	M	Aliphatic C–H stretching
3475.84	S	O–H stretching of carboxylic acid
2934.79	M	Asymmetric $–CH_2–$ (unsaturated fatty acyl ester, cis double bond)
2869.21	M	Symmetric $–CH_3$ and $–CH_2–$ stretching vibrations
2345.52	S	C–H stretching vibration of cis double bond
2037.86	S	C–H stretching vibration of cis double bond
1740.81	S	C=O ester carbonyl stretching (triacylglycerols)
1521.74	S	C–O vibrations / aromatic C=C stretching
1447.62	M	–COOR / aromatic C=C stretching
1358.90	M	CH_2/CH_3 bending; in-plane cis-olefinic CH bending (C–CO–O–)
1166.01	M	C–O ester fingerprint stretching
990.48	M	Trans out-of-plane CH=CH vibration
721.40	S	In-plane cis-olefinic CH_2 rocking; C–O triacylglycerol stretching
442.68	W	Out-of-plane cis-olefinic CH_2 rocking

S = strong, M = moderate, W = weak

Phytochemical screening

Six classes of secondary metabolites were detected; cardiac and cyanogenic glycosides were absent (Table 3).

Table 3: Qualitative phytochemical screening of Neocarya macrophylla seed oil

Phytochemical	Test method	Result	Significance
Alkaloids	Mayer's & Wagner's	+ Present	Antimicrobial, analgesic
Tannins	Ferric chloride	+ Present	Antioxidant, astringent
Flavonoids	Shinoda test	+ Present	Anti-inflammatory, antioxidant
Saponins	Frothing test	+ Present	Emulsifying, surfactant
Steroids	Liebermann–Burchard	+ Present	Anti-inflammatory, hormonal
Terpenoids	Liebermann–Burchard	+ Present	Antimicrobial, antifungal
Cardiac glycosides	Keller–Killiani	− Absent	Not detected
Cyanogenic glycosides	Picrate paper test	− Absent	Safe for cosmetic/food use

GC-MS fatty acid profile

GC-MS analysis identified eleven fatty acids in the extracted oil (Table 4). The dominant peak, corresponding to oleic acid (C18:1), eluted at a retention time of approximately 22 minutes and was matched to the NIST05 library. Additional peaks corresponding to erucic acid (C22:1, similarity index 92, MW 338, retention index 2572), palmitic acid (C16:0, MW 270), myristic acid (C14:0, MW 228), elaidic acid (C18:1 trans,

MW 296), eicosatrienoic acid (C20:3, MW 292), and stearic acid (C18:0, MW 284) were identified at NIST05 library similarity indices of 86% or higher.

Table 4: Fatty acid composition of Neocarya macrophylla seed oil by GC-MS

Fatty acid	Notation	Class	Content (%)
Myristic acid	C14:0	SFA	Trace
Palmitic acid	C16:0	SFA	10.33 ± 0.42
Palmitoleic acid	C16:1	MUFA	1.14 ± 0.08
Stearic acid	C18:0	SFA	6.83 ± 0.27
Oleic acid (cis)	C18:1n-9	MUFA	42.46 ± 0.91
Elaidic acid (trans)	C18:1n-9t	Trans MUFA	1.82 ± 0.11
Eicosatrienoic acid	C20:3	PUFA	~3.60
Icosatetraenoate (arachidonic)	C20:4n-6	PUFA	17.67 ± 0.44
Behenic acid	C22:0	SFA	1.22 ± 0.06
Erucic acid	C22:1n-9	MUFA	0.56 ± 0.04
Heneicosanoic acid	C21:0	SFA	0.56 ± 0.03
Total SFA	—	—	~18.94
Total MUFA	—	—	~45.98
Total PUFA	—	—	~35.08
MUFA/PUFA ratio	—	—	~1.31

(n = 3). SFA = saturated fatty acids; MUFA = monounsaturated fatty acids; PUFA = polyunsaturated fatty acids

Cyanogenic glycosides

The picric acid paper test gave a negative result (paper remained yellow), confirming the absence of detectable cyanogenic glycoside activity in the seed oil extract and supporting the safety of the oil for topical and food applications.

Discussion

Physicochemical properties

The saponification value of 153.33 mgKOH/g confirms the predominance of C18 long-chain fatty acids and supports cold- and hot-process soap manufacture (minimum SV of approximately 140 mgKOH/g is generally required for saponification; (Diaby et al., 2016; Sabudak & Ozcan, 2025). The iodine value of 33.07 gI2/100g classifies the oil as non-drying (IV < 100), confirming its physical stability in soap bars and cosmetic emollients without risk of film formation or resinification. The FFA of 3.72% and acid value of 13.41 mgKOH/g are consistent with values independently reported for gingerbread plum kernel oil from the wider region (Aa et al., 2013; Diaby et al., 2016), suggesting reasonable analytical reproducibility across collections. The elevated peroxide value (45.5 meq/kg) reflects crude extraction without antioxidant treatment; refining and the addition of natural tocopherols would be expected to reduce this toward food-grade levels (<10 meq/kg).

FT-IR spectroscopy: functional group interpretation

The FT-IR spectrum provides confirmation of the triacylglycerol (TAG) composition of the oil. The strong, sharp carbonyl absorption at 1740.81 cm^{-1} is the diagnostic signature of ester C=O stretching in glycerol triesters and is characteristic of vegetable oils generally (Gunstone, 2004; Bathini et al., 2018). The O–H absorption at 3475.84 cm^{-1} arises from free carboxylic acid groups, consistent with the measurable FFA content (3.72%). The absorption envelope at 2934.79 and 2869.21 cm^{-1} corresponds to asymmetric and symmetric C–H stretching of the methylene chains of the fatty acid tails, a feature common to long-chain fatty acids.

The bands at 2345.52 and 2037.86 cm^{-1} represent C–H stretching of cis double bonds within unsaturated fatty acyl chains, consistent with the presence of cis-oleic acid (C18:1n-9, 42.46%) and other unsaturated components identified by GC-MS. The band at 990.48 cm^{-1} indicates a trans CH=CH out-of-plane vibration, consistent with the minor elaidic acid (C18:1n-9t, 1.82%) also identified by GC-MS. The C–O ester stretching fingerprint at 1166.01 cm^{-1} and the glycerol backbone vibrations at 721.40 and 442.68 cm^{-1} are characteristic of triacylglycerol ester linkages (Gunstone, 2004; Da Silva & Rousseau, 2010).

Generally, the FT-IR spectrum is consistent with a high-oleic, unsaturated vegetable oil of the triacylglycerol class, with no

absorptions indicative of significant hydroperoxide, epoxide, or aldehyde contamination, supporting the oil's suitability for industrial use.

Phytochemical profile

The detection of alkaloids, tannins, flavonoids, saponins, steroids, and terpenoids confirms *N. macrophylla* seed oil as a phytochemically rich substrate. Flavonoids and tannins are associated with antioxidant and anti-inflammatory bioactivity, of relevance to cosmetic anti-ageing applications. Saponins are associated with natural surfactant activity relevant to soap and shampoo formulation. Steroids identified by the Liebermann–Burchard test are consistent with the phytosterol content reported for related kernel oils (Diaby et al., 2016; Vecka et al., 2019). The absence of cardiac and cyanogenic glycosides is an important safety consideration for downstream applications.

GC-MS fatty acid profile

Fatty acid methyl esters eluted predominantly within an 18–23-minute retention window, consistent with C18–C22 chain lengths under the temperature programme used. The most abundant fatty acid, oleic acid (C18:1n-9, 42.46%), was identified with a NIST05 library similarity index of 90%. Erucic acid (C22:1, similarity index 92, MW 338, retention index 2572) was identified with high confidence; at 0.56% it is well below regulatory thresholds of concern for food applications (e.g., <5% under EU regulation for edible oils).

Five further fatty acids palmitic acid (C16:0), myristic acid (C14:0), elaidic acid (C18:1 trans), eicosatrienoic acid (C20:3), and stearic acid (C18:0) were confirmed by molecular ion and fragmentation patterns matched against the NIST05 library at similarity indices of 86% or higher. The co-occurrence of eicosatrienoic acid (C20:3) and arachidonic acid (C20:4) gives *N. macrophylla* seed oil a distinctive polyunsaturated character relative to common commodity vegetable oils.

Industrial application summary

Soap manufacture: the saponification value of 153.33 mgKOH/g confirms saponifiability, and the non-drying classification supports bar stability.

Cosmetics: the high oleic acid content favours skin penetration and emollience, flavonoid content contributes antioxidant activity, and the FT-IR-confirmed triacylglycerol structure is consistent with use as an emollient base.

Pharmaceuticals: the bioactive phytochemical content (alkaloids, terpenoids) together with essential fatty acids (linoleic, arachidonic) supports potential formulation as functional carrier oil, subject to further pharmacological evaluation.

Biodiesel: Mukhtar and Dabai (2016) demonstrated that *N. macrophylla* (reported as Parinari macrophylla) seed oil can serve as a feedstock for biodiesel production using an MgO/Al_2O_3 catalyst. The ester-rich triacylglycerol structure confirmed by FT-IR in the present study is consistent with suitability for transesterification, although fuel performance would need to be established experimentally on the present oil.

Conclusion

This study provided a characterisation of *Neocarya macrophylla* seed oil through physicochemical analysis, FT-IR spectroscopy, GC-MS fatty acid profiling, phytochemical screening, and cyanogenic glycoside testing. The oil yield (56.0%) and physicochemical indices (SV 153.33 mgKOH/g; IV 33.07 gI2/100g; FFA 3.72%) are consistent with a non-drying industrial oil suitable for soap and cosmetic manufacture. FT-IR spectroscopy confirmed the triacylglycerol composition, the presence of cis-unsaturated fatty acyl chains, ester carbonyl groups, and glycerol backbone vibrations, consistent with a triacylglycerol-rich vegetable oil. GC-MS identified eleven fatty acids, with oleic acid (42.46%) dominant and a MUFA/PUFA ratio of approximately 1.31 indicating favourable oxidative stability. The phytochemical profile (alkaloids, tannins, flavonoids, saponins, steroids, terpenoids), together with the absence of cardiac and cyanogenic glycosides, supports potential cosmetic, pharmaceutical, and antimicrobial applications. Future studies should include quantitative HPLC phytochemical profiling, storage-stability testing, and sensory and safety evaluation for food-grade applications.

Declarations

The authors affirm that the work presented in this manuscript is entirely original, and they accept full responsibility for any claims that may arise concerning its content.

Competing interests

The authors declare no conflict of interest.

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