

Phytochemical Profiling of Parquetina Nigrescens Extracts by GC-MS, HPLC and FTIR

Abdulai Turay

abdulai.turay@usl.edu.sl

University of Sierra Leone

Olayinka Taiwo Asekun

University of Lagos

Moshood Olusola Akinleye

University of Lagos

Mamoud Massaquoi

University of Sierra Leone

Research Article

Keywords: Parquetina nigrescens, polarity-guided fractionation, phytochemical profiling, GC-MS, HPLC, ATR-FTIR, standardisation, quercetin, rutin, magnoflorine

Posted Date: January 14th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-8570194/v1>

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Additional Declarations: No competing interests reported.

Abstract

Background

Parquetina nigrescens is widely used in traditional medicine and has reported normoglycaemic potential. However, the specific active chemical constituents and mechanisms responsible for these effects remain insufficiently clarified, and variability between studies is likely when extracts are not chemically standardised. Systematic chemical profiling using polarity-guided fractionation, chromatographic separation, and marker quantification is therefore essential to define extract composition more reproducibly and provide a credible analytical foundation for subsequent pharmacological and mechanistic investigations.

Aim

To generate an integrated chemical profile of *Parquetina nigrescens* extract using polarity-guided solvent fractionation followed by complementary instrumental analyses (GC–MS, HPLC, and ATR-FTIR) in support of extract standardisation and future bioactivity-driven studies.

Methods

A *Parquetina nigrescens* extract (6.02 g) obtained from the Department of Pharmacognosy, Faculty of Pharmacy, University of Lagos, Nigeria, was dispersed in methanol (70 mL), distilled water (50 mL), and ethanol (10 mL) to obtain a partitionable mother solution. Sequential solvent–solvent partitioning was performed in triplicate using n-hexane (non-polar), dichloromethane (mid-polar), ethyl acetate (intermediate-polar), and an aqueous residue (polar). The n-hexane fraction was analysed by GC–MS using an Agilent 5977B GC/MSD system with an Elite-5MS column under electron ionisation at 70 eV (helium carrier gas at 1 mL/min; injection 1 µL, split 10:1; oven 100°C for 0.5 min then 20°C/min to 280°C, hold 2.5 min; mass range m/z 45–450). ATR-FTIR spectra of the dichloromethane, ethyl acetate, and aqueous extracts were acquired using an Agilent Cary 630 Diamond ATR accessory. HPLC profiling and quantification were carried out using external calibration with mixed standards under two methods (isocratic and gradient) on a C18 column with UV detection at 257–260 nm; extract (50 mg) was prepared at 10 mg/mL in methanol, filtered (0.45 µm), and injected (10 µL).

Results

GC–MS of the n-hexane fraction identified eight compounds (retention time 13.50–17.01 min) with a total oil content of 25.3%. The most abundant constituents by percentage composition were 3H-Naphth[1,8a-b]oxiren-2(1aH)-one (6.51%), hexadecanoic acid ethyl ester (5.10%), and ethyl 9,12,15-octadecatrienoate (4.54%). Additional constituents included linoleic acid ethyl ester (2.86%), phenol, 4-

[4,5-bis[4-(dimethylamino)phenyl]-4H-imidazol-2-yl]- (2.64%), octadecanoic acid ethyl ester (1.03%), and two sterol/terpenoid-like acetates (0.97–1.65%). HPLC profiling resolved three phytochemicals: quercetin (retention time 1.757 min; peak area 3593.212), magnoflorine (1.248 min; area 841.4059), and rutin (1.558 min; area 724.4042). Interpolated concentrations were quercetin 260.486 µg/mL, magnoflorine 63.03 µg/mL, and rutin 17.45 µg/mL. ATR-FTIR analysis across dichloromethane, ethyl acetate, and aqueous extracts showed bands consistent with O–H stretching ($\approx 3369\text{--}3280\text{ cm}^{-1}$), C–H stretching ($\approx 2929\text{--}2855\text{ cm}^{-1}$), carbonyl C = O ($\approx 1685\text{--}1636\text{ cm}^{-1}$), C–O/C–N stretching ($\approx 995\text{--}1275\text{ cm}^{-1}$), aromatic or alkene-associated absorptions ($\approx 1603\text{ cm}^{-1}$), and nitrile C $\equiv$ N features ($\approx 1938\text{--}2113\text{ cm}^{-1}$), supporting the presence of diverse chemical classes across fractions.

Conclusion

Polarity-guided solvent fractionation combined with GC–MS, HPLC, and ATR-FTIR provided a complementary framework for reproducible chemical profiling of *Parquetina nigrescens*. The non-polar fraction was enriched in fatty acid ethyl esters, while HPLC confirmed quercetin, magnoflorine, and rutin as quantifiable marker constituents. FTIR data further supported broad functional-group diversity consistent with phenolic-, alkaloid-, carbonyl-, nitrile-, and lipid-associated constituents. These findings provide fraction-specific and quantitative chemical evidence that can support standardisation, improve comparability between studies, and guide future isolation and bioactivity or mechanistic investigations.

INTRODUCTION

Herbal medicines remain integral to global health care as therapeutic resources, cultural health technologies, and important starting points for drug discovery. In many low- and middle-income settings, plant-based traditional medicine continues to be among the most accessible and affordable options for primary health needs, and international policy frameworks increasingly emphasize the need to strengthen regulation, quality assurance, and evidence generation for traditional and complementary medicine products and practices [1]. In Africa, reliance on traditional medicine remains substantial, reflecting health-system constraints, medicine affordability, and sustained community trust in local therapeutic knowledge [2].

From a pharmaceutical sciences perspective, the continuing importance of medicinal plants is reinforced by their contribution to modern therapeutics and the exceptional chemical diversity of natural products. Natural-product scaffolds and their derivatives continue to feature prominently among clinically used medicines, supporting sustained interest in botanical resources as reservoirs of bioactive secondary metabolites [3]. However, the pharmaceutical translation of herbal remedies requires more than ethnomedicinal popularity; it demands correct identity, reproducible preparation, and robust chemical characterisation to ensure dose-consistent exposure and meaningful comparability across studies [4].

A major challenge in herbal medicine research is chemical complexity and variability. Phytochemical composition can vary with plant part, geography, season, post-harvest processing, and storage, which can undermine reproducibility when crude preparations are used without standardisation. Analytical quality frameworks therefore emphasize developing chemical fingerprints and marker-based assays, alongside contaminant/adulterant surveillance, as foundational steps toward credible evaluation and product development [4]. Consequently, modern studies increasingly integrate chromatography and spectroscopy (e.g., TLC, GC–MS, HPLC, FTIR) to generate interpretable chemical profiles that can guide downstream isolation, quantification, and mechanistic investigations.

Within this broader context, diabetes mellitus (DM) represents a growing global public health burden, with rising prevalence and associated complications that strain health systems particularly in resource-limited settings. The International Diabetes Federation (IDF) Diabetes Atlas highlights the continuing global increase in diabetes burden, reinforcing the need for affordable and locally relevant interventions alongside conventional therapies [5]. In many African settings where access to medicines and long-term follow-up may be constrained, plant-based therapies remain widely used, further strengthening the rationale for scientifically grounded evaluation of medicinal plants commonly employed for metabolic disorders [2, 6].

Parquetina nigrescens (Afzel.) Bullock (Apocynaceae; Periplocoideae) is a perennial evergreen woody climber with a twinning stem and glossy leaves that commonly twine on other plants or surfaces in savannas, marshy areas, and gallery forests across parts of West Africa. It has been reported in ethnomedicine across countries including Sierra Leone, Ghana, Nigeria, and Senegal, where it is used traditionally for multiple conditions and is particularly cited in community-based management of ailments linked to blood and metabolic health [6]. Phytochemical reports and syntheses indicate that the plant contains multiple secondary metabolite classes commonly including alkaloids, tannins, saponins, flavonoids, cardenolides, and glycosides supporting its continued research interest [6].

Preclinical evidence further supports the relevance of *P. nigrescens* for metabolic research. For example, experimental studies in diabetic rat models have reported hypoglycaemic and related protective effects following administration of *P. nigrescens* extracts, providing biological plausibility for its traditional antidiabetic use and justifying deeper chemical investigations to identify constituents that may drive these effects [7, 8]. Nonetheless, despite its wide use and reported pharmacological potential, the mechanisms and active chemical constituents responsible for its normoglycaemic effects remain insufficiently clarified, and inter-study variability is likely when extracts are not chemically standardised.

Therefore, systematic chemical profiling of *Parquetina nigrescens* including polarity-guided fractionation, chromatographic separation, and marker quantification remains essential to (i) define its extract composition more reproducibly, (ii) support isolation and characterisation of key constituents (especially phenolic-associated compounds), and (iii) provide a credible analytical foundation for subsequent pharmacological and mechanistic studies using established platforms such as HPLC, GC–MS, and FTIR [4].

MATERIALS AND METHODS

This research applied polarity-guided solvent fractionation followed by chromatographic and spectroscopic techniques to characterise the chemical constituents of *Parquetina nigrescens* extract. The crude extract was first separated into fractions of different polarities by solvent–solvent partitioning to simplify the complex mixture and concentrate chemically related constituents into the same fraction, thereby improving downstream profiling and interpretation [9]. The resulting fractions were then analysed using GC–MS for profiling of constituents enriched in the non-polar fraction under electron ionisation conditions [12], ATR-FTIR to identify dominant functional-group features supporting preliminary chemical-class inference [11], and HPLC to support chromatographic profiling or quantification using mixed standards under defined isocratic and gradient conditions [13].

Source of *Parquetina nigrescens* extract

The *Parquetina nigrescens* extract was obtained from the Department of Pharmacognosy, Faculty of Pharmacy, University of Lagos, Nigeria. The sample was used as the starting material for solvent fractionation and instrumental analyses. The extract mass used for fractionation was measured using an electronic compact scale (SF-400C), and 6.02 g of sample was weighed into a beaker.

Solvent–solvent partitioning of *Parquetina nigrescens* extract

The weighed extract (6.02 g) was dispersed to obtain a partitionable mother solution by adding 70 mL methanol, followed by 50 mL distilled water and 10 mL ethanol to facilitate effective dissolution. The mixture was then fractionated sequentially using immiscible organic solvents according to polarity. In this approach, non-polar constituents preferentially distribute into n-hexane, moderately polar constituents partition into dichloromethane or ethyl acetate, while more polar constituents remain predominantly in the aqueous phase [9]. Each partitioning step was performed in triplicate before proceeding to the next solvent.

Partitioning with n-hexane (non-polar fraction).

To the prepared mother solution, 100 mL n-hexane was added and the mixture was transferred into a separatory funnel. The contents were gently sonicated, clamped on a retort stand, and allowed to separate into two layers. The organic n-hexane (upper) layer was collected as the n-hexane fraction for subsequent analysis, while the residual aqueous phase was retained for further partitioning.

Partitioning with dichloromethane (mid-polar fraction).

The residual aqueous phase was returned into the separatory funnel and extracted with 100 mL dichloromethane. The mixture was gently sonicated, allowed to separate, and the dichloromethane layer was collected as the dichloromethane fraction. The remaining aqueous phase was retained for the next step.

Partitioning with ethyl acetate (intermediate-polar fraction).

The residual aqueous phase was then extracted with 100 mL ethyl acetate using the separatory funnel, followed by gentle sonication and phase separation. The ethyl acetate layer was collected as the ethyl acetate fraction, while the remaining aqueous phase represented the polar residue or fraction for storage and further assessment as required.

Gas Chromatography–Mass Spectrometry (GC–MS) analysis

GC–MS analysis of the n-hexane fraction of *Parquetina nigrescens* was performed using an Agilent 5977B GC/MSD system coupled with an Agilent 8860 auto-sampler. Separation was achieved on an Elite-5MS capillary column (5% diphenyl/95% dimethyl polysiloxane; 30 × 0.25 mm ID × 0.25 µm df). Detection used an electron ionisation source operating in electron impact mode at 70 eV, which supports reproducible fragmentation useful for library-based compound identification [12]. Helium (99.999%) was used as carrier gas at 1 mL/min constant flow. An injection volume of 1 µL was used with a split ratio of 10:1. The injector temperature was maintained at 300°C and ion-source temperature at 250°C. The oven temperature programme was 100°C (isothermal for 0.5 min) then increased at 20°C/min to 280°C (held for 2.5 min). Mass spectra were acquired at 70 eV with a scanning interval of 0.5 s over a mass range of m/z 45–450, with a solvent delay of 0–3 min [12].

Fourier-Transform Infrared Spectroscopy (FTIR) analysis

ATR-FTIR spectra were acquired using an Agilent Cary 630 ATR-FTIR spectrometer equipped with a Diamond ATR accessory. ATR-FTIR was used to obtain rapid information on dominant functional groups in the extract or fractions (e.g., O–H, C = O, C–H, C–O), supporting chemical interpretation alongside chromatographic findings [11]. For spectrum acquisition, the sample press knob was turned counter-clockwise to open the press so the tip was elevated from the diamond sampling window. A small amount of the *Parquetina nigrescens* sample was placed on the diamond crystal and spread to cover the surface area to improve contact, after which the press was engaged and spectra were collected [11].

High-Performance Liquid Chromatography (HPLC) analysis

HPLC analysis was performed using external calibration with mixed standards and defined chromatographic conditions. Mixed-standard calibration supports efficient quantification across multiple analytes when appropriately applied, and two methods were used in this study: Method A (isocratic) and Method B (gradient), differing in standard composition and elution mode [13].

Preparation of sample solution.

A 50 mg portion of dried or concentrated *Parquetina nigrescens* extract was weighed, dissolved in methanol, and made up to 5 mL with methanol to obtain 10 mg/mL (10,000 µg/mL). The solution was filtered using a 0.45 µm syringe (Millipore) filter, transferred into HPLC vials, placed in the autosampler tray, and 10 µL was injected.

Preparation of mixed standards (Method A: isocratic).

Formononetin, rutin, magnoflorine, luteolin, and quercetin standards were each prepared by dissolving 5 mg of each standard in 5 mL methanol to obtain 1000 µg/mL solutions (prepared separately). Exactly 2 mL from each standard solution was combined and made up to 10 mL, yielding a mixed standard of 200 µg/mL for each analyte. From this stock, graded concentrations of 20, 40, 60, 80, and 100 µg/mL were prepared, transferred to vials, and 10 µL was injected in duplicate [13].

Preparation of mixed standards (Method B: gradient).

Gallic acid, magnoflorine, luteolin, and pinostrobin standards were each prepared as 1000 µg/mL solutions by dissolving 5 mg of each standard in 5 mL methanol. Exactly 2 mL from each of the four standards (total 8 mL) was combined and 2 mL methanol was added to make 10 mL, giving 200 µg/mL for each analyte. Graded concentrations of 20, 40, 60, 80, and 100 µg/mL were prepared and injected in duplicate at 10 µL [13].

HPLC conditions (Method A: isocratic).

The mobile phase was methanol:acetonitrile:water (40:15:45) containing 1% acetic acid. A C18 column (150 × 4.6 mm, 5 µm) was used. Detection was at 257 nm, temperature was ambient, flow rate was 1 mL/min, and injection volume was 10 µL [13].

HPLC conditions (Method B: gradient).

Mobile phase A was acetonitrile:TFA (100:0.5) and mobile phase B was acetonitrile:water:TFA (20:80:0.01). The column was C18 (150 × 4.6 mm, 5 µm) with detection at 260 nm, ambient temperature, flow rate 1 mL/min, and injection volume 10 µL [13].

RESULTS

Overview of phytochemical profiling of *Parquetina nigrescens*

The chemical profile of *Parquetina nigrescens* was evaluated using complementary instrumental methods (GC–MS, HPLC, and FTIR) to provide an integrated description of constituents detectable in the prepared fractions/extracts. The GC–MS analysis described the non-polar n-hexane extract, HPLC provided targeted chromatographic profiling of selected phytochemicals, and FTIR supported functional-group level interpretation across dichloromethane, ethyl acetate, and aqueous extracts [14].

Gas Chromatography–Mass Spectrometry (GC–MS) analysis

GC–MS analysis of the n-hexane extract of *Parquetina nigrescens* identified eight (8) compounds, with retention times ranging from 13.50 to 17.01 min (Table 4.1). The total oil content detected for the n-hexane extract was 25.3%. The chromatographic profile showed that the most abundant compounds by percentage composition were 3H-Naphth[1,8a-b]oxiren-2(1aH)-one (6.51%; quality 27%), Hexadecanoic acid, ethyl ester (5.10%; quality 98%), and Ethyl 9,12,15-octadecatrienoate (4.54%; quality 98%). Additional constituents included Linoleic acid ethyl ester (2.86%; quality 96%), Phenol, 4-[4,5-bis[4-(dimethylamino)phenyl]-4H-imidazol-2-yl]- (2.64%; quality 45%), Octadecanoic acid, ethyl ester (1.03%; quality 98%), and two sterol/terpenoid-like acetates with lower quality matching values (0.97–1.65%; quality 35–38). The quality scores reported alongside each compound reflect the strength of library matching under the applied EI-GC–MS method, indicating high confidence for several fatty acid ester identifications and lower confidence for certain aromatic/complex structures under the same conditions [15].

Table 1
Chemical composition of the n-hexane extract of *Parquetina nigrescens* by GC-MS

S/N	Compound	RT (min)	% Composition	Quality (%)
1	Hexadecanoic acid, ethyl ester	13.50	5.10	98
2	3H-Naphth[1,8a-b]oxiren-2(1aH)-one	14.66	6.51	27
3	Phenol, 4-[4,5-bis[4-(dimethylamino) phenyl]-4H-imidazol-2-yl]-	14.73	2.64	45
4	Linoleic acid ethyl ester	14.80	2.86	96
5	Ethyl 9,12,15-octadecatrienoate	14.86	4.54	98
6	Octadecanoic acid, ethyl ester	15.02	1.03	98
7	9,19-Cycloergost-24(28)-en-3-ol,14-dimethyl-, acetate	16.96	0.97	38
8	9,19-Cyclolanost-24-en-3-ol, acetate	17.01	1.65	35

Total oil content (n-hexane fraction): 25.3%.

Mass Spectra of some major compounds from Total Ion Chromatogram of *Parquetina nigrescens* n-hexane extracts.

Figure 2.

Mass spectrum of 3H-Naphth[1,8a-b]oxiren-2(1aH)-one

Hexadecanoic acid and ethyl ester (Figs. 2 and 4), constituted 5.10% of the total area with a high identification quality of 98%. Additionally, 3H-Naphth[1,8a-b]oxiren-2(1aH)-one is observed at 6.51% area but with a lower identification quality of 27%.

High-Performance Liquid Chromatography (HPLC) profiling

HPLC profiling of *Parquetina nigrescens* extract showed three (3) phytochemicals resolved and reported with their average peak areas and retention times (Table 2). Quercetin showed the largest peak area (3593.212) and eluted at 1.757 min, indicating the highest relative abundance among the three reported compounds under the applied chromatographic conditions. Magnoflorine (area 841.4059; RT 1.248 min) and rutin (area 724.4042; RT 1.558 min) were also detected, with lower peak areas relative to quercetin [16].

Table 2
HPLC extract profiling of *Parquetina nigrescens*

Phytochemicals	Average Area (%)	Average Retention Time
Quercetin	3593.212	1.757
Rutin	724.4042	1.558
Magnoflorine	841.4059	1.248

Linearity and interpolated concentrations

Calibration/linearity datasets for quercetin, rutin, and magnoflorine were reported using graded standard concentrations and corresponding peak areas. Based on the entered extract peak areas, the interpolated concentrations in the *Parquetina nigrescens* extract were reported as quercetin: 260.486 µg/mL at area 3593.21, rutin: 17.45 µg/mL at area 724.40 and magnoflorine: 63.03 µg/mL at area 841.40 [17].

Calibration curve determination

Quercetin standard

Table 3
presented the Quercetin
standard concentrations
and corresponding peak
areas used to generate the
calibration curve (Fig. 8).

Conc (µg/ml)	Area
20	177.45
40	324.25
60	502.45
80	
100	1329.5

Concentration of Quercetin in *Parguetina nigresens*

Table 4 presented the interpolated concentration of quercetin in *Parguetina nigresens*. This data suggests that at an area of 3593.21, quercetin identified in *Parguetina nigresens* had an interpolated concentration of 260.486 µg/ml.

Table 4
Concentration of Quercetin in
Parguetina nigresens

Conc (µg/ml) (Interpolated)	Area (Entered)
260.486	3593.21

Calibration curve determination

Rutin standard

Table 5
presented the Rutin
standard concentrations
and corresponding peak
areas used to generate the
calibration curve (Fig. 9).

Conc (µg/ml)	Area
20	867.85
40	1849.95
60	2706.15
80	4352
100	4736.3

Concentration of Rutin in *Parguetina nigresens*

Table 6 revealed at average area of 724.40, the rutin identified from the HPLC chromatogram showed an interpolated concentration of 17.45µg/ml.

Table 6
Concentration of Rutin in
Parguetina nigresens

Conc (µg/ml) (Interpolated)	Area (Entered)
17.45	724.40

Calibration curve determination Magnoflorine standard

Table 7 presented the Magnoflorine standard concentrations and corresponding peak areas used to generate the calibration curve (Fig. 10).

Conc (µg/ml)	Area
20	247.718
40	520.5009
60	767.6525
80	1061.068
100	1395.266

Concentration of Magnoflorine in *Parguetina nigresens*

Table 8 showed that the concentration of Magnoflorine in *Parguetina nigresens* extract at an average area of 841.40, was 63.03µg/ml.

Table 8
Concentration of
Magnoflorine in *Parguetina
nigresens*

Conc. (µg/ml) (Interpolated)	Area (Entered)
63.03	841.40

Fourier-Transform Infrared Spectroscopy (FTIR) analysis

FTIR analysis was used to describe dominant functional groups across extracts prepared in dichloromethane, ethyl acetate, and water. The band assignments were interpreted using standard FTIR functional-group regions to support chemical-class level inference in plant-derived mixtures (e.g., C–H stretching, O–H stretching, carbonyl bands, nitrile bands, and aromatic or alkene-associated absorptions) [18].

FTIR profile of the dichloromethane extract

The dichloromethane extract presented fourteen (14) absorption peaks. Key reported bands included 715.64 cm⁻¹ (alkanes/alkyl), 995.19 cm⁻¹ (C–O or C–N), 1028.74 cm⁻¹ (C–N; amines/amides), 1684.75 cm⁻¹ (C = O; ketone/aldehyde region), 2113.40 cm⁻¹ (C ≡ N; nitrile), and 3369.51 cm⁻¹ (O–H; alcohol). The full set of interpreted bands is summarised in Table 11 [18].

Table 9
FTIR interpretation of dichloromethane extract of *Parquetina nigrescens*

S/N	Functional Groups	Absorption Location (cm ⁻¹)	Absorption Intensity
1	Alkanes or Alkyl Groups	715.64	Medium to weak
2	C-H Stretching (Alkynes, Alkenes, Aromatic)	827.46	Weak
3	C-O or C-N Stretching (Alcohols, Ethers, Amines)	995.19	Medium to weak, sharp
4	C-N Stretching (Amines or Amides)	1028.74	Medium to strong, sharp
5	C-N or C-O Stretching (Amines, Amides, Esters)	1166.65	Medium to weak
6	C-N Stretching (Amines or Amides)	1274.75	Medium to weak
7	Carbonyl (C = O) or C-O Stretching (Esters)	1375.38	Weak
8	C-H Bending (Alkanes or Alkyl Groups)	1457.38	Medium to weak
9	Carbonyl (C = O) Stretching (Ketones or Aldehydes)	1684.75	Medium to strong, sharp
10	C = C Stretching (Alkenes or Aromatic Rings)	1990.39	Weak
11	C $\equiv$ N Triple Bond (Nitrile Group)	2113.40	Weak
12	C-H Stretching (Alkanes)	2855.14	Medium to weak
13	C-H Stretching (Alkanes or Alkyl Groups)	2922.23	Medium to weak
14	O-H Stretching (Alcohols)	3369.51	Weak, broad

FTIR profile of the ethyl acetate extract

The ethyl acetate extract showed fourteen (14) absorption peaks, including bands at 924.37 cm⁻¹ (C–C/C–H; alkanes/alkyl), 995.19 cm⁻¹ (C–O/C–N), 1028.74 cm⁻¹ (C–N), 1513.29 cm⁻¹ (carbonyl/C–O region as stated), 1636.30 cm⁻¹ (carbonyl region), 1938.21 and 2087.30 cm⁻¹ (C $\equiv$ N; nitrile), 2929.68 cm⁻¹ (C–H), and 3332.24 cm⁻¹ (O–H). The interpreted peak set is summarised in Table 10 [18].

Table 10
FTIR interpretation of compounds of Ethylacetate extract of *Parguetina nigresens*

S/N	Functional Groups	Absorption Location (cm ⁻¹)	Absorption Intensity
1	C-C or C-H Stretching (Alkanes, Alkyl Groups)	924.37	Weak
2	C-O or C-N Stretching (Alcohols, Ethers, Amines)	995.19	Medium to weak
3	C-N Stretching (Amines or Amides)	1028.74	Medium to weak, broad
4	C-H Bending (Alkanes or Alkyl Groups)	1252.38	Weak
5	C-H Bending (Alkanes or Alkyl Groups)	1341.84	Weak
6	Carbonyl (C = O) or C-O Stretching (Esters)	1513.29	Weak
7	Carbonyl (C = O) Stretching (Ketones or Aldehydes)	1636.30	Weak, broad
8	C $\equiv$ N Triple Bond (Nitrile Group)	1938.21	Weak
9	C $\equiv$ N Triple Bond (Nitrile Group)	2087.30	Weak
10	C-H Stretching (Alkanes)	2929.68	Weak
11	O-H Stretching (Alcohols)	3332.24	Medium to weak
12	C-C or C-H Stretching (Alkanes, Alkyl Groups)	924.37	Weak
13	C-O or C-N Stretching (Alcohols, Ethers, Amines)	995.19	Medium to weak
14	C-N Stretching (Amines or Amides)	1028.74	Medium to weak, broad

FTIR profile of the aqueous extract

The aqueous extract showed eleven (11) absorption peaks, with key bands at 775.28, 820.01, and 864.74 cm⁻¹ (C–H bending; alkanes/alkyl), 1028.73 cm⁻¹ (C–N; amines/amides), 1602.8 cm⁻¹ (C = C; alkenes/aromatic), 2926.07 cm⁻¹ (C–H; alkanes), and 3280.15 cm⁻¹ (O–H; alcohol). The interpreted bands are presented in Table 11 [18].

Table 11
FTIR interpretation of compounds of aqueous extract of *Parquetina nigrescens*

S/N	Functional Groups	Absorption Location (cm ⁻¹)	Absorption Intensity
1	C-H Bending (Alkanes or Alkyl Groups)	775.28	Medium to weak
2	C-H Bending (Alkanes or Alkyl Groups)	820.01	Medium to weak
3	C-H Bending (Alkanes or Alkyl Groups)	864.74	weak
4	C-C or C-H Stretching (Alkanes, Alkyl Groups)	924.37	Medium to weak
5	C-H Bending (Alkanes or Alkyl Groups)	991.47	Medium to strong
6	C-N Stretching (Amines or Amides)	1028.73	Medium to weak
7	C-H Bending (Alkanes or Alkyl Groups)	1244.96	Weak, broad
8	C-H Bending (Alkanes or Alkyl Groups)	1341.86	Weak, broad
9	C = C Stretching (Alkenes or Aromatic Rings)	1602.8	weak
10	C-H Stretching (Alkanes)	2926.07	Weak
11	O-H Stretching (Alcohols)	3280.15	Medium to weak, broad

Discussion

The present study applied polarity-guided solvent fractionation combined with GC–MS, HPLC, and FTIR analyses to generate an integrated chemical profile of *Parquetina nigrescens* extract. This approach aligns with modern phytochemical research strategies aimed at reducing extract complexity, improving compound detectability, and supporting reproducible chemical characterisation of medicinal plants [9, 19]. The results demonstrate clear polarity-dependent distribution of constituents and provide quantitative and functional-group–level evidence supporting the chemical diversity previously reported for *P. nigrescens*.

GC–MS profiling of the non-polar n-hexane fraction identified eight compounds, with a total oil content of 25.3%. The dominance of fatty acid ethyl esters, particularly hexadecanoic acid ethyl ester, linoleic acid ethyl ester, and ethyl 9,12,15-octadecatrienoate, is consistent with earlier studies reporting lipid-rich fractions in medicinal plants extracted with non-polar solvents [23, 26]. Similar fatty acid derivatives have been reported in *Parquetina nigrescens* and related species, where they are often associated with membrane-stabilising, antimicrobial, and anti-inflammatory activities [6, 26].

The detection of aromatic and sterol or terpenoid-like acetates, albeit with lower library match quality, reflects the limitations of EI-GC–MS for highly substituted or thermolabile compounds, but still supports earlier reports describing structural diversity in *P. nigrescens* extracts [6, 7]. Previous phytochemical investigations of *P. nigrescens* leaves and stems have reported sterol-related constituents and phenolic derivatives using chromatographic techniques, supporting the present findings [6, 8]. The relatively higher confidence scores for fatty acid esters compared with aromatic compounds further highlight the suitability of GC–MS for profiling volatile and semi-volatile lipid constituents rather than complex polyphenols [12, 23].

HPLC analysis revealed quercetin, rutin, and magnoflorine as the major chromatographically resolved phytochemicals in the extract. Quercetin exhibited the highest peak area and interpolated concentration (260.486 µg/mL), followed by magnoflorine (63.03 µg/mL) and rutin (17.45 µg/mL). These findings agree with earlier reports identifying flavonoids and alkaloids as prominent secondary metabolites in *Parquetina nigrescens* and other African medicinal plants [6, 17].

The predominance of quercetin is particularly noteworthy, as quercetin has been widely documented for its antioxidant, antidiabetic, and anti-inflammatory activities [17, 18]. Studies on related medicinal plants have similarly reported higher concentrations of quercetin relative to other flavonoids when ethanol or methanol-based extraction and reversed-phase HPLC methods are employed [24, 26]. The detection of magnoflorine, an isoquinoline alkaloid, corroborates previous pharmacological studies reporting haematinic and antidiabetic effects of *P. nigrescens*, as alkaloids are often implicated in glucose modulation and hematopoietic activity [7, 8].

Rutin, although present at lower concentration, remains pharmacologically relevant due to its reported vascular-protective and antioxidant properties. The observed quantitative differences among these compounds may reflect solvent polarity effects, plant chemotype, geographical origin, or post-harvest processing conditions, all of which are known to influence phytochemical abundance [4, 20].

FTIR analysis of dichloromethane, ethyl acetate, and aqueous extracts revealed characteristic absorption bands corresponding to O–H, C–H, C = O, C–O, C–N, and C ≡ N functional groups. These findings support the presence of alcohols, phenolics, carbonyl-containing compounds, alkaloids, and nitrile-related functionalities across fractions, consistent with phytochemical classes previously reported for *P. nigrescens* [6, 22, 25].

The dichloromethane extract showed prominent aromatic and phenolic-associated bands, suggesting enrichment of moderately polar phenolic constituents, which aligns with the HPLC detection of flavonoids in the extract. Similar FTIR profiles have been reported in studies of medicinal plant extracts where phenolics and alkaloids co-exist across mid-polar fractions [22, 25]. The aqueous extract exhibited dominant O–H and C–H bands, reflecting the retention of polar constituents, including sugars and highly oxygenated metabolites, as commonly observed in water-soluble plant fractions [4, 25].

Overall, the present study's findings are consistent with earlier phytochemical and pharmacological investigations of *Parquetina nigrescens*, which have documented the presence of flavonoids, alkaloids, fatty acids, and glycosides using qualitative assays and bioactivity models [6–8]. However, the current work advances existing knowledge by providing polarity-guided fractionation, GC–MS profiling of non-polar constituents, and quantitative HPLC data for selected marker compounds, thereby addressing gaps in reproducible chemical standardisation.

Compared with earlier studies that relied primarily on crude extracts or qualitative screening, the present analytical workflow strengthens the chemical evidence base needed for quality control, standardisation, and future bioactivity-guided isolation. This approach aligns with WHO recommendations for the scientific evaluation of traditional medicinal plants and supports their potential integration into regulated healthcare frameworks [1, 4].

Despite these strengths, the study has limitations. Only selected phytochemicals were quantified by HPLC, and comprehensive LC–MS/MS profiling was not performed, which may have enabled broader metabolite coverage. In addition, structural confirmation relied on library matching and functional-group inference rather than full spectroscopic elucidation (e.g., NMR). Finally, no direct biological assays were conducted to correlate chemical composition with pharmacological activity. Future studies should therefore integrate advanced metabolomics, compound isolation, and bioactivity evaluation to strengthen causal links between chemistry and therapeutic effects.

Conclusion

This study demonstrates that polarity-guided solvent fractionation combined with GC–MS, HPLC, and FTIR provides a robust and complementary framework for chemical profiling of *Parquetina nigrescens*. The non-polar fraction was enriched in fatty acid esters, while HPLC profiling confirmed quercetin, magnoflorine, and rutin as key phytochemical markers. FTIR analysis further supported the presence of diverse functional groups corresponding to phenolic, alkaloid, and lipid-related constituents. These findings are consistent with previous reports on *P. nigrescens* and extend current knowledge by offering quantitative and fraction-specific chemical evidence. Collectively, the results support the pharmaceutical relevance of *P. nigrescens* and provide a foundation for future standardisation, isolation, and bioactivity-driven investigations.

Abbreviations

ACEDHARS: African Centre of Excellence for Drug Research, Herbal Medicine Development and Regulatory Science.

ATR-FTIR: Attenuated total reflectance–Fourier transform infrared spectroscopy

C=O: Carbonyl

$C\equiv C$: Alkyne

$C\equiv N$: Nitrile

Da: Dalton

El: Electron ionisation

GC–MS: Gas chromatography–mass spectrometry

HPLC: High-performance liquid chromatography

mAU: Milli-absorbance units

R_f: Retention factor

R²: Coefficient of determination

TFA: Trifluoroacetic acid

TLC: Thin layer chromatography

UV: Ultraviolet

Declarations

Ethics approval and consent to participate

Not applicable. No animal model or human participants were involved; therefore, ethical approval was not required.

Consent for publication

Not applicable.

Availability of data and materials

The datasets generated and/or analysed during the current study are available from the corresponding author on reasonable request.

Competing interests

The authors declare that they have no competing interests.

Funding

This work was supported by the African Centre of Excellence for Drug Research, Herbal Medicine Development and Regulatory Science (ACEDHARS).

Authors' contributions

A.T: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Writing original draft, Writing review and editing.

O.T.A: Supervision, Methodology oversight, Writing review and editing.

M.O.A: Resources, Technical support, Writing review and editing.

M.M: Writing review and editing.

All authors read and approved the final manuscript.

Acknowledgements

Thanks to Prof. Olayinka T. Asekun, Dr. Moshood O. Akinleye, the ACEDHARS leadership and coordinators, and staff of the University of Lagos for guidance, facilities, and technical support. The authors also acknowledge the support of colleagues and family during the study.

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Figures

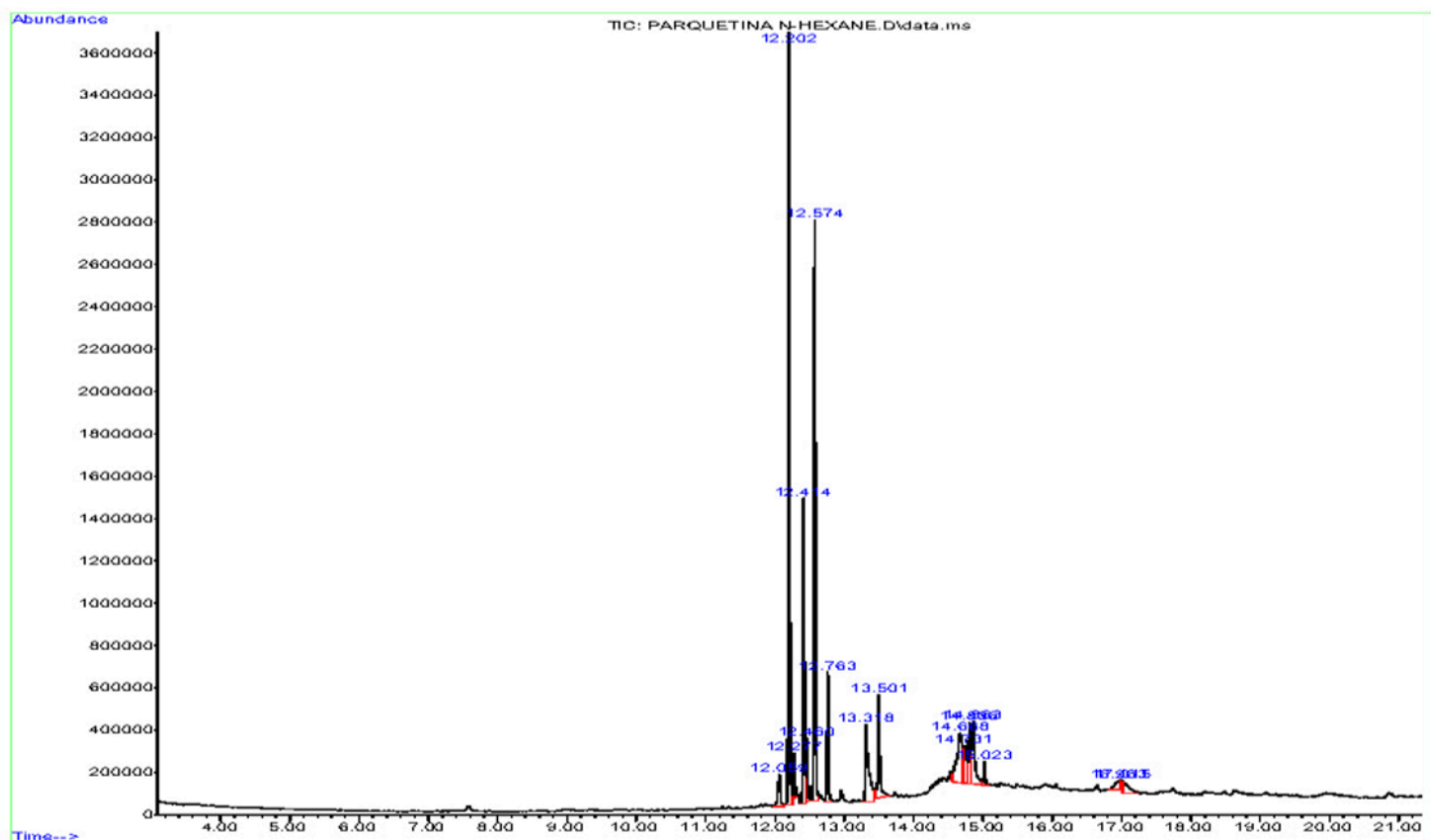


Figure 1

Total ion chromatogram of *Parquetina nigrescens* n-hexane extracts

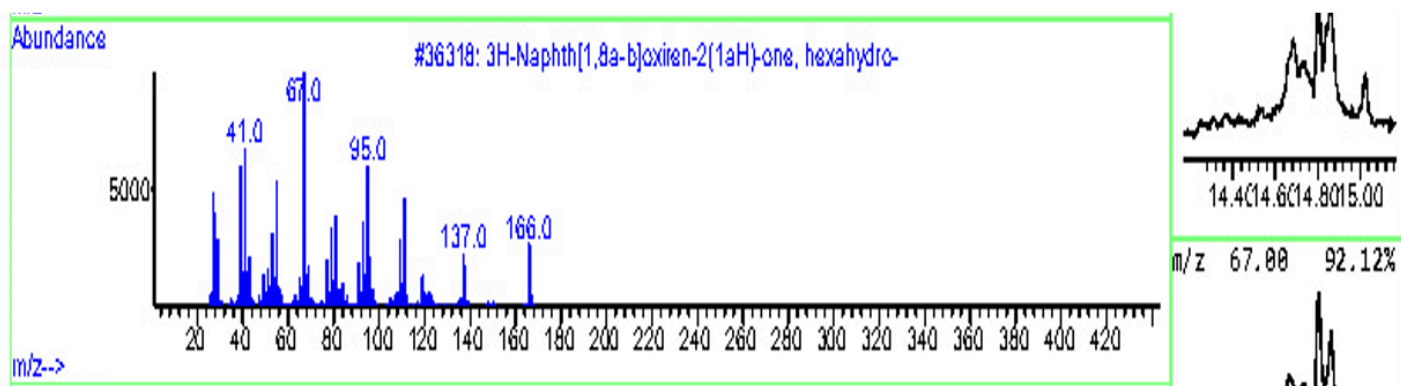


Figure 2

Mass spectrum of 3H-Naphth[1,8a-b]oxiren-2(1aH)-one

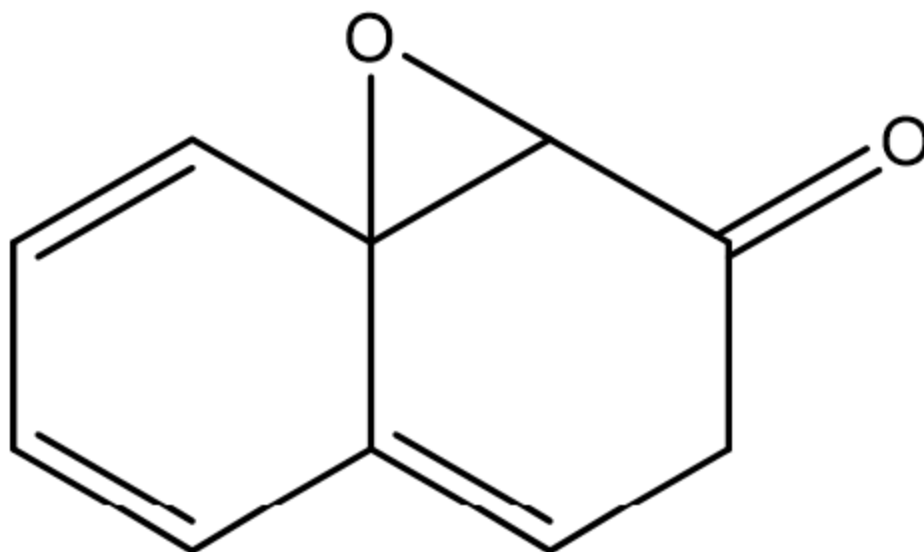


Figure 3

Structure of 3H-Naphth[1,8a-b]oxiren-2(1aH)-one (6.51%)

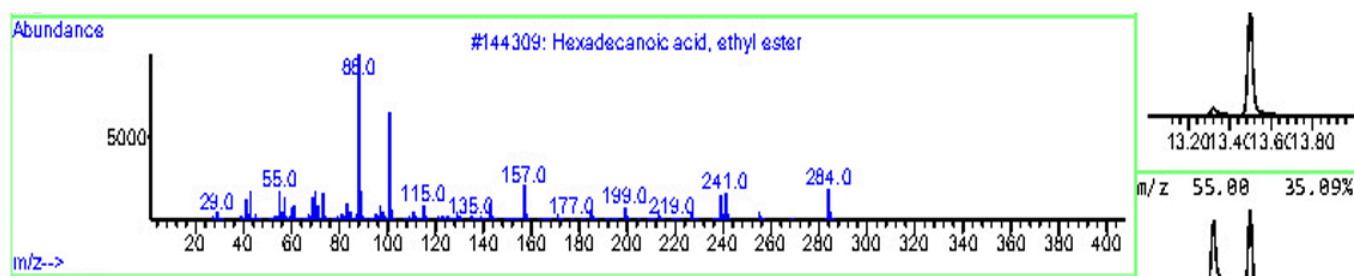


Figure 4

Mass spectrum of Hexadecanoic acid, ethyl ester

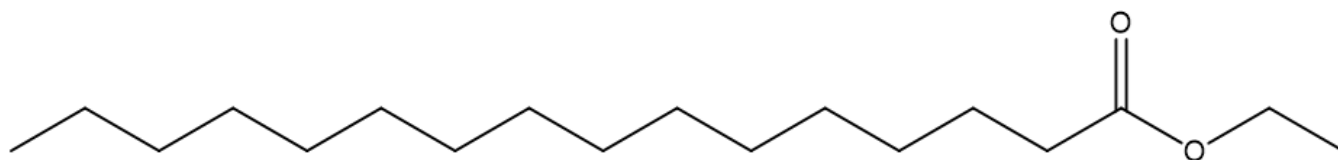


Figure 5

Structure of Hexadecanoic acid, ethyl ester (5.10%)

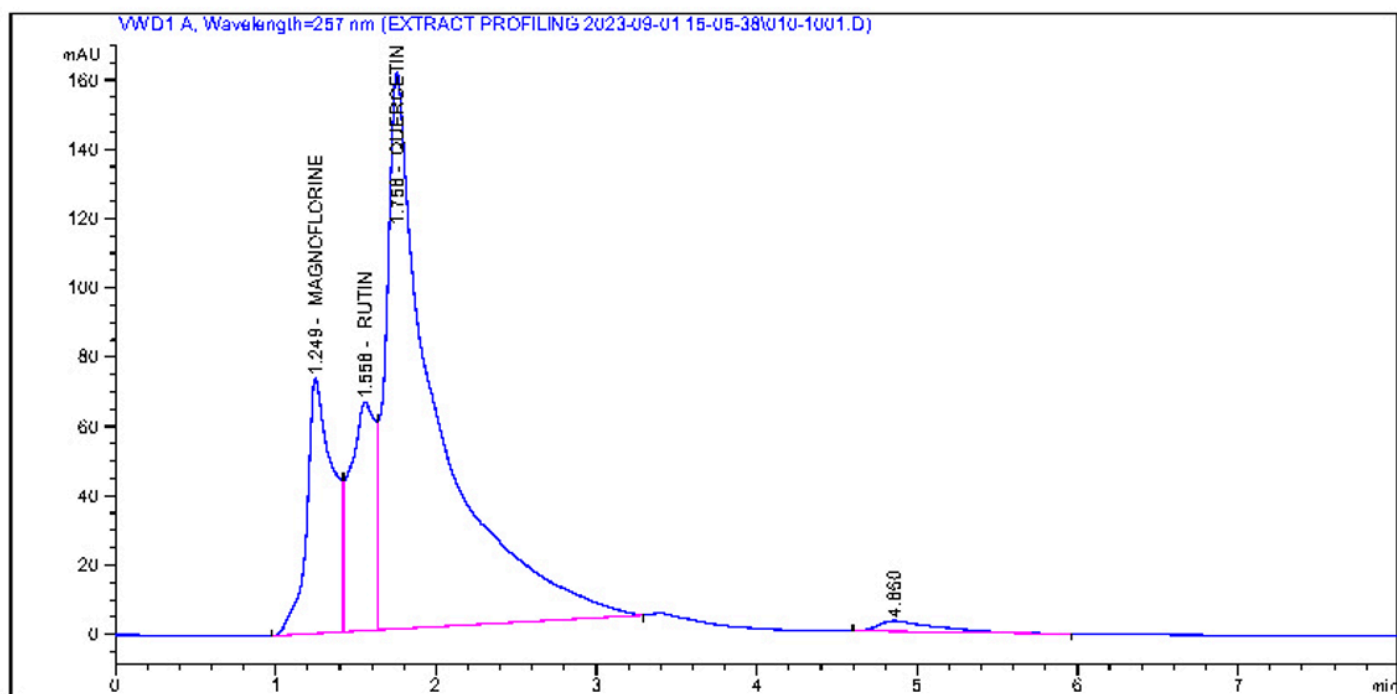


Figure 6

Chromatogram of extract Profiling of *Parguetina nigresens* (RUN A)

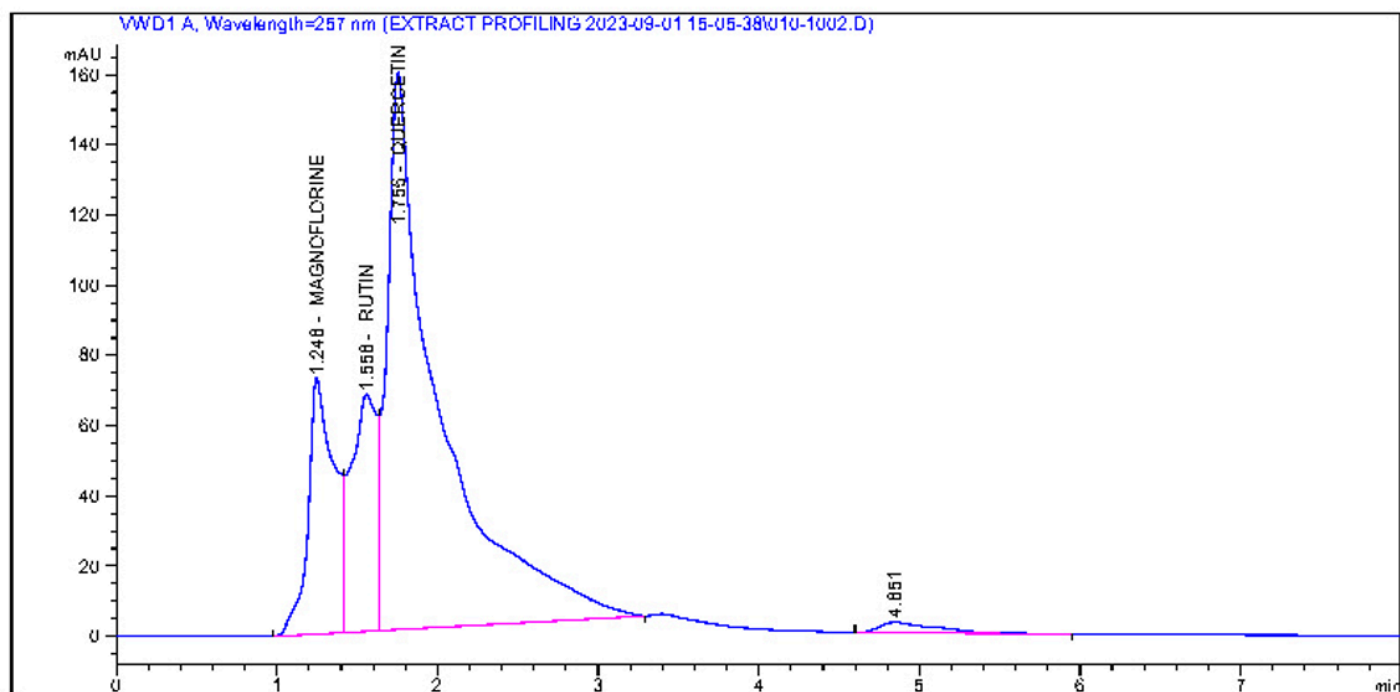


Figure 7

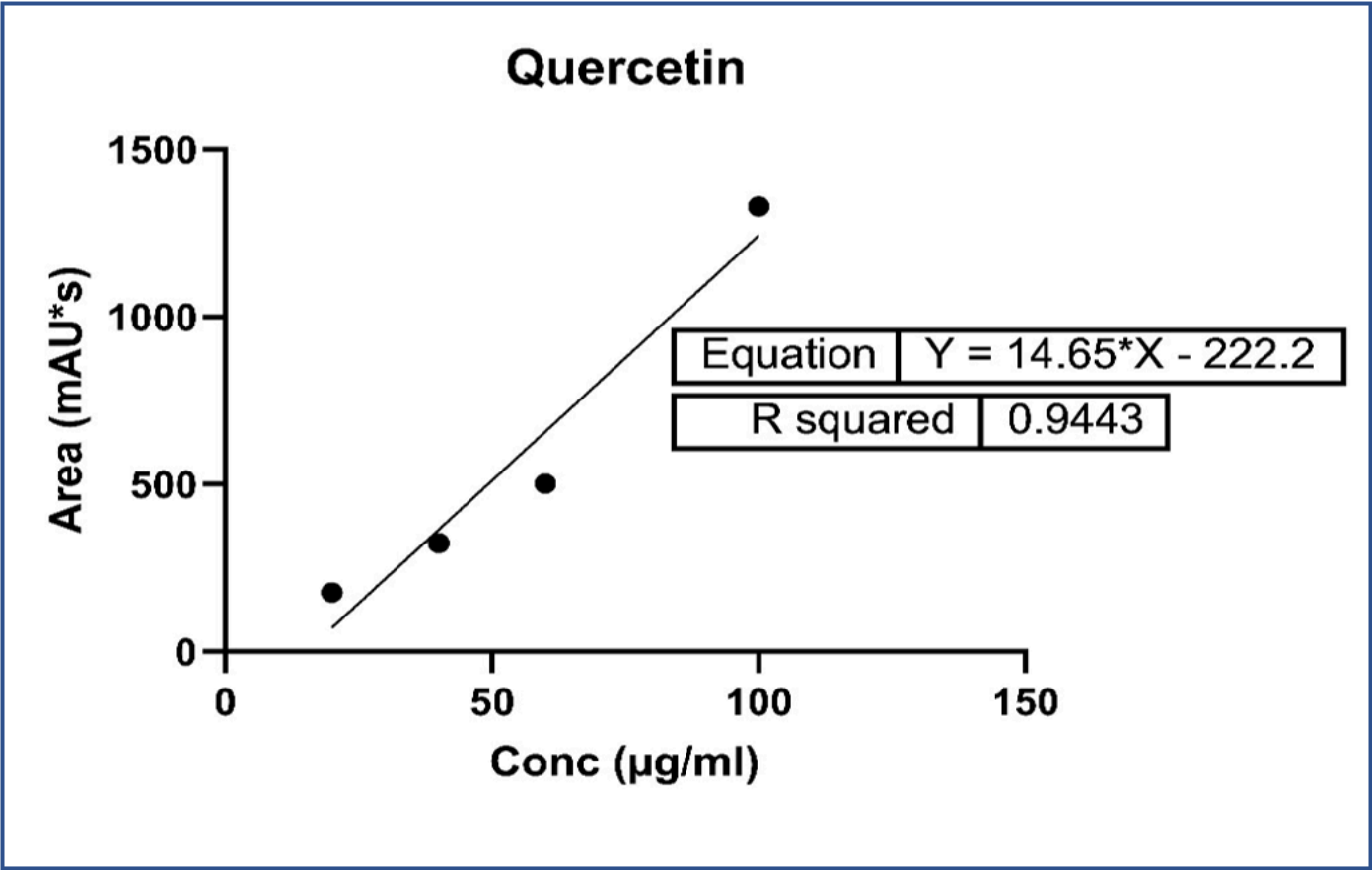


Figure 8

Linearity plot for quercetin standard

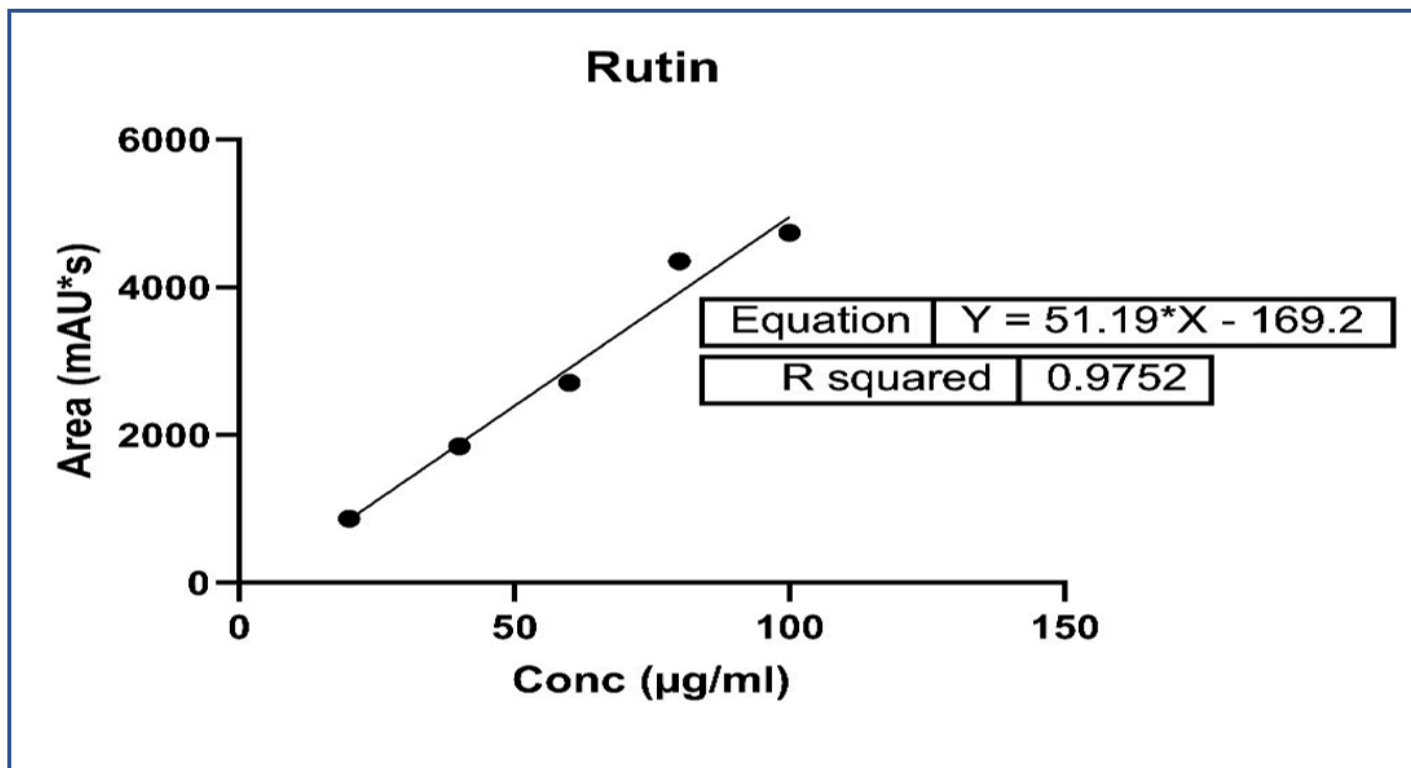


Figure 9

Calibration plot for Rutin standard

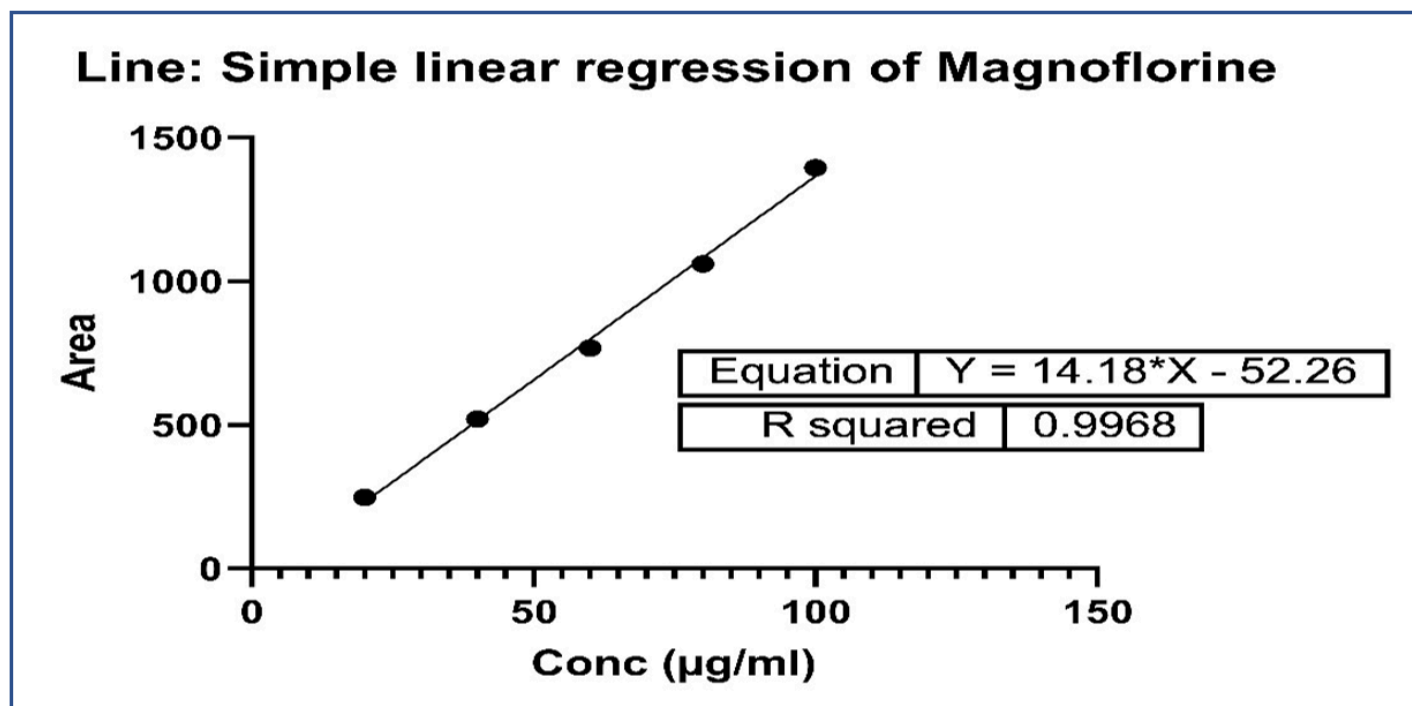


Figure 10

Calibration plot for Magnoflorine standard.

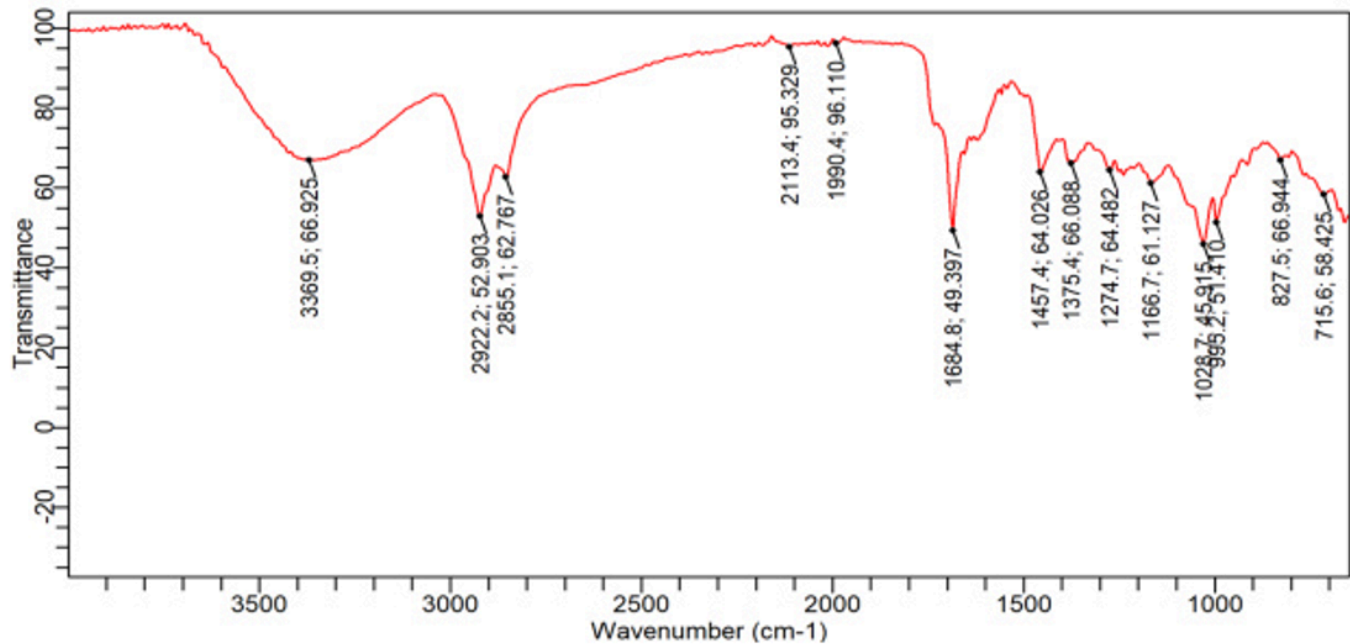


Figure 11

FTIR spectrum analysis of the dichloromethane extract of the *Parguetina nigresens* plant.

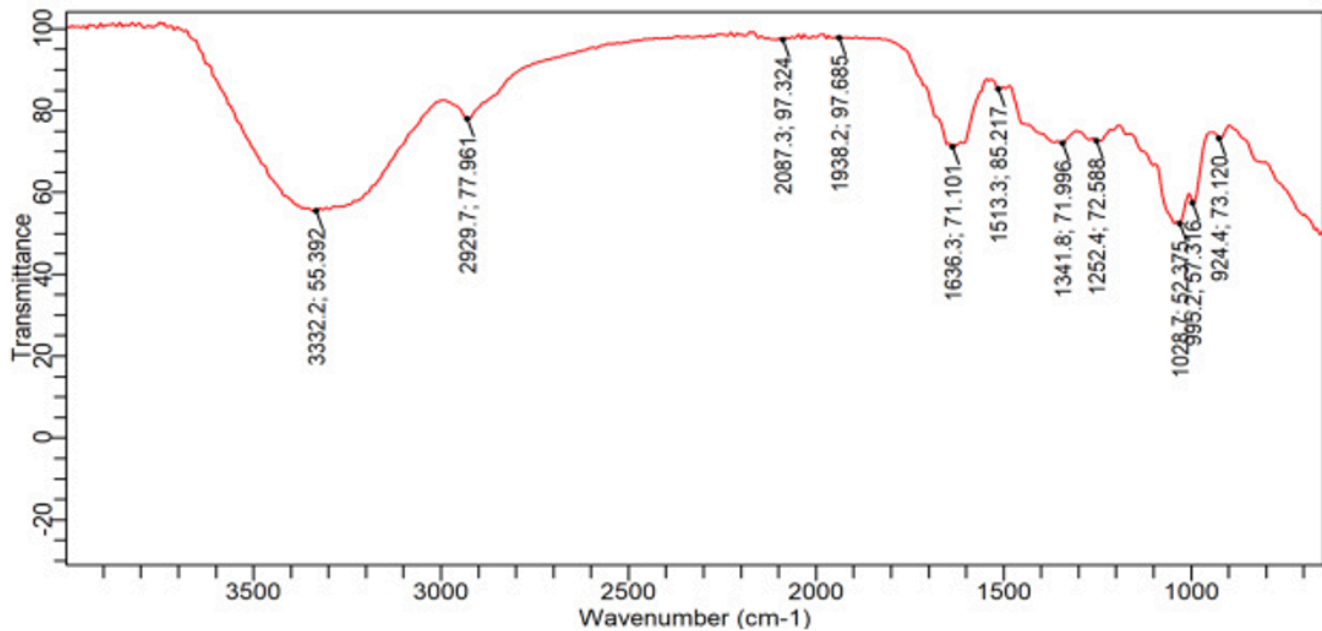


Figure 12

FTIR spectrum analysis of the ethyl acetate extract of the *Parguetina nigresens* plant.

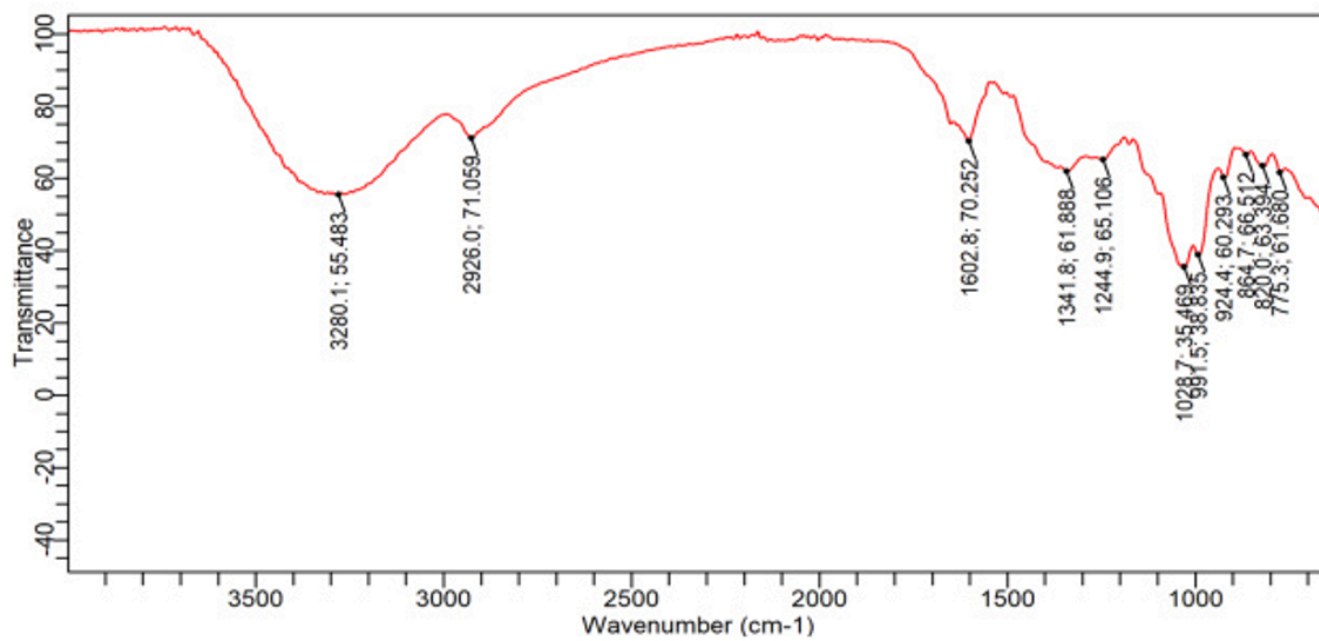


Figure 13

FTIR spectrum analysis of the aqueous extract of the *Parguetina nigresens* plant.