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Original Research Article

Phytochemical profiling and bioactive compound variation in *Jatropha landraces* from Nigeria: Implications for agricultural and medicinal applications

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Abstract

Purpose: *To determine the phytochemical composition of various Jatropha landraces from different regions of Nigeria in order to identify key bioactive compounds and regional variations for future agricultural and pharmacological applications.*
Methods: *A total of 40 Jatropha landraces were collected from traditional farmers in Nigeria, identified by local names and morphological features. Dried leaves (50 g) were extracted with ethanol (hot percolation) using Soxhlet apparatus, concentrated to 50 mL under reduced pressure in desiccators and lyophilized for further analysis. A total of 6 samples representing the six geopolitical zones were selected for gas chromatography-mass spectrometry (GC-MS), while principal component analysis (PCA) was used to identify the bioactive compounds.*
Results: *GC-MS analysis identified 122 phytochemicals, predominantly fatty acids, with oleic acid and linoleic acid being the most common. The sample from Enugu had the highest phytochemical diversity (33 compounds), followed by Nasarawa (22), Delta (21), Borno (20), Kano (14), and Lagos (12). Principal component analysis (PCA) revealed that PC1 contributed 64.2 % of the total variation, with Borno showing the highest loading value (0.521), followed by Lagos (0.599) on PC2, Nasarawa (0.708) on PC3, and Enugu (0.639) on PC4. Furthermore, PCA revealed that Borno had the highest contribution to variations in phytochemical composition.*
Conclusion: *This study confirms substantial phytochemical diversity of Jatropha landraces across Nigeria, and highlights its potential for breeding programs aimed at selecting plants with specific bioactive compounds.*

Keywords: *Jatropha, Phytochemical composition, GC-MS (Gas Chromatography-Mass Spectrometry), Principal Component Analysis (PCA), Bioactive compounds*

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INTRODUCTION

Nigeria's tropical and subtropical forests are teeming with biodiversity, particularly rich in plant species with substantial potential to fulfill basic human needs such as food, raw materials and various services [1]. Among these, Jatropha stands out as a fruit tree with considerable economic and medicinal significance. The genus Jatropha originates from the Greek words *jatros* (physician) and *trophe* (food), suggesting the traditional use of its species for medicinal and

nutritional purposes [2]. In Nigeria, Jatropha species are used for dye production and tanning. The oil-rich seeds are ideal for biodiesel production, while the medicinal leaves serve as livestock feed and local vegetables [3]. These applications stem from its diverse phytochemical content. Phytochemicals, which are biologically active compounds derived from plants, support the development and defense mechanisms of the host plant against pathogens, competitors, or predators [4].

Recently, attention has been drawn to phytochemicals due to the potential health impacts of certain plant compounds, which are either protective or harmful to living organisms [4]. Moreover, plants capable of producing new chemical defenses may have an evolutionary advantage, potentially leading to the diversification of plant lineages with preserved chemical phenotypes [5]. Despite the considerable economic and ecological value of Jatropha species, its potential remains largely untapped in Nigeria [6]. While Jatropha species have been studied worldwide, there is limited research on the phytochemical profiles of various *Jatropha landraces* within Nigeria. This study investigated the phytochemical diversity of *Jatropha landraces* from the six geopolitical regions in Nigeria.

EXPERIMENTAL

Sample collection

The study analyzed 40 leaf samples of Jatropha species collected from 25 states across Nigeria (Table 1). These samples were obtained from local farmers and validated by a taxonomist, Dr EA Effa of the Department of Plant and Ecological Studies, Faculty of Biological Sciences, University of Calabar. Voucher specimens were deposited at the herbarium of the University of Calabar for future reference. This study was conducted at Docchy Analytical and Environmental Services Ltd, Awka, Anambra State, Nigeria.

Phytochemical analysis

A total of 6 leaf samples representing each of Nigeria's geopolitical zones were selected for comprehensive phytochemical analysis.

Extraction and preparation of bioactive compounds

Leaves of *Jatropha spp*. were collected and air-dried for 2 weeks and finely powdered (Qlink-Q15L40 blender). Thereafter, 50 g of dried Jatropha leaf powder was extracted with ethanol (hot percolation) using a Soxhlet apparatus [7]. The *Jatropha landraces* ethanol extract (JLEE) was concentrated at 50 mL under reduced pressure in desiccators and subsequently lyophilized for further analysis.

Phytochemical compound identification

Phytochemical analysis was performed on Jatropha leaves using cold maceration following procedures outlined by Adamu *et al* [8] and Ananthi and Giri [9].

Gas chromatography-mass spectrometry (GC-MS) analysis

The GC-MS analysis was performed using a Shimadzu 2010 Plus instrument, equipped with an AOC-20i auto-sampler and a gas chromatograph interfaced with a mass spectrometer. The following parameters were used for optimal analysis: RTX-5Ms column (0.32 mm diameter, 30 m length, 0.50 µm thickness), electron impact mode at 70 eV and helium (99.99 %) as the carrier gas at a flow rate of 1.73 mL/min with an injection volume of 0.5 µL (split ratio 10:1). The injector temperature was set to 270 °C, and the ion-source temperature was 200 °C. The GC oven temperature program began with an isothermal hold at 40 °C for 2 min, followed by a ramp of 8 °C/min to 150 °C, then another ramp of 8 °C/min to 250 °C, with a final isothermal hold at 280 °C for 20 min. Mass spectra were recorded at 70 eV, with a scan interval of 0.5 s and a range of fragments from 40 to 450 Da, resulting in a total GC run-time of 51.25 mins. Data from the GC-MS were analyzed with Turbo Mass software (version 5.20). Compound identification was achieved by matching mass spectra with entries in the National Institute of Standards and Technology (NIST) library, which includes over 62,000 known patterns. For each detected component, the software provided molecular weight, structural details and relative abundance based on average peak area percentages [9].

GC-MS data processing and analysis

The data pre-treatment process followed several preprocessing steps [10]. Initially, a filtering step was applied to eliminate peaks that account for less than 50 % within a single group. Missing values were then addressed through imputation, where half the minimum detected values were used as a substitute. Subsequently, normalization was carried out using an internal standard method to quantify phytochemical

compounds. The concentration of each phytochemical was determined using Eq 1.

$$Ci = (A_i/A_o)(M_o/M) \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where C_i represents the content of the phytochemical compound, Ai is each compound's peak area, A_o is the internal standard substance's peak area of the internal standard substance, M_o is the mass, and M is the sample taken.

Data analysis

Data analysis was conducted using Soft Independent Modelling of Class Analogy-Projection (SIMCA-P 11) software (Sartorius Stedim, Germany). Principal component analysis (PCA) was conducted using multivariate data analysis.

RESULTS

Phytochemical composition of selected Jatropha samples

A total of 122 peaks, indicating 122 compounds, were detected from the six (6) *Jatropha* landraces. The predominant compounds common to all landraces were oleic acid and linoleic acid. The metabolites were mostly fatty acids. Borno sample contained 20 identified phytochemicals, with linoelaidic acid (24.92 %) being the most abundant. Lagos sample had 12 detected compounds, with cis-vaccenic acid (40.39 %) being the most abundant.

Table 1: Samples of *Jatropha spp* used in the study and their locations

Sample no.	Location	Latitude	Longitude
1	KaruKarama, Jos, Plateau	9.744537	8.837208
2	Ndegwu, Owerri, Imo	5.543245	6.986405
3	Rumodome, Rivers	4.888140	7.007098
4	Kanshio, Asuir, Benue	7.697007	8.537146
5	Rimi, kokona, Nassarawa	8.915968	7.889378
6	Amassoama, Bayelsa	4.971469	6.124349
7	Aba, Abia	5.135215	7.354580
8	Kaba, Kubwa, FCT	9.126189	7.312542
9	Kudy-kogin, Dutse, Jigawa	11.725733	9.367135
10	Opi, Nsukka, Enugu	6.769912	7.434066
11	Obubra, Cross River	5.991089	8.258368
12	Ashaka, Gombe	10.915930	11.480775
13	Faggae, Kano	12.024042	8.528676
14	Aguata, Anambra	6.018366	7.075524
15	Uyo, Akwa-Ibom	5.008406	7.898525
16	Yola, Adamawa	9.203496	12.495390
17	Ikorodu, Lagos	6.629484	3.518274
18	Bauchi	11.398440	6.793149
19	Ozoro, Delta	5.538727	6.228469
20	Ekete, Orhuwhorun, Delta	5.500385	5.820495
21	Biu Emirates, Borno	10.617181	12.152730
22	Abakaliki, Ebonyi	6.336659	8.087300
23	Jalingo, Taraba	8.903073	11.314469
24	Umuonaje, Asaba, Delta	6.196002	6.718493
25	Alafia, Ibadan, Oyo	7.362198	3.819935
26	Ota, Ogun	6.592366	3.201195
27	Ojota, Lagos	6.584031	3.376412
28	Safana, Katsina	12.402568	7.405300
29	Ushafa, FCT	9.228900	7.390215
30	Newkaru, Karu, Nassarawa	9.013259	7.632999
31	Ado, Abuja, FCT	9.040931	7.584636
32	Vandelkya, Benue	6.811492	9.050438
33	Calabar South, Calabar, Cross River	4.982873	8.334503
34	Calabar Municipal, Calabar, Cross River	5.026875	8.373303
35	Nung-ukana, Ibesikpo, Akwa-Ibom	4.921256	7.966280
36	Obudu, Cross River	6.672476	9.163086
37	Ita, Uyo, Akwa-Ibom	4.989842	7.888318
38	Ikot–Ekpene, Akwa-Ibom	5.200653	7.700433
39	Itu, Akwa-Ibom	5.050375	7.889212
40	Idomi, Cross River	5.758464	8.084197

In the Kano sample, 14 compounds were identified, and linoelaidic acid (32.99 %) was the most abundant. The Delta sample contained twenty-one phytochemicals, with the highest abundance recorded for 9,12-octadecadienoic acid (28.37 %). Sample from Nasarawa had 22 identified compounds, with (R*, R*)-5-hydroxy-4-methyl-3-heptanone (22.87 %) being the most prevalent. Furthermore, samples from Enugu exhibited a diverse profile of 33 compounds, with oleic acid (12.54 %) being the most prevalent (Tables 2 - 7).

Table 2: Phytochemicals identified by GC-MS in JLEE sample 21 (Biu Emirates, Borno State)

S/no.	Retention time (min)	Peak area (%)	Compound
1	9.840	1.07	5-Octadecene
2	12.828	0.98	Pyrimidine-4
3	12.8793	0.81	Trichloroacetic acid
4	13.113	2.69	Dodecanoic acid
5	15.408	2.11	Tetradecanoic acid
6	16.880	0.66	Carbonic acid
7	16.952	1.44	Hexadecenoic acid
8	17.410	2.14	n-Hexadecenoic
9	17.538	7.12	n-Hexadecenoic
10	18.743	6.63	10-Octadecenoic acid
11	18.980	0.88	Heptadecanoic acid
12	19.301	24.92	Linoleic acid
13	19.497	7.73	Octadecanoic acid
14	19.753	2.98	9,12-Octadecadienoic acid
15	19.869	4.56	9,12-Octadecadienoic acid
16	19.999	2.91	9,12-Octadecadienoic acid
17	20.137	5.76	Linoleic acid
18	20.900	10.94	6-Octadecenoic acid
19	30.931	12.97	Oleic acid
20	31.429	0.72	Ethyl oleate

Table 3: Phytochemicals identified by GC-MS in JLEE sample 17 (Ikorodu, Lagos State)

S/no.	Retention time (min)	Peak area (%)	Compound
1	7.087	0.69	Dimethyl Sulfoxide
2	9.220	4.86	Phthalic anhydride
3	12.944	2.56	Dodecanoic acid
4	15.369	1.84	Tetradecanoic acid
5	17.534	13.21	n-Hexadecenoic acid
6	18.735	1.14	Cis-13-octadecenoic acid
7	19.338	40.39	Cis-Vaccenic acid
8	19.516	10.33	Octadecanoic acid
9	19.743	11.52	9,12-Octadecadienoic acid
10	19.974	2.47	9,12-Octadecadienoic acid
11	20.117	9.84	Linoleic acid
12	23.163	1.15	3H-Pyrazol-3-one

Table 4: Phytochemicals identified by GC-MS in JLEE sample 13 (Faggae, Kano State)

S/no.	Retention time (min)	Peak area (%)	Compound
1	9.164	1.53	Phthalic anhydride
2	15.405	1.14	2,2-Dichloroethylpropylcarbonate
3	16.422	1.12	Dibutyl phthalate
4	17.322	0.91	n-Hexadecenoic acid
5	17.400	1.33	n-Hexadecenoic acid
6	17.530	6.80	n-Hexadecanoic acid
7	18.744	0.76	9-Oxabicyclo (6.1.0) nonane
8	19.307	32.99	Linoleic acid
9	19.498	14.81	Nonanoic acid
10	19.742	17.12	z,z-10,12-Hexadecadien-1-olacetate
11	19.984	5.35	z,z-10,12-Hexadecadien-1-olacetate
12	20.120	12.08	Cyclohexene
13	23.191	2.89	10H-Phenoxaphosphine
14	23.395	1.17	3H-Pyrazol-3-one

Table 5: Phytochemicals Identified by GC-MS in JLEE sample 24 (Umuonaje, Asaba, Delta State)

S/n	Retention time (min)	Peak area (%)	Compound
1	5.77	3.89	2-Chloroethylmethylsulfoxide
2	7.089	1.01	Dimethyl Sulfoxide
3	9.221	3.67	Phthalic anhydride
4	9.849	1.96	2-chloroethylchlorobromoethylsulfoxide
5	12.896	0.63	Dimethyl sulfoxide
6	15.404	1.48	Carbonic acid
7	16.954	0.75	Benzene sulfonyl Chloride
8	17.403	2.25	n-Hexadecenoic acid
9	17.533	9.01	n-Hexadecenoic acid
10	18.412	0.67	S-Methylmethanethiosulfinate
11	18.592	1.40	(S)-(-)-2-Chloropropionic acid
12	18.745	3.07	9-Oxabicyclo (6.1.0) nonane
13	18.983	0.51	Heptadecanoic acid
14	19.308	28.37	9,12-Octadecadienoic acid
15	19.496	10.26	Oleic acid
16	19.737	9.81	9,12-Octadecadienoic acid
17	19.979	3.41	9,12-Octadecadienoic acid
18	20.128	6.53	9,12-Octadecadienoic acid
19	23.193	6.12	3H-Pyrazol-3-one
20	23.449	4.17	3H-Pyrazol-3-one
21	23.779	1.02	9,12-Octadecadienoic acid

Table 6: Phytochemicals identified by GC-MS in JLEE sample 5 (Rimi, Nassarawa State)

S/n	Retention time (min)	Peak area (%)	Compound
1	11.877	22.87	(R*, R*)-5-hydroxy-4-methyl-3-heptanone
2	12.460	5.45	Decanoic acid
3	12.699	0.96	Butoxyacetic acid
4	14.435	6.31	Ether
5	14.527	1.70	Docosyloctyl ether
6	14.703	2.49	3-Deoxy-d-mannoic lactone
7	15.474	2.39	Oxazole
8	16.982	2.94	Hexadecenoic acid
9	17.486	1.17	1,2-Benzenedicarboxylic acid
10	17.621	12.12	n-Hexadecenoic acid
11	18.208	0.66	1-Octenylsuccinicanhydride
12	18.800	5.41	Cis-13-Octadecenoic acid
13	19.102	6.18	1H-cycloprop[e]azulene
14	19.425	12.69	Cis-Vaccenic acid
15	19.604	5.64	Oleic acid
16	19.915	1.63	Oleic acid
17	20.268	2.33	7-Pentadecyne
18	20.564	0.75	2-Propenoicacid
19	23.602	2.60	6-Octadecenoicacid
20	23.931	1.54	4-Thiazolidinone
21	26.110	1.24	Glycemic acid
22	29.714	0.95	Octa siloxane

Loading values

The results show that the first four Principal Components account for over 90 % of the total variations observed in phytochemical composition. Principal Component 1 had an eigenvalue of 302.412 and contributed the highest percentage of 64.208 % to the total variation in the phytochemical composition of the different landraces. Sample 21 from Borno had the highest loading value of 0.521 contribution on PC1 to the total observed variations in the phytochemical composition (Table 8, Figure 1).

Identification of phytochemicals accounting for variation in *Jatropha* samples

The data from GC-MS was used as the subject of the PCA model. Principal Component 1 explained 64.2 % of the variation while PC2 explained 22 % of the variation, and PC3 and PC4 accounted for 5.4 % and 3.7 % of the variation, respectively (Table 9). The

phytochemicals in PC1 and 2 included cyclopentane undecanoic acid, trans-13-octadecenoic acid, methyl stearate, dimethyl-12-tetradecen-1-ol, oleicacid,6-Octadecenoicacid, *p*-menth-8(10)-en-9-ol, octadec-9-enoic acid, 9-octadecenoic acid, 9,17-octadecadienal, 3, 7, 11-tridecatrienoic acid, 2,5-furandione, 6-methylhe-5-cyclohex-2-enol, 1H-indene,1,2-hydrazinedicarbothioamide, benzoic acid, 6-octadecenoic acid, bicyclo (4.2.0)oct-2-ene (Table 9).

DISCUSSION

The importance of medicinal plants in the development of pharmacopeias cannot be overstated, as they have long been used for the treatment of various diseases and ailments. Phytochemicals, the bioactive compounds found in plants, are primarily responsible for varying therapeutic properties, such as prophylaxis and treatment [11]. Jatropha species, in particular, have gained significant attention due to their medicinal properties, including high nutritional content in leaves and oil-rich seeds.

Table 8: Loading values for the landraces across the principal components

Location	PC1	PC2	PC3	PC4
Enugu	-0.188	-0.086	0.283	0.639
Nasarawa	0.462	-0.356	-0.708	0.108
Delta	0.478	0.299	0.145	0.307
Kano	0.387	0.596	-0.023	-0.345
Lagos	0.314	0.599	-0.024	0.560
Borno	0.521	-0.246	0.629	-0.228

Table 9: Variations in *Jatropha* Samples using the PCA model

PC value	1	2	3	4
Eigen value	302.412	103.771	25.8163	17.4812
% variance	64.208	22.033	5.4813	3.7116
Cumulative %	64.208	86.211	91.960	95.490

Table 7: Phytochemicals identified by GC-MS in JLEE sample 10 (Opi, Nsukka, Enugu)

S/n	Retention time (min)	Peak area (%)	Compound
1	7.070	0.82	3-Methyl-6-hepten-1yn-3-ol
2	7.722	1.19	Chitral
3	16.990	3.74	Hexadecenoic acid
4	17.638	6.98	n-Hexadecenoic acid
5	17.866	0.34	Cyclopentane undecanoic acid
6	18.804	8.69	Trans-13-octadecenoic acid
7	19.051	4.27	Methyl stearate
8	19.217	0.86	11,13, Dimethyl-12-tetradecane-1-acetate
9	19.434	12.54	Oleic acid
10	19.601	7.17	6-Octadecenoic acid
11	19.795	0.92	p-menthyl-8(10)-en-9-ol
12	19.830	1.02	Octadec-9-enoic acid
13	19.981	4.54	9-Octadecenoic acid
14	20.228	8.63	Oleic acid
15	20.328	1.92	9-Octadecenoic acid
16	20.601	9.31	1,3-Dioxolane
17	20.712	3.49	Cyclopropane carboxamide
18	20.807	1.15	Octadec-9-enoic acid
19	20.934	2.13	9,17-Octadecadienal
20	21.044	2.35	3,7,11-Tridecatrienoic acid
21	21.646	2.74	Trimethylsilyl-di-(trimethylsilyl)-silane
22	21.777	2.24	Glycemic acid (ISP-TFA)
23	23.479	0.61	2,5-Furandione
24	23.550	1.08	Oleic acid
25	23.601	0.57	(1R,4R)-1-methyl-4-(6-Methylhept-5-en-2-yl) cyclohex 2 enol
26	24.481	0.82	1H-Indene
27	26.076	0.99	1,2-hydrazinedicarbothioamide
28	26.640	0.20	9-Octadecenoic acid
29	28.039	0.96	3,7,11-Tridecatrienoic acid
30	28.113	1.09	Benzoic acid
31	28.926	1.71	3,7,11-Tridecatrienoic acid
32	29.751	2.64	6-octadecenoic acid
33	30.011	2.31	Bicyclo[4.2.0]oct-2-ene

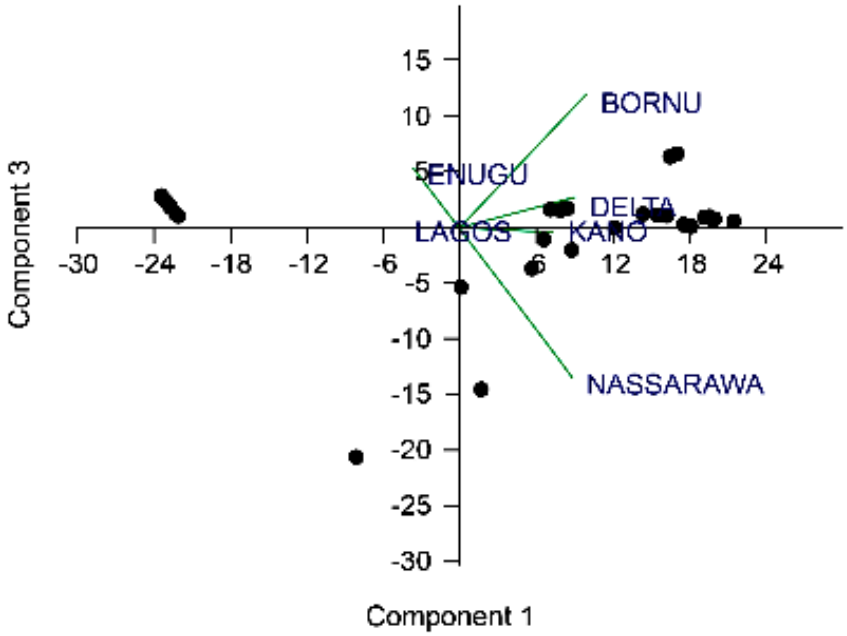

Figure 1: Principal component analysis plot based on the phytochemical components among six (6) landraces of *Jatropha* spp

This has led to an increased interest in Jatropha for its potential in drug discovery and other medicinal applications. Historically, the breeding and domestication of plants for the production of pharmacologically active compounds relied on morphological and genetic markers [12]. However, recent advancements suggest that phytochemicals themselves may serve as biomarkers for distinguishing different varieties of plants.

Earlier studies [13] emphasized that phytochemicals are not neutral to environmental influences and management practices, suggesting they reflect variations due to geographical and climatic factors. As such, understanding the phytochemical diversity within different *Jatropha landraces* is fundamental for identifying region-specific bioactive compounds. Environmental factors play significant role in shaping the phytochemical profile of plants. Findings from this study revealed that phytochemical content of the 6 *Jatropha landraces* demonstrated significant variation based on geographic location, which is in tandem with previous studies [14]. The phytochemicals in Jatropha samples collected from different States in Nigeria exhibited distinct patterns that corresponded to their respective environments. In particular, linolelaidic acid was predominantly found in landraces from northern Nigeria, such as Borno, Nasarawa and Kano, while oleic acid was common in samples from Borno, Kano, Enugu and Delta states. Other compounds, including 9,12-octadecadienoic acid and n-hexadecanoic acid, were found across all six states, suggesting a widespread presence of these bioactive molecules in the Jatropha species studied. These variations may be attributed to the complex interaction between genetic factors and environmental conditions.

Production of secondary metabolites in plants is often an adaptive response to various biotic and abiotic pressures in the environment, which may explain the observed differences in the phytochemical composition of Jatropha samples from different locations [15]. Results from PCA analysis further highlighted the importance of geographical factors in shaping the phytochemical profile of *Jatropha landraces*. The highest loading value on PC1, indicating the greatest contribution to the variation in phytochemical composition, was observed in the sample from Borno (0.521), followed by the sample from Lagos (0.599) on PC2, Nasarawa (0.708) on PC3 and Enugu (0.639) on PC4. These findings emphasize the strong geographical influence on the diversity of bioactive compounds present in *Jatropha landraces*.

The GC-MS analysis revealed several key phytochemicals with known medicinal properties, such as antioxidant, antimicrobial, anti-inflammatory and insecticidal activities. These findings are consistent with previous studies that have documented the therapeutic potential of *Jatropha* species [16,17]. A total of 33 phytochemicals were common to at least two samples across the 6 landraces, while 122 distinct phytochemicals were identified in total.

The common compounds identified include 9,12-octadecadienoic acid (known for its antifungal properties), cis-vaccenic acid (which has antibacterial and hypolipidemic effects) and n-hexadecanoic acid (noted for its anti-inflammatory activity), underlining the medicinal potential of Jatropha and its wide application in pharmacology. The decline in the cultivation of traditional *Jatropha landrace*, as they are often replaced by improved varieties, poses great risk to the genetic diversity of the species [18]. This loss of genetic diversity may impact the availability of specific bioactive compounds, making it imperative to conserve and characterize *Jatropha landraces* for future biotechnological and pharmacological applications.

CONCLUSION

This study demonstrates the impact of environmental factors on the phytochemical composition of *Jatropha* landraces. The presence of bioactive compounds across various regions of Nigeria highlights the potential for developing region-specific medicinal products. Given the ongoing loss of genetic diversity in Jatropha, efforts to preserve these landraces and explore their bioactive properties are crucial for sustaining their medicinal value.

DECLARATIONS

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Ethical approval

None required.

Use of Artificial intelligence/Large language models

We also declare that we did not use Generative artificial intelligence (AI) and AI-assisted technologies in writing the manuscript.

Availability of data and materials

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

Conflict of interest

No conflict of interest is associated with this work.

Contribution of authors

We declare that this work was done by the author(s) named in this article, and all liabilities pertaining to claims relating to the content of this article will be borne by the authors. Ndem E. Edu supervised and designed the experiment. Lilian G. Uzoma carried out the experiment and Dr. Uduak L. Edem prepared the manuscript for publication. Pius A. Obua, Idu J. lsorshe and Henderson O. Egbaji contributed to the work.

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