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Data Article

Dataset on phytochemical screening, FTIR and GC–MS characterisation of *Azadirachta indica* and *Cymbopogon citratus* as reducing and stabilising agents for nanoparticles synthesis

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ABSTRACT

The dataset for this article contains phytochemical and FTIR data for three different extracts from two indigenous medicinal plants obtained from Ogun State, Southwest Nigeria and the GC–MS characterisation data for their ethanolic extracts. To obtain this data, the leaves of *Azadirachta indica* and *Cymbopogon citratus* were collected from the premises of Covenant University, Nigeria. The plants were dried, pulverized and extracted with ethanol, distilled water and ethanol:water (50:50), before phytochemical screening (qualitative and quantitative), FTIR and GC–MS analyses were carried out. The dataset provides insight into the presence of bioactive phyto-constituents such as polyphenols and tannins as potential precursors for green-based nanoparticle synthesis.

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Specifications Table

Subject area	*Chemistry, Biology*
More specific subject area	*Analytical Chemistry, Phytochemistry and Nanotechnology*
Type of data	*Table, figure, image*
How data was acquired	*Fourier Transform Infrared Spectroscopy (FTIR, AGILENT CARY 630)* *Gas Chromatography-Mass Spectroscopy (GC–MS, AGILENT 7890A GC/5977 MS)*
Data format	*Raw, analysed*
Experimental factors	*Phytochemicals (Fresh leaves were air-dried, pulverized, extracted with ethanol, distilled water, ethanol/water (1:1) and concentrated using rotary extractor under reduced pressure. Crude extracts were used for qualitative phytochemical analysis)* *FTIR (Range – 4000-650 cm^{-1}, Resolution – 8 cm^{-1}, Microlab PC software with ATR sampling unit)* *GCMS (Column - 30 mm × 0.25 mm ID × 0.25 μm film, Carrier gas - Helium, flow - 1.0 ml/min, electron ionization - 70 Ev, Software - Masshunter)*
Experimental features	*Phytochemical analysis of carbohydrates, tannins, saponins, flavonoids, alkaloids, anthocyanins, betacyanins, quinones, glycosides, cardiac glycosides, terpenoids, triterpenoids, phenols, coumarins, steroids, acids, FTIR scan of functional groups and GCMS scan of bioactive constituents.*
Data source location	*Ota, Nigeria*
Data accessibility	*Data included in this article*
Related research article	[1] P. Dubey, P. Sharma, V. Kumar, FTIR and GC–MS spectral datasets of wax from *Pinus roxburghii Sarg*. needles biomass, Data Brief. 15 (2017) 615–622. doi:10.1016/j.dib.2017.09.074. [2] K.M. Hammi, M. Hammami, C. Rihouey, D. Le Cerf, R. Ksouri, H. Majdoub, GC-EI-MS identification data of neutral sugars of polysaccharides extracted from *Zizyphus lotus* fruit, Data Brief. 18 (2018) 680–683. doi:10.1016/j.dib.2018.01.085.

Value of the data

- The dataset provides insight into the exact phyto-constituents, which are responsible for stabilization and reduction of metal ions during nanoparticles formation, thereby aiding proposition of mechanistic pathways for these reactions.
- The data provides information on the most potent of the locally selected plants for biosynthesis of nanoparticles using readily available indigenous plants in Southwest Nigeria.
- The methods used can be extended to other indigenous plants, forming a large database capable of informing researchers on the active plant(s) for nanoparticle synthesis.
- The dataset can be used for educational purposes, drug synthesis and multidisciplinary research. Similar data articles can be found in [1,2].

1. Data

The dataset on phytochemical screening of three extracts of *Azadirachta indica* and *Cymbopogon citratus* is presented in Table 1. FTIR spectra and data of different crude extracts of each plant are presented in Figs. 1 and 2 and Table 2, respectively. GC–MS chromatogram/TIC of phyto-constituents

Table 1
Phytochemical screening of ethanol, water and ethanol/water (1:1) extracts of *Azadirachta indica* and *Cymbopogon citratus* leaves.

Biochemicals / Inference																
	CHO	TAN	SAP	FLA	ALK	ANTHO	BETA	QUIN	GLY	CARD-GLY	TER	TRI-TERP	PHE	COU	STE	ACIDS
Ethanol extract																
C. citratus	–	+		+	+	+	+	+	–	+	+	–	+	+	–	–
A. indica	–	+++		+	++	–	–	–	–	–	+	–	+	–	–	–
Ethanol:water (1:1) extract																
C. citratus	–	++		–	–	–	–	+	–	+	++	–	+	+	–	–
A. indica	–	+++		–	+	+	+	–	–	–	+	–	+	+	–	–
Water extract																
C. citratus	–	+		–	–	+	+	–	–	+	+	–	–	+	–	–
A. indica	–	+++		–	–	+	+	–	–	–	+	–	–	+	–	–

+ = trace amount; ++ = moderately present; +++ = highly present; - = absent.
CHO – Carbohydrates, TAN – Tannins, SAP – Saponins, FLA – Flavonoids, ALK – Alkaloids, ANTHO – Anthocyanins, BETA – Betacyanin, QUIN – Quinones, GLY – Glycosides, CARD-GLY – Cardiac.
Glycosides, TER – Terpenoids, TRI-TERP – Triterpenoids, PHE – Phenols, COU – Coumarins, STE – Steroids.

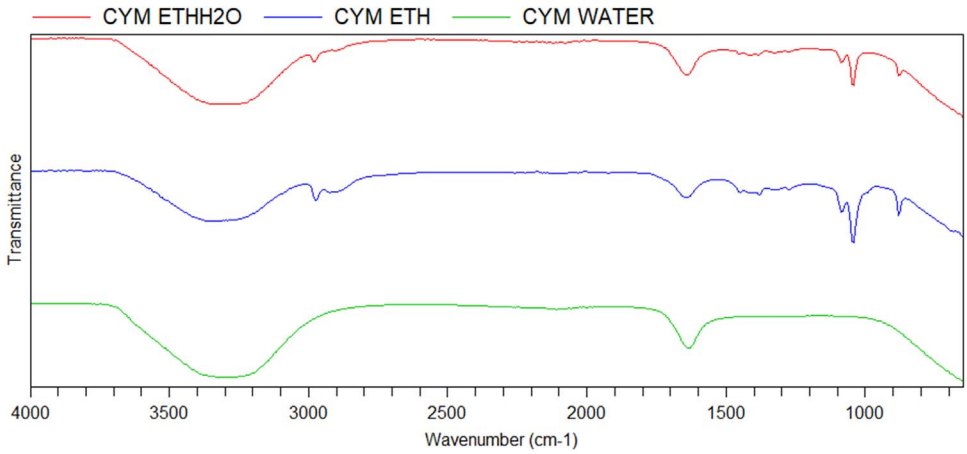

Fig. 1. FTIR spectrum of three extracts of *Cymbopogon citratus* leaves.

of ethanolic extracts of plants and identification data of each constituent is provided in Figs. 3 and 4 and Tables 3 and 4, respectively.

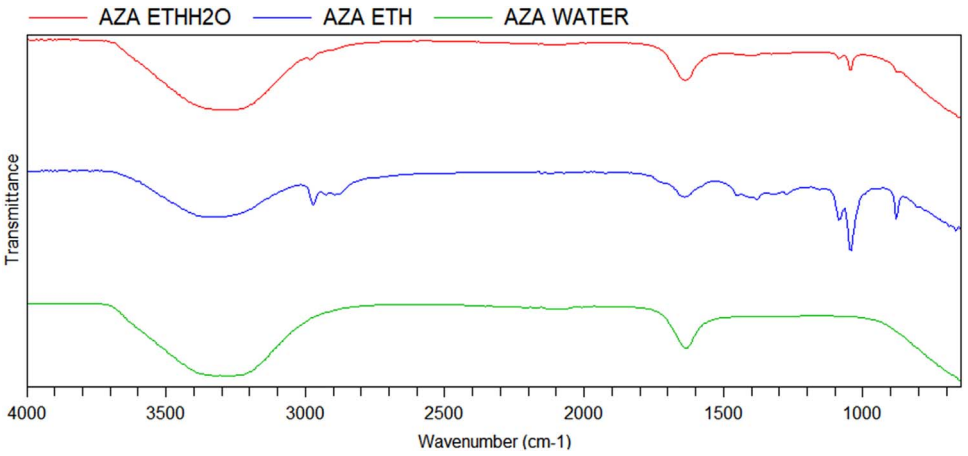

Fig. 2. FTIR spectrum of three extracts of *Azadirachta indica* leaves.

Table 2
FTIR frequency/intensity table for ethanol, water and ethanol/water extracts of *Cymbopogon citratus* and *Azadirachta indica* leaves.

FTIR Absorption frequency (cm^{-1})/intensity											
***C. citratus* extracts**											
Ethanol	881 (m)	1048 (s)	1089 (m)	1275 (w)	1383 (w)	1640 (w)	2929 (w)	2974 (w)	3357(m,b)	–	–
Ethanol/water	881 (m)	1048 (m)	1089 (w)	–	–	1640 (m)	–	2891 (w)	3316 (s,b)	–	–
Water	–	–	–	–	–	1640 (m)	–	–	3316 (s,b)	–	–
***A. indica* extracts**											
Ethanol	881 (m)	1048 (s)	1089 (m)	1383 (w)	1640 (w)	2892 (w)	2929 (w)	2974 (w)	3361(m,b)	–	–
Ethanol/water	881 (w)	1048 (w)	1089 (w)	–	1640 (m)	–	–	–	3264(s,b)	–	–
Water	–	–	–	–	1637 (m)	–	–	–	3331(s,b)	–	–

m – medium, s – strong, w – weak, b – broad.

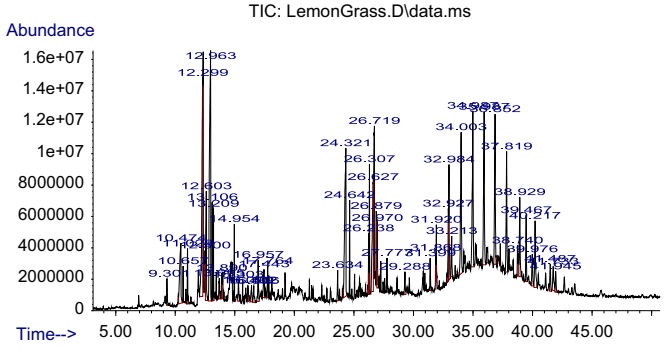

Fig. 3. TIC of *Cymbopogon citratus* ethanolic extract.

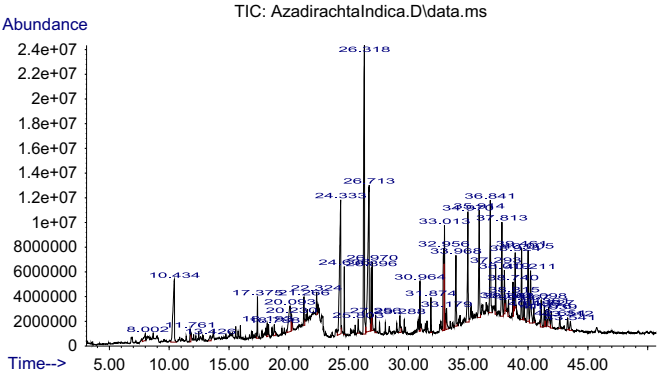

Fig. 4. TIC of *Azadirachta indica* ethanolic extract.

Table 3
Identification of phyto-constituents in ethanolic extract of *C. citratus* leaves using GC–MS.

Ret. time	Area %	IUPAC name of compound	Mol formular	Mol. wt.
6.92	0.2126	Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)-	C_9H_{18}	126.2392
9.14	0.2154	2-Acetylcyclopentanone	$C_7H_{10}O_2$	126.1531
9.30	0.4783	1,6-Octadien-3-ol, 3,7-dimethyl- OR Linalool	$C_{10}H_{18}O$	154.2493
10.47	2.6532	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	$C_6H_8O_4$	144.1253
10.65	0.5139	Cyclooctane, ethenyl-	$C_{10}H_{18}$	138.2499
10.88	0.2167	Furan-2-carbohydrazide, N2-(1-methylhexylideno)-		
11.02	0.7758	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethenyl)-	$C_{10}H_{16}O$	152.2334
11.87	0.2083	Oxiranecarboxaldehyde, 3-methyl-3-(4-methyl-3-pentenyl)-	$C_{10}H_{16}O_2$	168.2328
11.93	0.2702	Benzofuran, 2,3-dihydro-	C_8H_8O	120.1485
12.29	6.6959	2,6-Octadienal, 3,7-dimethyl-, (Z)-	$C_{10}H_{16}O$	152.2334
12.49	0.6401	Geraniol	$C_{10}H_{18}O$	154.2493
12.60	2.545			
12.96	9.4115	Citral	$C_{10}H_{16}O$	152.2334
13.10	1.1612	Epoxy-linalooloxide		
13.20	1.1323			
13.44	0.3872	Cyclopentane, (1-methylethyl)-	C_8H_{16}	112.2126
13.69	0.4762	2-Methoxy-4-vinylphenol	$C_9H_{10}O_2$	150.1745
13.88	0.5025	Bicyclo[2.2.2]octan-1-amine		
13.98	0.3829	3-Cyclopropylcarbonyloxydodecane		
14.49	0.217	Triallylsilane	$C_9H_{16}Si$	152.3088
14.58	0.1855	3-Heptanol, 2-methyl-	$C_8H_{18}O$	130.2279
14.64	0.1943	1,5-Heptadiene, 3,3-dimethyl-, (E)-		
14.95	0.8738	Geranyl acetate	$C_{12}H_{20}O_2$	196.2860
15.17	0.2231	Cyclopropanemethanol,.alpha.,2-dimethyl-2-(4-methyl-3-pentenyl)-, [1.alpha. (R*),2.alpha.]-		
15.30	0.514	Vanillin	$C_8H_8O_3$	152.1473
15.65	0.3534	3,5-Heptadienal, 2-ethylidene-6-methyl-	$C_{10}H_{14}O$	150.2176
16.09	0.4413	Adamantane	$C_{10}H_{16}$	136.2340
16.40	0.4469	3-Cyclopentylpropionic acid, but-3-yn-2-yl ester		
16.59	0.4452	2-Propanol, 1,1,1-trichloro-2-methyl-	$C_4H_7Cl_3O$	177.457
16.95	0.9541	2,6-Octadienal, 3,7-dimethyl-, (Z)-	$C_{10}H_{16}O$	152.2334
17.44	0.7992	3-Cyclohexene-1-acetaldehyde,.alpha.,4-dimethyl-	$C_{10}H_{16}O$	152.2334
17.76	0.6387	3-n-Propyl-2-pyrazolin-5-one	$C_6H_{10}N_2O$	126.1564
17.85	0.3297	4-Methyl-5H-furan-2-one	$C_5H_6O_2$	98.0999
18.11	0.3635	Dodecanoic acid	$C_{12}H_{24}O_2$	200.3178
19.00	0.1681	1-Methyl-3-n-propyl-2-pyrazolin-5-one	$C_7H_{12}N_2O$	140.1830
19.21	0.4101	Selina-6-en-4-ol		

Table 3 (*continued*)

Ret. time	Area %	IUPAC name of compound	Mol formular	Mol. wt.
19.76	0.1779	2-(2-Hydroxyethylthio)propionic acid		
20.89	0.2064	Phenylacetylformic acid, 4-hydroxy-3-methoxy-		
21.25	0.3042	Tetradecanoic acid	$C_{14}H_{28}O_2$	228.3709
21.45	0.2678	Benzene, 1,1'-ethylidenebis-	$C_{14}H_{14}$	182.2610
21.56	0.2124	Pyridine, 4-[(1,1-dimethylethyl)thio]-		
22.30	0.3018	p-Hydroxycinnamic acid, ethyl ester		
23.02	0.3948	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-	$C_{10}H_{10}O_4$	194.1840
23.63	0.5611	p-Fluoroethylbenzene	C_8H_9F	124.1555
24.32	5.9637	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256.4241
24.64	1.1441	Hexadecanoic acid, ethyl ester	$C_{18}H_{36}O_2$	284.4772
25.05	0.3111	Heptadecanoic acid	$C_{17}H_{34}O_2$	270.4507
25.47	0.3151	3-Methyl-2-butenoic acid, 2-tridecyl ester		
26.23	0.7845	Phytol	$C_{20}H_{40}O$	296.5310
26.30	1.6582	Diboroxane, triethyl[(4-methyl-2-pyridyl)amino]-		
26.62	3.8736	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	280.4455
26.71	3.6845	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	$C_{18}H_{30}O_2$	278.4296
26.79	0.1683	Cyclooctene, 3-ethenyl-		
26.87	0.9543	Linoleic acid ethyl ester	$C_{20}H_{36}O_2$	308.4986
26.97	0.988	Ethyl 9,12,15-octadecatrienoate		
27.11	0.2389	p-Menth-2-en-9-ol, trans-		
27.25	0.3594	Octadecanoic acid, ethyl ester	$C_{20}H_{40}O_2$	312.5304
27.44	0.2377	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	$C_{13}H_{22}O$	194.3132
27.57	0.2752	Naphtho[2,1-b:3,4-b']difuran, 2,3,8,9-tetrahydro-2,9-dimethyl-		
27.77	0.4932	Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	$C_{10}H_{18}O$	154.2493
28.62	0.2172	1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)-	$C_{20}H_{34}O$	290.4834
29.28	0.4722	Eicosanoic acid	$C_{20}H_{40}O_2$	312.5304
29.65	0.2219	Methyl 19-methyl-eicosanoate		
30.77	0.3075	9-Tricosene, (Z)-	$C_{23}H_{46}$	322.6113
31.86	0.527			
34.22	0.2424			
30.82	0.2058	Heptadecane	$C_{17}H_{36}$	240.4677
30.95	0.237	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$C_{19}H_{38}O_4$	330.5026
31.39	0.5588	Dichloroacetic acid, heptadecyl ester		
31.91	0.6148	Hexacosane	$C_{26}H_{54}$	366.7070
32.79	0.2052	Cyclohexane, 1,1'-[4-(3-cyclohexylpropyl)-1,7-heptanediyl]bis-	$C_{28}H_{52}$	388.7125
32.92	1.2801	1-Nonadecene	$C_{19}H_{38}$	266.5050
32.98	1.9114	Tetracosane	$C_{24}H_{50}$	338.6538
34.00	3.8594			
36.85	3.8693			
37.81	2.8508			
38.92	2.0079			
33.21	0.8589	Butane, 2,2-bis(5-acetyl-2-thienyl)-		
34.32	0.1678	Squalene	$C_{30}H_{50}$	410.7180
34.98	4.4543	Nonacosane	$C_{29}H_{60}$	408.7867
35.21	0.2288	Nonadecyl heptafluorobutyrate		
35.26	0.2462	Heptacosyl acetate		
35.93	4.1869	Triacontane	$C_{30}H_{62}$	422.8133
36.15	0.2301	Triacontyl acetate	$C_{32}H_{64}O_2$	480.8494
37.29	0.4097	dl-.alpha.-Tocopherol	$C_{29}H_{50}O_2$	430.7061
38.01	0.2942	Benzene, 1-nitro-4-(phenylthio)-	$C_{12}H_9NO_2S$	231.270
38.37	0.3256	Campesterol	$C_{28}H_{48}O$	400.6801
38.74	0.5393	Stigmasterol	$C_{29}H_{48}O$	412.6908
38.81	0.3692	1,2,3,4-4H-Isoquinolin-1,3-dione, 4,4,5,6,8-pentamethyl-		
39.46	1.3421	.gamma.-Sitosterol	$C_{29}H_{50}O$	414.7067
39.97	0.8629	2-Furancarboxamide, N-[3-methyl-1-(phenylmethyl)-1H-pyrazol-5-yl]-		
40.21	1.9876	Tetratriacontane	$C_{34}H_{70}$	478.9196
40.48	0.2395	9,19-Cyclolanost-24-en-3-ol, (3.beta.)-	$C_{30}H_{50}O$	426.7174
41.09	0.4235	4-[5-(3,4-Diethoxy-benzyl)-[1,2,4]oxadiazol-3-yl]-furazan-3-ylamine		

Table 3 (*continued*)

Ret. time	Area %	IUPAC name of compound	Mol formular	Mol. wt.
41.48	0.6734	Cannabidiol	$C_{21}H_{30}O_2$	314.4617
41.73	0.8292	Eicosane	$C_{20}H_{42}$	282.5475
43.54	0.3269			
41.94	0.5473	Cyclopropane-1-carboxamide, 2-butyl-N-(5,6,7,8-tetrahydro-7,7-dimethyl-5-oxoquinazolin-2-yl)-		
42.67	0.382	3-Methoxy-17beta-(O-nitrobenzoyloxy)-estra-1,3,5(10)-triene		
43.30	0.1722	2-(Acetoxymethyl)-3-(methoxycarbonyl)biphenylene		

Table 4
Identification of phyto-constituents in ethanolic extract of *A. indica* leaves using GC–MS.

Ret. time	Area %	IUPAC name of compound	Mol formular	Mol weight
6.85	0.263	Thiazole, 4,5-dihydro-2-methyl-	C_4H_7NS	101.170
8.00	0.4441	2-Hexenoic acid	$C_6H_{10}O_2$	114.1424
8.67	0.1883	2-Fluoro-5-methoxypyrimidine		
10.43	4.0847	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	$C_6H_8O_4$	144.1253
10.88	0.1569	Isopropyl isothiocyanate	C_4H_7NS	101.170
11.42	0.2128	N-Aminopyrrolidine	$C_4H_{10}N_2$	86.1356
11.76	0.4228	Benzofuran, 2,3-dihydro-	C_8H_8O	120.1485
11.83	0.2203	D-Alanine, N-allyloxycarbonyl-, decyl ester		
12.04	0.1826	2(1H)Pyrimidinone,4-amino-1,N-dimethyl-	$C_6H_9N_3O$	139.1552
12.23	0.1549	2,6-Octadienal, 3,7-dimethyl-, (Z)-	$C_{10}H_{16}O$	152.2334
12.47	0.2256	Geraniol OR 2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-	$C_{10}H_{18}O$	154.2493
12.61	0.2274	N-[5-(3,4-Dimethoxy-benzyl)-[1,3,4]thiadiazol-2-yl]-3-fluoro-benzamide		
13.42	0.3247	Malic Acid	$C_4H_6O_5$	134.0874
13.67	0.2593	2-Methoxy-4-vinylphenol	$C_9H_{10}O_2$	150.1745
15.56	0.2434	1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-	$C_{15}H_{24}$	204.3511
15.75	0.1914	trans-Cinnamic acid	$C_9H_8O_2$	148.1586
15.94	0.2789	.gamma.-Elemene OR γ-Elemene	$C_{15}H_{24}$	204.3511
17.37	0.8838	2-Hydroxy-1-(1'-pyrrolidiyl)-1-buten-3-one		
17.96	0.1632	L-Proline, 1-acetyl-	$C_7H_{10}NO_3$	156.1592
18.08	0.1893	Dodecanoic acid	$C_{12}H_{24}O_2$	200.3178
18.19	0.3327	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-	$C_{15}H_{24}$	204.3511
18.30	0.2576	Fumaric acid, cyclobutyl ethyl ester		
18.59	0.2391	Phosphine, methyl(1-methylethyl)phenyl-		
18.78	0.4281	Carbamic acid, methylphenyl-, ethyl ester	$C_{10}H_{13}NO_2$	179.2157
20.09	2.4879	Ethyl.alpha.-d-glucopyranoside		
20.22	0.3267	.beta.-D-Glucopyranoside, methyl	$C_7H_{14}O_6$	194.1825
20.29	0.2465	d-Glycero-l-gluco-heptose		
21.26	0.7649	2(1H)-Pyrimidinone, 5-methyl-		
21.54	0.2506	Sorbitol	$C_6H_{14}O_6$	182.1718
22.32	0.5687	Piperidine, 1-(1-pentenyl)-		
22.53	0.2716	Galactitol	$C_6H_{14}O_6$	182.1718
22.90	0.2182	Cyclohexane, 1,5-diisopropyl-2,3-dimethyl-		
23.91	0.2894	Palmitoleic acid	$C_{16}H_{30}O_2$	254.4082
24.33	7.424	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256.4241
24.40	0.1754	11-Oxa-tricyclo[4.4.1.0(1,6)]undecan-2-ol		
24.63	1.0398	Hexadecanoic acid, ethyl ester	$C_{18}H_{36}O_2$	284.4772
25.54	0.1899	Heptadecanoic acid	$C_{17}H_{34}O_2$	270.4507
25.80	0.4054	3-Heptanol, 3,5-dimethyl-	$C_9H_{20}O$	144.2545
26.31	11.5639	Phytol	$C_{20}H_{40}O$	296.5310
26.71	9.7212	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	$C_{18}H_{30}O_2$	278.4296
26.89	1.5401	Octadecanoic acid	$C_{18}H_{36}O_2$	284.4772

Table 4 (*continued*)

Ret. time	Area %	IUPAC name of compound	Mol formular	Mol weight
26.97	1.4276	Ethyl 9,12,15-octadecatrienoate		
27.25	0.329	Octadecanoic acid, ethyl ester	$C_{20}H_{40}O_2$	312.5304
27.58	0.2923	Naphtho[2,1-b:7,8-b']difuran, 1,2,9,10-tetrahydro-2,9-dimethyl-		
28.06	0.2169	1-Heneicosyl formate	$C_{22}H_{44}O_2$	340.5836
28.40	0.2843	Benzyl.beta.-d-glucoside		
29.02	0.213	Z,Z-8,10-Hexadecadien-1-ol acetate		
29.28	0.6416	Eicosanoic acid	$C_{20}H_{40}O_2$	312.5304
29.65	0.2674	Methyl 19-methyl-eicosanoate		
29.75	0.1501	(1S,15S)-Bicyclo[13.1.0]hexadecan-2-one		
30.78	0.2073	Cyclotetradecane, 1,7,11-trimethyl-4-(1-methylethyl)-	$C_{20}H_{40}$	280.5316
30.82	0.245	Eicosane	$C_{20}H_{42}$	282.5475
30.96	1.0086	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$C_{19}H_{38}O_4$	330.5026
31.07	0.254	Glycerol 1-palmitate	$C_{19}H_{38}O_4$	330.5026
31.41	0.2199	Bis(2-ethylhexyl) phthalate	$C_{24}H_{38}O_4$	390.5561
31.55	0.2299	Docosanoic acid	$C_{22}H_{44}O_2$	340.5836
31.87	0.6983	Nonadecanoic acid, ethyl ester	$C_{21}H_{42}O_2$	326.5570
32.64	0.2932	Cyclopentadecanone, 2-hydroxy-	$C_{15}H_{28}O_2$	240.3816
32.70	0.2054	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-	$C_{20}H_{34}O_2$	306.4828
32.95	3.8689	Ethanol, 2-(octadecyloxy)-	$C_{20}H_{42}O_2$	314.5463
33.01	1.9763	Linolenic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (Z,Z,Z)-	$C_{21}H_{36}O_4$	352.5081
33.09	0.309			
33.17	0.8062	Benzene, 1,2-dimethoxy-4-nitro-	$C_8H_9NO_4$	183.1614
33.48	0.1631	Fumaric acid, pent-4-en-2-yl tridecyl ester		
33.96	2.3197	Octacosane	$C_{28}H_{58}$	394.7601
34.31	0.1787	Squalene	$C_{30}H_{50}$	410.7180
34.96	3.6131	Nonacosane	$C_{29}H_{60}$	408.7867
35.19	0.1721	Octacosyl acetate	$C_{30}H_{60}O_2$	452.7962
35.25	0.2752	1-Nonadecene	$C_{19}H_{38}$	266.5050
35.66	0.1803			
35.91	3.7204	Tetracosane	$C_{24}H_{50}$	338.6538
36.84	4.1428			
36.14	0.2142	Triacontyl acetate	$C_{32}H_{64}O_2$	480.8494
36.21	0.165			
36.62	0.1643			
36.50	0.1834	.gamma.-Tocopherol	$C_{28}H_{48}O_2$	416.6795
37.29	0.9935	Vitamin E	$C_{29}H_{50}O_2$	430.7061
37.81	3.0663	Octadecane	$C_{18}H_{38}$	254.4943
38.92	1.5839			
38.01	1.0458	Pregn-4-ene-3,20-dione, 16-hydroxy-, (16.alpha.)-		
38.09	0.4445	2,6,10,14-Tetramethyl-7-(3-methylpent-4-enylidene) pentadecane		
38.36	0.4534	Campesterol	$C_{28}H_{48}O$	400.6801
38.74	0.8867	Stigmasterol	$C_{29}H_{48}O$	412.6908
38.81	0.3705	4-Cyclohexene-1,2-dicarboximide, N-butyl-, cis-		
39.46	2.0086	.gamma.-Sitosterol	$C_{29}H_{50}O$	414.7067
39.66	0.5223	4,4,6a,6b,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one		
40.00	2.5958	2-Furancarboxamide, N-(8-methyl-2H-[1,2,4]thiadiazolo[2,3-a]pyridin-2-ylidene)-		
40.21	2.2065	Eicosane	$C_{20}H_{42}$	282.5475
41.72	0.9181			
43.54	0.4271			
40.48	0.4548	4,22-Stigmastadiene-3-one	$C_{29}H_{46}O$	410.6749
41.09	0.9555	D:A-Friedoursan-3-one		
41.36	0.7263	Stigmast-4-en-3-one	$C_{29}H_{48}O$	412.6908
41.47	0.5	Cyclopropane-1-carboxamide, 2-butyl-N-(5,6,7,8-tetrahydro-7,7-dimethyl-5-oxoquinazolin-2-yl)-		
41.61	0.1877	Hexahydropyridine, 1-methyl-4-[4,5-dihydroxyphenyl]-		
41.93	0.6689	Cannabidiol	$C_{21}H_{30}O_2$	314.4617
42.65	0.3853	1H-1,2,4-Triazole-5(4H)-thione, 4-allyl-3-(3-furyl)-		

Table 4 (*continued*)

Ret. time	Area %	IUPAC name of compound	Mol formular	Mol weight
43.00	0.1593	1,2-Bis(trimethylsilyl)benzene		
43.31	0.4858	Pyrido[2,3-d]pyrimidine, 4-phenyl-		
45.73	0.2579	2-(Acetoxymethyl)-3-(methoxycarbonyl)biphenylene		

2. Experimental design, materials and methods

2.1. Sample collection

Fresh leaves of two (2) indigenous plants namely *Cymbopogon citratus and Azadirachta indica* were collected in March 2018 from Covenant University, Nigeria. The leaf samples were thoroughly washed in distilled water before air-drying at room temperature for 21 days. Dried leaves were then pulverized and preserved in airtight containers until further use.

2.2. Sample preparation and characterisation

For phytochemical screening, 25 g of pulverized plant leaves was extracted with 125 mL of three solvents namely; ethanol, distilled water and ethanol/water (1:1) for 72 h. The plant extracts were filtered and concentrated using rotary evaporator under reduced pressure. Preliminary phytochemical analysis was carried out to test for the presence of tannins, saponins, flavonoids, alkaloids, anthocyanins, betacyanins, quinones, glycosides, cardiac glycosides, terpenoids, triterpenoids, phenols, coumarins, steroids and acids in all the three extracts following the standard test methods [3,4].

Also, 10 g of each powdered plant material was extracted with ethanol, distilled water and ethanol/distilled water (1:1), respectively, for 72 h. The extracts were filtered and concentrated to 1 mL using BUCHI rotary evaporator under reduced pressure. Then, 1 mL of crude ethanolic, water and ethanol/water extracts were taken for FTIR analysis, while 1 mL ethanolic extracts were taken in amber GC vials for GC–MS analysis.

2.3. Fourier transform infrared spectroscopy analysis

The extracts were analysed using Agilent Cary 630 FTIR spectrometer equipped with Microlab PC software with ATR sampling unit with a resolution of 8 cm^{-1} and scan range of 4000 cm^{-1} to 650 cm^{-1}.

2.4. Gas chromatography mass spectroscopy analysis

The GC–MS analysis was carried out using Agilent 7890 A gas chromatograph coupled with a 5977 A mass spectrometer. The temperature programme of the GC was maintained at an initial temperature of 50 °C with a hold for 1 min, followed by gradual increase to 300 °C at 7 °C/min for 14 min. 1 μL of each sample was injected in the split mode (split ratio 1:10). The identification of components was based on retention time on the capillary column and matching the GC mass spectra with the National Institute of Standards and Technology (NIST) library.

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Transparency document. Supporting information

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