Data Article

Dataset on analytical characterization of bioactive components from *Azadirachta indica*, *Canna indica*, *Magnifera indica* and *Moringa oleifera* leaf extracts and their applications in nanoparticles biosynthesis

Oladotun P. Bolade, Akan B. Williams, Nsikak U. Benson*

Department of Chemistry, Covenant University, Km 10 Idiroko Road, Ota, Nigeria

**ABSTRACT**

This paper presents data on the bioactive phytoconstituents in *Azadirachta indica*, *Canna indica*, *Magnifera indica*, and *Moringa oleifera* analyzed using quantitative and qualitative phytochemical screening methods, Fourier Transform Infrared Spectroscopy and Gas Chromatography-Mass Spectrometry (GC-MS). Extracts were prepared in water, ethanol (EtOH) and EtOH:water mix. Identification of bioactive components was based on their spectral data and retention times compared with National Institute of Standards and Technology (NIST) mass spectral library. The most prominent absorption bands indicated are O-H stretching vibration, C-H stretch of polyols, aromatic C=C stretching vibration, O-H stretch of polyols, C-H stretching vibration and C-OH polyols. The GC-MS characterization for *A. indica* showed the presence of phenols, organic acids and carbohydrates with cannabidiol as the most abundant. Crude extracts of *M. oleifera* showed six phenolic compounds with 4-hydroxy-benzoic acid and cannabidiol present prominently. Six phenolic phytoconstituents were identified in *M. indica* extracts with 1,2,3-benzenetriol as the major polyphenolic compound. Biogenic
Iron oxide nanoparticles were synthesized and the formation was confirmed using a UV spectrometer (UV-3000 ORI, Germany) between 200 and 800 nm spectral range. X-ray diffraction (XRD) characterization of the biosynthesized iron oxide nanoparticles was carried out using Empyrean, Malvern PanAnalytical.

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### Specifications Table

| Subject                                      | Chemistry                  |
|----------------------------------------------|----------------------------|
| Specific subject area                        | Analytical Chemistry, Nanotechnology |
| Type of data                                 | Table, figure, spectra      |
| How data was acquired                        | FTIR Agilent Cary 630, Range = 4000 – 650 cm⁻¹. Resolution – 8 cm⁻¹, Microlab PC software with ATR sampling unit. GC-MS Agilent 7890A GC/5977 MS, Column - 30 × 0.25 mm ID × 0.25 μm film, Carrier gas - Helium, flow - 1.0 mL/min, electron ionization - 70 eV, Software - Masshunter) UV spectrometer (UV-3000 ORI, Germany) between 200 and 800 nm spectral range. X-ray Diffractometer (Empyrean, Malvern PanAnalytical). |
| Data format                                  | Raw spectra data, analyzed  |
| Parameters for data collection               | Azadirachta indica, Canna indica, Magnifera indica and Moringa oleifera leaves were air-dried and ground to a fine powder using a clean auto-operated grinder; ground leaves were separately extracted using ethanol (EtOH), distilled water, and a mixture of EtOH/water in the ratio 1:1. |
| Description of data collection              | Raw extracts of A. indica, C. indica, M. indica and M. oleifera were subsequently filtered and concentrated to 1.0 mL using a BUCHI rotary evaporator under controlled pressure. 1.0 mL of crude extracts obtained separately from water, ethanol, water/ethanol (50:50%) were taken for analysis using FTIR and gas chromatography. Qualitative phytochemical analysis to determine bioactive components as reducing and stabilizing agents for the synthesized green-based nanoparticles was also carried out. |
| Data source location                         | Institution: Covenant University |
|                                              | City: Ota                   |
|                                              | Country: Nigeria            |
| Data accessibility                           | All data is included in this article. |
| Related research article                     | O. P. Bolade, A. A. Akinsiku, O. S. Oluwafemi, A. B. Williams, N. U. Benson, Biogenic iron oxide nanoparticles and activated sodium persulphate for hydrocarbon remediation in contaminated soil, Environmental Technology & Innovation, 9(4), 105801, (2021), https://doi.org/10.1016/j.jece.2021.105801. |

### Value of the Data

- The dataset provides insight into the specific phytochemicals in A. indica, C. indica, M. indica and M. oleifera that could serve as stabilizing agents for the synthesis of green-based nanoparticles.
• The dataset provides valuable information on phytochemicals responsible for the reduction of metal ions as well as stabilizing agents for the newly formed nanoparticles.
• The data is invaluable to the scientific community because it provides novel information about bioactive components of *A. indica*, *C. indica*, *M. indica* and *M. oleifera* collected from a tropical region.
• The spectral datasets and phytochemical profile data of constituents from locally sourced *A. indica*, *C. indica*, *M. indica* and *M. oleifera* could be used in comparative studies of same plant species in other regions.
• The method and data provide very valuable information on possible phyto-constituents that could serve as precursors for drug synthesis and biosynthetic production of nanoparticles.

1. Data Description

The dataset of this article provides a comprehensive phytomapping of ethanolic extracts obtained from the leaves of *A. indica*, *C. indica*, *M. indica* and *M. oleifera* by gas chromatography (Tables 1–4). The data also show the Fourier Transform Infrared Spectroscopy (FTIR) spectra and characterization data of water only, ethanol (EtOH) only, and EtOH-water (1:1) mixture extracts of *A. indica*, *C. indica*, *M. indica* and *M. oleifera* in Fig. 1a–d and Table 5, respectively. The FTIR spectra provide information on the functional groups present in the samples. The associated data for the phytochemical screening of extracts is presented in Table 6, while the GC-MS total ion chromatogram (TIC) of phyto-constituents of ethanolic extracts of each plant is provided in Figs. 2–5.

![FTIR spectra](image-url)

*Fig. 1.* FTIR spectra of *A. indica* [A], *C. indica* [B], *M. indica* [C] and *M. oleifera* [D] leaves extracts in three solvent media.
Table 1
GC-MS derived phytoconstituents in ethanolic extract of *M. indica* leaves.

| Retention time | Area %  | IUPAC name of compound                                                                 | Molecular formula | Molecular weight |
|----------------|---------|---------------------------------------------------------------------------------------|-------------------|------------------|
| 08.84          | 0.1353  | 4,5-Diamo-no-2-hydroxy pyrimidine                                                      | C_{6}H_{12}O_{4}  | 144.1253         |
| 10.23          | 0.3373  | 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-                                    | C_{6}H_{10}O_{4}  | 146.1412         |
| 10.69          | 0.1053  | Ethyl hydrogen succinate                                                              | C_{6}H_{10}O_{4}  | 150.1745         |
| 12.22          | 0.0999  | 5-Diethoxymethyl-3-ethoxy-4,5-dihydro-isoxazole                                       | C_{6}H_{10}O_{2}  | 103.186          |
| 13.66          | 0.1684  | 4-Hydroxy-2-methylacetophenone                                                         | C_{6}H_{10}O_{2}  | 126.1100         |
| 14.19          | 0.0979  | Thiomorpholine                                                                       | C_{6}H_{12}NS     |                  |
| 14.97          | 0.1524  | 1,2,3-Benzeneritrol                                                                  | C_{6}H_{12}O_{3}  |                  |
| 15.56          | 0.632   | 1H-Cyclopentylezulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,14,7-tetramethyl-              | C_{15}H_{24}      | 204.3511         |
| 15.75          | 0.2804  | Caryophyllene                                                                         | C_{15}H_{24}      | 204.3511         |
| 16.37          | 0.2207  | Humulene                                                                              | C_{15}H_{24}      | 204.3511         |
| 16.49          | 0.0873  | Alloaromadendrene                                                                     | C_{15}H_{24}      | 204.3511         |
| 16.69          | 0.0907  | Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethyl)-                  | C_{15}H_{24}      | 204.3511         |
| 16.95          | 0.6406  | Naphthalene                                                                            | C_{15}H_{24}      | 204.3511         |
| 17.09          | 0.3032  | decalhydro-4-a-methyl-1-methylene-7-(1-methylethenyl)-                                | C_{15}H_{24}      | 204.3511         |
| 17.25          | 0.108   | Benzoic acid, 4-hydroxy-                                                              | C_{15}H_{24}      | 138.1207         |
| 17.32          | 0.2091  |                                                                                      |                   |                  |
| 17.43          | 0.0878  |                                                                                      |                   |                  |
| 18.64          | 0.2695  | Caryophyllene oxide                                                                   | C_{15}H_{24}O     | 220.3505         |
| 18.97          | 0.1386  | Sorbitol                                                                              | C_{6}H_{12}O_{6}  | 182.1718         |
| 19.07          | 0.2918  | Naphthalene, decalhydro-                                                              | C_{15}H_{18}      | 138.2499         |
| 19.35          | 0.1451  | L-Arabinitol                                                                           | C_{5}H_{12}O_{5}  | 152.1458         |
| 20.28          | 0.2396  |                                                                                      |                   |                  |
| 19.40          | 0.0933  | Ribitol                                                                                | C_{5}H_{12}O_{5}  | 152.1458         |
| 19.78          | 0.2046  | 1-[4-Hydroxy-1-methylproline                                                         | C_{5}H_{12}O_{5}  | 270.4507         |
| 21.21          | 0.1211  | Tetradecanoic acid                                                                    | C_{14}H_{28}O_{2} | 228.3709         |
| 22.44          | 0.1883  | 6-Octen-1,1-ol, 3,7-dimethyl- formate                                                 | C_{14}H_{22}O_{2} | 184.2753         |
| 24.21          | 4.7148  | n-Hexadecanoic acid                                                                   | C_{16}H_{32}O_{2} | 256.4241         |
| 24.62          | 0.3464  | Hexadecanoic acid, ethyl ester                                                        | C_{16}H_{30}      | 284.7772         |
| 24.94          | 2.9483  | 4-Cardboxycyclohexanone                                                                |                   |                  |
| 25.04          | 0.2215  | α-D-Glucopyranose, 4-O-β-D-galactopyranosyl-                                          | C_{14}H_{22}O_{11} | 342.2965         |
| 25.49          | 0.139   | Heptadecanoic acid                                                                    | C_{17}H_{24}O_{2} | 270.4507         |
| 26.23          | 1.6559  | Phytol                                                                                | C_{17}H_{30}O      | 296.5310         |
| 26.48          | 0.799   | 9,12-Octadecadienoic acid (Z)-                                                       | C_{18}H_{32}O_{2} | 280.4455         |
| 26.57          | 3.6134  | 9,12,15-Octadecatrienic acid, (Z,Z,Z)-                                              | C_{18}H_{34}O_{2} | 278.4296         |
| 26.81          | 0.5386  | Octadecanoic acid                                                                     | C_{18}H_{32}O_{2} | 284.7772         |
| 26.94          | 0.2266  | Ethyl 9,12,15-octadecatrienoate                                                        | C_{18}H_{32}O_{2} | 284.7772         |
| 27.55          | 0.119   | Norharmane, N-trimethylsilyl-                                                          |                   |                  |
| 28.01          | 0.2059  | Benzyl-β-d-glucoside                                                                   |                   |                  |
| 28.34          | 0.1053  | 2-Tridecanone                                                                          | C_{18}H_{32}O      | 198.3449         |
| 29.00          | 0.1016  | 5-Octen-2-one, 3,6-dimethyl-                                                          |                   |                  |
| 29.22          | 0.1253  | 7-Methyl-Z-tetradecen-1-ol acetate                                                    |                   |                  |
| 30.67          | 0.1071  | Bacchotticineatin c                                                                    |                   |                  |
| 30.76          | 0.0977  | Cycloctadecane, 1,7,11-trimethyl-4-(1-methylethyl)-                                    | C_{20}H_{40}       | 280.5316         |
| 30.94          | 0.9165  | Glycerol 1-palmitate                                                                  | C_{20}H_{38}O_{4}  | 330.5026         |
| 31.07          | 0.1529  | Fumaric acid, decyl 2-fluorophenyl ester                                              | C_{20}H_{38}O_{2}  | 312.5304         |
| 31.86          | 0.1269  | Octadecanoic acid, 17-methyl-, methyl ester                                           | C_{20}H_{38}O_{2}  | 296.4879         |
| 32.64          | 0.2174  | 13-Octadecenoic acid, methyl ester                                                    | C_{20}H_{38}O_{2}  | 238.4088         |
| 32.92          | 2.5892  | cis-9-Hexadecenal                                                                     | C_{20}H_{38}O      | 352.5081         |
| 32.98          | 2.3466  | Linolenic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (Z,Z,Z)-                       | C_{20}H_{38}O_{4}  |                  |
| 33.09          | 0.4883  | 9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-                                  | C_{20}H_{38}O_{2}  | 306.4828         |
| 33.16          | 0.6126  | N-[4-(Acridin-9-ylamino)-phenyl]-acetamide                                            |                   |                  |

(continued on next page)
Table 1 (continued)

| Retention time | Area %  | IUPAC name of compound                                      | Molecular formula | Molecular weight |
|----------------|---------|-------------------------------------------------------------|-------------------|------------------|
| 33.47          | 0.2293  | Benz[e]azulene-3,8-dione, 5-[(acetyloxy)methyl]-3a,4,6a,7,9,10,10a,10b-octahydro-3a,10a-dihydroxy-2,10-dimethyl-,(3a-α,6a-α,10-β,10a-β,10b-β)-<+>-E-6-Tetradecen-1-ol acetate | C_{28}H_{58}       | 394.7601         |
| 33.66          | 0.095   | Octacosane                                                  | C_{38}H_{80}O_{2} | 240.3816         |
| 34.21          | 0.0878  | Cyclopentadecanone, 2-hydroxy-                             | C_{20}H_{42}O_{2} | 410.7180         |
| 34.31          | 0.5064  | Squalene                                                    | C_{29}H_{48}O_{2} | 254.4028         |
| 34.63          | 0.106   | 1-Bromo-11-iodoundecane                                    | C_{29}H_{50}O_{2} | 266.5050         |
| 34.95          | 3.9573  | Heptadecane                                                 | C_{28}H_{50}O_{2} | 210.3987         |
| 35.19          | 0.1548  | Nonadecyl trifluoroacetate                                  | C_{28}H_{52}O_{2} | 282.5475         |
| 35.25          | 0.2779  | 13-Tetradecen-1-ol acetate                                  | C_{29}H_{50}O_{2} | 210.3987         |
| 35.33          | 0.094   | 1-Nonadecene                                                | C_{29}H_{50}O_{2} | 282.5475         |
| 37.06          | 0.1873  | 13-Nonadecane                                               | C_{29}H_{50}O_{2} | 282.5475         |
| 37.50          | 0.2588  | γ-Tocopherol                                                | C_{29}H_{50}O_{2} | 282.5475         |
| 38.06          | 0.2096  | Triacontyl acetate                                          | C_{32}H_{64}O_{2} | 480.8494         |
| 38.28          | 1.883   | Vitamin E                                                   | C_{29}H_{52}O_{2} | 338.6538         |
| 38.32          | 2.020   | 1-Tricosene                                                | C_{29}H_{52}O_{2} | 338.6538         |
| 38.50          | 0.2588  | γ-Tocopherol                                                | C_{29}H_{52}O_{2} | 338.6538         |
| 38.62          | 0.1592  | Tetracosyl acetate                                          | C_{32}H_{64}O_{2} | 480.8494         |
| 38.68          | 6.3061  | 1-Nonylcycloheptane                                        | C_{29}H_{50}O_{2} | 282.5475         |
| 39.23          | 1.2872  | Stigmastadiene-3-one                                       | C_{29}H_{50}O_{2} | 282.5475         |
| 39.45          | 3.9062  | β-Sitosterol                                                | C_{29}H_{50}O_{2} | 282.5475         |
| 39.66          | 0.9882  | Stigmast-24[28]-en-3-one, (5.alpha)-                        | C_{29}H_{50}O_{2} | 282.5475         |
| 40.03          | 8.8682  | 5-Bromophthaldehydeic acid                                  | C_{29}H_{50}O_{2} | 282.5475         |
| 40.48          | 0.8571  | 4,22-Stigmastadiene-3-one                                   | C_{29}H_{50}O_{2} | 282.5475         |
| 40.83          | 0.0953  | 1,2-Bis(trimethylsilyl)benzene                              | C_{29}H_{50}O_{2} | 282.5475         |
| 40.98          | 0.0838  | 2-〈(Acetoxymethyl)〈-(methoxycarbonyl)biphenylene           | C_{29}H_{50}O_{2} | 282.5475         |
| 41.09          | 1.6569  | D:A-Friedoursan-3-one                                      | C_{29}H_{50}O_{2} | 282.5475         |
| 41.36          | 1.3446  | Stigmast-4-en-3-one                                         | C_{29}H_{50}O_{2} | 282.5475         |
| 41.47          | 0.9061  | Cannabidiol                                                 | C_{29}H_{50}O_{2} | 282.5475         |
| 41.61          | 0.3742  | 1,2-Bis(trimethylsilyl)benzene                              | C_{29}H_{50}O_{2} | 282.5475         |
| 41.93          | 1.353   | 4-Acetamido-6-methoxy-8-aminoquinoline                      | C_{29}H_{50}O_{2} | 282.5475         |
| 42.65          | 0.7311  | Indano[1,2,3-kl]naphtho[7,8,8a,1,2,3-tuvwx]hexaphene        | C_{29}H_{50}O_{2} | 282.5475         |
| 43.00          | 0.2624  | 2,4-Cyclohexadien-1-one, 3,5-bis[1,1-dimethyl]4-hydroxy-     | C_{29}H_{50}O_{2} | 282.5475         |
| 43.32          | 2.6803  | Cyclopentenol[4,3-b]tetrahydrofuran, 3-[(4-methyl-5-oxo-3-phenylthio)tetrahydrofuran-2-yloxymethylene]- | C_{30}H_{50}O_{2} | 370.3449         |
| 43.54          | 0.7559  | Tetratriacontane, 17-hexacycl-                              | C_{30}H_{50}O_{2} | 370.3449         |
| 45.76          | 0.5625  | Cyclotrisiloxane, hexamethy-                                | C_{6}H_{14}O_{3}Si_{3} | 222.4618         |
| 50.24          | 0.7175  | Cyclotrisiloxane, hexamethyl-                              | C_{6}H_{14}O_{3}Si_{3} | 222.4618         |
| Retention time | Area %  | IUPAC name of compound | Molecular formula | Mol weight |
|----------------|--------|------------------------|-------------------|------------|
| 6.8576         | 0.263  | Thiazole, 4,5-dihydro-2-methyl- | C₄HₛNS           | 101.170    |
| 8.002          | 0.4441 | 2-Hexenoic acid         | C₆H₁₀O₂           | 114.1424   |
| 8.6715         | 0.1883 | 2-Fluoro-5-methoxypyrimidine |                     |            |
| 10.4339        | 0.8047 | 4H-Pyrany-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- | C₆H₈O₄           | 144.1253   |
| 10.8802        | 0.1569 | Isopropyl isothiocyanate | C₅H₈NS           | 101.170    |
| 11.4238        | 0.2128 | N-Aminopyrrolidine       | C₁₇H₂₀N₂         | 286.358    |
| 11.7614        | 0.4228 | Benzoquin, 2,3-dihydro-   | C₁₆H₂₆O₂         | 250.319    |
| 11.8357        | 0.2203 | D-Alanine, N-allyloxyiminobenzyl, decyl ester | C₆H₈N₃O         | 139.1552   |
| 12.0417        | 0.1826 | (2H)Pyrimidinone,4-amino-1N-dimethyl- | C₁₀H₁₂O₃         | 152.2334   |
| 12.2306        | 0.1549 | 2,6-Octadienal, 3,7-dimethyl- (Z)- | C₁₀H₁₂O₃         | 154.2493   |
| 12.4709        | 0.2256 | Geraniol                 | C₁₀H₁₆O₂         | 154.2493   |
| 12.6139        | 0.2274 | N-[5-(3,4-Dimethoxy-benzyl)]-[1,3,4]thiadiazol-2-yl]-3-fluorobenzamide |           |            |
| 13.4265        | 0.3247 | Malic Acid               | C₆H₈O₃           | 134.0874   |
| 13.6782        | 0.2593 | 2-Methoxy-4-vinylphenol  | C₁₀H₁₀O₂         | 150.1745   |
| 15.5608        | 0.2434 | 1H-Cyclopropylazulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl- | C₁₅H₂₈        | 204.3511   |
| 15.7553        | 0.1914 | trans-Cinnamic acid      | C₁₀H₁₂O₂         | 148.1586   |
| 15.9498        | 0.2789 | gamma,Elemene OR gamma,Elemene | C₁₅H₂₈        | 204.3511   |
| 17.3746        | 0.8838 | 2-Hydroxy-1-(1'-pyrrolyl)-1-buten-3-one | C₁₅H₆O₃        | 156.1592   |
| 17.964         | 0.1632 | L-Proline, 1-acyetyl-    | C₁₂H₁₆O₃         | 202.3178   |
| 18.0841        | 0.1893 | Dodecanoic acid          | C₁₂H₂₆O₂         | 202.3178   |
| 18.1929        | 0.3327 | Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethenylidene)- | C₁₅H₃₄        | 204.3511   |
| 18.3073        | 0.2576 | Fumaric acid, cyclobutyl ethyl ester |                       |            |
| 18.5934        | 0.2391 | Phosphine, methyl[1-methylbenzyl]phenyl- |                     |            |
| 18.7879        | 0.4281 | Carbamic acid, methylphenyl-, ethyl ester | C₁₀H₁₂O₂         | 179.2157   |
| 20.0925        | 2.4879 | Ethyl alpha-d-glucopyranoside |                       |            |
| 20.2299        | 0.3267 | beta-D-Glucopyranoside, methyl | C₁₆H₁₄O₆         | 194.825    |
| 20.2928        | 0.2465 | d-Glycero-1-gluco-heptose | C₁₈H₁₄O₆         | 205.3511   |
| 21.2656        | 0.7649 | 2(1H)-Pyrimidinone, 5-methyl- | C₁₂H₁₄O₆         | 182.1718   |
| 21.5402        | 0.2506 | Sorbitol                 | C₁₅H₃₄           | 182.1718   |
| 22.3241        | 0.5687 | Piperidine, 1-(1-penteny)- | C₁₂H₂₆O₃         | 182.1718   |
| 22.5358        | 0.2716 | Galactitol               | C₁₅H₃₄           | 182.1718   |
| 22.902         | 0.2182 | Cyclohexane, 1,5-diisopropyl-2,3-dimethyl- |                     |            |
| 23.9148        | 0.2894 | Palmitoleic acid         | C₁₆H₃₀O₂         | 254.4082   |
| 24.3325        | 7.424  | n-Hexadecanoic acid      | C₁₆H₃₀O₂         | 256.4241   |
| 24.4012        | 0.1754 | 11-Oxa-tricyclo[4.4.10]6]decane-2-ol |                     |            |
| 24.6358        | 1.0398 | Hexadecanoic acid, ethyl ester | C₁₆H₃₀O₂         | 284.4772   |
| 25.5456        | 0.1899 | Heptadecanoic acid       | C₁₇H₃₂O₂         | 270.4507   |
| 25.8031        | 0.4054 | 3-Heptanol, 3,5-dimethyl- | C₁₅H₃₀O₂         | 284.4772   |
| 26.318         | 11.5639 | Phytol                   | C₁₆H₃₀O₂         | 278.4296   |
| 26.7129        | 9.7212 | 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- | C₁₈H₃₀O₂         | 278.4296   |
| 26.896         | 1.5401 | Octadecanoic acid        | C₁₈H₃₂O₂         | 284.4772   |
| 26.9704        | 1.4276 | Ethyl 9,12,15-octadecatrienoate |                     |            |
| 27.2565        | 0.329  | Octadecanoic acid, ethyl ester | C₁₈H₃₂O₂         | 312.5304   |
| 27.5826        | 0.2923 | Naphtho[2,1-b:7,8-b']difuran, 1,2,9,10-tetrahydro-2,9-dimethyl- | C₂₃H₂₄O₂         | 340.5836   |
| 28.069         | 0.2169 | 1-Hetricosyl formate     | C₂₂H₂₄O₂         | 340.5836   |
| 28.4009        | 0.2843 | Benzyl beta-d-glucoside  | C₂₀H₂₂O₂         | 312.5304   |
| 29.0245        | 0.213  | ZZ-8,10-Hexadecadien-1-ol acetate |                     |            |
| 29.2878        | 0.6416 | Eicosanoic acid          | C₂₀H₄₀O₂         | 328.5475   |
| 29.654         | 0.2674 | Methyl 19-methyl-eicosanoate |                     |            |
| 29.757         | 0.1501 | (1S,15S)-Bicyclo[13.1.0]hexadecan-2-one |                     |            |
| 30.7812        | 0.2073 | Cycloketadecane, 1,7,11-trimethyl-4-(1-methylethyl)- | C₂₀H₄₀O₂         | 280.5316   |
| 30.8212        | 0.245  | Eicosane                 | C₂₀H₄₂           | 282.5475   |
| 30.9643        | 1.0086 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C₂₀H₃₈O₄         | 330.5026   |

(continued on next page)
| Retention time | Area % | IUPAC name of compound | Molecular formula | Mol weight |
|----------------|--------|------------------------|-------------------|------------|
| 31.0787        | 0.254  | Glycerol 1-palmitate   | C₁₉H₃₂O₄         | 330.5026   |
| 31.4163        | 0.2199 | Bis(2-ethylhexyl) phthalate | C₁₉H₃₂O₄         | 390.5561   |
| 31.5537        | 0.2299 | Docosanoic acid        | C₁₂₂H₂₄O₂        | 340.5836   |
| 31.8741        | 0.6983 | Nonadecanoic acid, ethyl ester | C₁₉₂H₃₂O₂        | 326.5570   |
| 32.6408        | 0.2932 | Cyclopentadecanone, 2-hydroxy- | C₁₀₂H₁₆O₂        | 240.3816   |
| 32.7095        | 0.2054 | 9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)- | C₁₀₂H₁₆O₂        | 306.4828   |
| 32.9555        | 3.8689 | Ethanol, 2-(octadecyloxy)- | C₁₉₂H₃₂O₂        | 314.5463   |
| 33.0128        | 1.9763 | Linolenic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (Z,Z,Z)- | C₁₀₂H₁₆O₂        | 352.5081   |
| 33.0986        | 0.309  | Nonadecanoic acid, ethyl ester | C₁₀₂H₂₀O₂        | 352.5081   |
| 33.1787        | 0.8062 | Benzene, 1,2-dimethoxy-4-nitro- | C₈H₈NO₄         | 183.1614   |
| 33.4877        | 0.1631 | Fumaric acid, pent-4-en-2-yl tridecyl ester | C₁₉H₃₂O₄         | 430.4780   |
| 33.9683        | 2.3197 | Octacosane             | C₁₀₀H₁₆O₂        | 394.7601   |
| 34.3174        | 0.1787 | Squalene               | C₁₀₂H₂₀O₂        | 410.7180   |
| 34.9697        | 3.6131 | Nonacosane             | C₁₀₀H₂₀O₂        | 408.7867   |
| 35.1986        | 0.1721 | Octacosyl acetate      | C₁₀₂H₂₀O₂        | 452.7962   |
| 35.2558        | 0.2752 | 1-Nonadecene           | C₁₀₀H₂₀O₂        | 266.5050   |
| 35.6678        | 0.1803 | Tetracosane            | C₁₂₂H₂₄O₂        | 338.6538   |
| 35.9138        | 3.7204 | Tetracosane            | C₁₂₂H₂₄O₂        | 338.6538   |
| 36.9408        | 4.1428 | Triacetylacetate       | C₁₂₂H₂₄O₂        | 480.8494   |
| 36.2171        | 0.165  | Triacetylacetate       | C₁₂₂H₂₄O₂        | 480.8494   |
| 36.6292        | 0.1643 | Triacetylacetate       | C₁₂₂H₂₄O₂        | 480.8494   |
| 36.5032        | 0.1834 | 1,2-Bis(trimethylsilyl)benzene | C₁₂₂H₂₄O₂        | 461.6795   |
| 37.2928        | 0.9935 | Vitamin E              | C₁₀₂H₂₀O₂        | 430.7061   |
| 37.8135        | 3.0663 | Octadecane             | C₁₀₀H₂₀O₂        | 254.4943   |
| 38.9235        | 1.5839 | Octadecane             | C₁₀₀H₂₀O₂        | 254.4943   |
| 38.0195        | 1.0458 | Pregn-4-ene-3,20-dione, 16-hydroxy-, (16,alphah)- | C₁₀₀H₂₀O₂        | 254.4943   |
| 38.0996        | 0.4445 | 1,2-Bis(trimethylsilyl)benzene | C₁₂₂H₂₄O₂        | 369.6795   |
| 38.3628        | 0.4534 | Campesterol            | C₁₀₀H₂₀O₂        | 400.6801   |
| 38.7405        | 0.8867 | Stigmasterol           | C₁₀₀H₂₀O₂        | 412.6908   |
| 38.8148        | 0.3705 | 4-Cyclohexene-1,2-dicarboximide, N-butyl-, cis-| C₁₀₀H₂₀O₂        | 414.7067   |
| 39.4614        | 2.0086 | 4-Cyclohexene-1,2-dicarboximide, N-butyl-, cis- | C₁₀₀H₂₀O₂        | 414.7067   |
| 39.6674        | 0.5223 | 4-Cyclohexene-1,2-dicarboximide, N-butyl-, cis- | C₁₀₀H₂₀O₂        | 414.7067   |
| 40.005         | 2.5958 | 2-Furancarboxamide, N-(8-methyl-2H-[1,2,4]thiadiazolo[2,3-a]pyridin-2-ylidene)- | C₁₀₀H₂₀O₂        | 282.5475   |
| 40.211         | 2.2065 | 2,6,10,14-Tetramethyl-7-(3-methylpent-4-ylidene)-penta decane | C₁₀₀H₂₀O₂        | 282.5475   |
| 41.7273        | 0.9181 | 2,6,10,14-Tetramethyl-7-(3-methylpent-4-ylidene)-penta decane | C₁₀₀H₂₀O₂        | 282.5475   |
| 43.5412        | 0.4271 | 2,6,10,14-Tetramethyl-7-(3-methylpent-4-ylidene)-penta decane | C₁₀₀H₂₀O₂        | 282.5475   |
| 40.4857        | 0.4548 | 4,22-Stigmastadiene-3-one | C₁₀₀H₂₀O₂        | 410.6749   |
| 41.0979        | 0.9555 | D:4-Friedoursan-3-one  | C₁₀₀H₂₀O₂        | 412.6908   |
| 41.3611        | 0.7263 | Stigmaster-4-en-3-one  | C₁₀₀H₂₀O₂        | 412.6908   |
| 41.4756        | 0.5    | Cyclopropane-1-carboxamide, 2-butyl-N-(5,6,7,8-tetrahydro-7,7-dimethyl-5-oxoquinazolin-2-yl)- | C₁₀₀H₂₀O₂        | 412.6908   |
| 41.6186        | 0.1877 | Hexahydropyridine, 1-methyl-4-[4,5-dihydroxyphenyl]-Cannabidiol | C₁₀₀H₂₀O₂        | 314.4617   |
| 41.939         | 0.6689 | D:4-Friedoursan-3-one  | C₁₀₀H₂₀O₂        | 314.4617   |
| 42.6543        | 0.3853 | 1H-1,2,4-Triazole-5(4H)-thione, 4-allyl-3-(3-furyl)- | C₁₀₀H₂₀O₂        | 314.4617   |
| 43.0033        | 0.1593 | 1,2-Bis(trimethylsilyl)benzene | C₁₀₀H₂₀O₂        | 314.4617   |
| 43.3123        | 0.4858 | Pyrido[2,3-d]pyrimidine, 4-phenyl- | C₁₀₀H₂₀O₂        | 314.4617   |
| 45.7384        | 0.2579 | 2-(Acetoxyethyl)-3-(methoxycarbonyl)biphenylene | C₁₀₀H₂₀O₂        | 314.4617   |
| Retention time | Area % | IUPAC name of compound | Molecular formula | Mol weight |
|----------------|--------|------------------------|-------------------|------------|
| 12.23          | 0.5467 | 2,6-Octadienial, 3,7-dimethyl- | C_{18}H_{36}O     | 152.2334   |
| 12.44          | 0.1904 | OR 2,6-Octadien-1-ol, 3,7-dimethyl- | C_{18}H_{36}O     | 154.2493   |
| 12.80          | 0.6749 | OR 2,6-Octadienial, 3,7-dimethyl- | C_{18}H_{36}O     | 152.2334   |
| 13.28          | 0.3461 | Indole                 | C_{6}H_{5}N       | 117.1479   |
| 16.99          | 0.1062 | 2-Methyl-3-isopropylpyrazine | C_{8}H_{12}N_{2}   | 136.1943   |
| 18.06          | 0.1089 | Dodecanoic acid        | C_{2}H_{22}O_{2}   | 200.3178   |
| 18.82          | 0.0892 | 1-Oxaspiro[2.5]octane, 4,4-dimethyl-8-methylene-2-propyl- | C_{6}H_{16}O_{6}   | 182.1718   |
| 19.29          | 0.1037 | Sorbitol               | C_{6}H_{12}O_{6}   | 154.229    |
| 20.48          | 0.0885 | p-(Methylthio)benzyl alcohol | C_{6}H_{10}OS      | 178.2277   |
| 21.09          | 0.1822 | Benzene, 1,2-dimethoxy-4-(1-propenyl)- | C_{16}H_{22}O_{2}  | 288.3709   |
| 21.24          | 0.1231 | Tetradecanoic acid      | C_{16}H_{28}O_{2}  | 212.2439   |
| 21.44          | 0.1036 | Benzyl Benzoate         | C_{16}H_{22}O_{2}  | 222.2802   |
| 21.51          | 0.1437 | Cycloptanececarboxaldehyde, 2-methyl-3-methylene- | C_{16}H_{24}O_{3}  | 222.2802   |
| 21.86          | 1.3486 | 2-Cyclohexen-1-one, 4-hydroxy-3,5,6-trimethyl-4-(3-oxo–butenyl)- | C_{16}H_{24}O_{3}  | 268.4778   |
| 22.25          | 0.103  | Bicyclo[2.2.1]heptan-2-one, 5-hydroxy-4,7,7-trimethyl- | C_{16}H_{24}O_{3}  | 268.4778   |
| 22.54          | 0.181  | 2-Pentadecanone, 6,10,14-trimethyl- | C_{16}H_{24}O_{3}  | 268.4778   |
| 22.66          | 0.0906 | 1-Cyclobutanol, 1-methyl-2-(2,2-dimethyl-6-methylenecyclohexyl) | C_{16}H_{24}O_{3}  | 268.4778   |
| 22.73          | 0.0942 | Pentadecanoic acid      | C_{16}H_{30}O_{2}  | 242.3975   |
| 22.91          | 0.1045 | Tricyclo[4.3.1][3,8]undecane-1-carboxylic acid, methyl ester | C_{16}H_{30}O_{2}  | 242.3975   |
| 23.54          | 0.2442 | Indole-6-carboxylic acid | C_{16}H_{30}O_{2}  | 262.4302   |
| 23.63          | 0.1808 | 5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl- | C_{18}H_{30}O_{2}  | 254.4082   |
| 23.89          | 0.0916 | Palmitoleic acid        | C_{16}H_{32}O_{2}  | 256.4241   |
| 24.27          | 4.3774 | n-Hexadecanoic acid     | C_{16}H_{32}O_{2}  | 284.4772   |
| 24.64          | 0.769  | Hexadecanoic acid, ethyl ester | C_{16}H_{32}O_{2}  | 270.4507   |
| 25.52          | 0.1612 | Heptadecanoic acid      | C_{17}H_{34}O_{2}  | 296.5310   |
| 26.26          | 4.7447 | Phytol                 | C_{20}H_{40}O_{4}  | 280.4455   |
| 26.50          | 1.111  | 9,12-Octadecadienoic acid (Z,Z)- | C_{18}H_{32}O_{2}  | 282.4614   |
| 26.58          | 1.1892 | Oleic Acid              | C_{18}H_{32}O_{2}  | 308.4986   |
| 26.85          | 0.7642 | 9,12-Octadecadienoic acid, ethyl ester | C_{20}H_{36}O_{2}  | 312.5304   |
| 26.94          | 0.3246 | 14-Pentadecenoic acid   | C_{18}H_{32}O_{2}  | 254.4943   |
| 27.24          | 0.2336 | Octadecanoic acid, 17-methyl-, methyl ester | C_{18}H_{36}O_{2}  | 232.6113   |
| 27.30          | 0.1564 | Octadecane              | C_{18}H_{38}O_{2}  | 266.5050   |
| 27.57          | 0.2966 | Naphthal[2,1-b:3,4-b′]diferan, 2,3,7,9-tetrahydro-2,9-dimethyl- | C_{2}H_{26}O_{2}  | 322.6113   |
| 28.46          | 0.5524 | 9-Tricosene, (Z)-        | C_{2}H_{26}O_{2}  | 240.4677   |
| 28.53          | 0.674  | Heptadecane             | C_{17}H_{36}O_{3}  | 280.5316   |
| 29.02          | 0.1115 | Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)- | C_{20}H_{40}O_{4}  | 280.5316   |
| 29.11          | 0.0859 | 1-Eicosene               | C_{20}H_{40}O_{4}  | 280.5316   |
| 32.66          | 0.0859 | 1-Nonadecene             | C_{19}H_{38}O_{2}  | 266.5050   |
| 29.45          | 0.1016 | Cyclotetrasocane         | C_{24}H_{48}O_{2}  | 336.6379   |
| 29.59          | 0.4245 |                          |                    |            |
| 29.65          | 1.3267 |                          |                    |            |
| 29.95          | 0.3418 |                          |                    |            |
| 30.39          | 0.0819 |                          |                    |            |
| 32.19          | 0.5337 |                          |                    |            |

(continued on next page)
| Retention time | Area %  | IUPAC name of compound                  | Molecular formular | Mol weight   |
|----------------|---------|----------------------------------------|--------------------|-------------|
| 29.72          | 1.8179  | Tetracosane                            | C_{24}H_{50}       | 338.6538    |
| 30.87          | 1.8751  |                                        |                    |             |
| 31.98          | 4.4291  |                                        |                    |             |
| 34.04          | 8.1295  |                                        |                    |             |
| 38.94          | 2.9929  |                                        |                    |             |
| 29.76          | 0.2311  | 1-Docosene                             | C_{22}H_{44}       | 308.5848    |
| 30.54          | 0.0776  |                                        |                    |             |
| 30.81          | 2.4887  |                                        |                    |             |
| 34.25          | 0.4713  |                                        |                    |             |
| 35.23          | 0.473   |                                        |                    |             |
| 30.22          | 0.1309  | 3-Eicosene, (E)-                       | C_{20}H_{40}       | 280.5316    |
| 31.21          | 0.1385  | Octacosyl acetate                      | C_{20}H_{40}O_{2}  | 452.7962    |
| 31.34          | 0.0906  | 1-Nonadecene                           | C_{19}H_{38}       | 266.5050    |
| 31.54          | 0.1031  |                                        |                    |             |
| 32.42          | 0.1088  |                                        |                    |             |
| 31.43          | 0.6062  | Bis(2-ethylhexyl) phthalate            | C_{24}H_{38}O_{4}  | 390.5561    |
| 31.70          | 0.1813  | Oleyl alcohol, trifluoroacetate        |                    |             |
| 32.14          | 0.1758  |                                        |                    |             |
| 32.29          | 0.0995  | 1-Hexacosene                           | C_{26}H_{52}       | 364.6911    |
| 32.71          | 0.1786  | Cyclooctacosane                        | C_{28}H_{56}       | 392.7442    |
| 32.81          | 0.1506  | Oxirane, tetradecyl-                   | C_{16}H_{32}O      | 240.4247    |
| 33.87          | 0.157   |                                        |                    |             |
| 33.03          | 4.1376  | Heptacosane                            | C_{27}H_{56}       | 380.7335    |
| 33.19          | 0.4429  | Butane, 2,2-bis(5-acetyl-2-thienyl)-    |                    |             |
| 33.24          | 0.2147  | 9-Hexacosene                           | C_{26}H_{52}       | 364.6911    |
| 33.69          | 0.1802  | Octacosyl acetate                      | C_{20}H_{40}O_{2}  | 452.7962    |
| 34.30          | 0.1039  | Oleyl alcohol, trifluoroacetate        |                    |             |
| 35.02          | 7.8384  | Nonacosane                             | C_{29}H_{60}       | 408.7867    |
| 35.29          | 0.5216  | 1-Tricosene                            | C_{23}H_{46}       | 322.6113    |
| 35.96          | 6.9585  | Triacontane                            | C_{30}H_{62}       | 422.8133    |
| 36.17          | 0.3705  | Heptacosyl acetate                     |                    |             |
| 36.87          | 5.6464  | Heptacosane, 1-chloro-                 | C_{27}H_{55}Cl     | 415.179     |
| 37.09          | 0.1352  | Triacontyl acetate                     | C_{22}H_{42}O_{2}  | 480.8494    |
| 37.30          | 0.5733  | dl-alpha.-Tocopherol                   | C_{29}H_{50}O_{2}  | 430.7061    |
| 37.53          | 0.0981  | Eicosane                               | C_{20}H_{42}       | 282.5475    |
| 41.74          | 0.4685  |                                        |                    |             |
| 43.55          | 1.0959  |                                        |                    |             |
| 37.83          | 4.0475  | Dotriacontane                          | C_{32}H_{66}       | 450.8664    |
| 38.03          | 0.7766  | Silane, dimethyl(2,2,2-trichloroethoxy)undecyloxy-| C_{32}H_{66}O_{8}  | 412.6908    |
| 38.75          | 0.5823  | Stigmasterol                           | C_{29}H_{48}O_{2}  | 231.270     |
| 38.82          | 0.8672  | Benzene, 1-nitro-4-(phenylthio)-       | C_{12}H_{7}NO_{2}S | 250.4626    |
| 39.26          | 0.6337  | Cyclohexane, 1,1’-(2-propyl-1,3-propanediyl)bis-| C_{20}H_{34}O_{2}  | 414.7067    |
| 39.47          | 1.6513  | .beta.-Sitosterol                      |                    |             |
| 39.99          | 1.0972  | Cyclopropane carboxamide,              |                    |             |
| 40.22          | 2.6996  | 2-cyclopropyl-2-methyl-N-(1-cyclopropylethyl)-| C_{34}H_{30}       | 478.9196    |
| 41.11          | 0.2358  | 2-Methyl-7-phenylindole                |                    |             |
| 41.49          | 1.2484  | 4-tert-pentylphenol, trifluoroacetate ester |                    |             |
| 41.95          | 0.7345  | Isobenzofuran-[1(3H)-one, 3,3-diheptyl-|                    |             |
| 42.67          | 0.6008  | Diacenaphthol[1,2-j:1’2’-j]fluoranthen | C_{38}H_{18}       | 450.5281    |
| 43.31          | 0.3566  | 5-Methyl-2-trimethylsilyloxy-acetophenone |                    |             |
| Ret. time | Area %  | IUPAC name of identified compound                                                                 | Mol. formula | Mol. wt  |
|-----------|---------|----------------------------------------------------------------------------------------------------|--------------|----------|
| 10.25     | 0.1956  | 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-                                             | C₈H₁₀O₄      | 144.1253 |
| 10.76     | 0.2414  | Benzoic acid                                                                                      | C₇H₆O₂       | 122.1213 |
| 11.77     | 0.126   | 5-Hydroxymethylfurfural                                                                        | C₆H₁₀O₃      | 126.1100 |
| 11.93     | 0.1363  | Citronnellol                                                                                      | C₈H₁₀O₂      | 156.2652 |
| 12.45     | 0.4528  | Benzeneacetic acid                                                                               | C₈H₁₀O₂      | 136.1479 |
| 12.63     | 0.3047  | Niacin                                                                                           | C₈H₁₅NO₂     | 123.1094 |
| 12.79     | 0.282   | Citral                                                                                            | C₉H₁₈O       | 152.2334 |
| 13.28     | 0.2957  | Indole                                                                                            | C₈H₈N        | 117.1479 |
| 14.50     | 0.5301  | Geranic acid                                                                                     | C₁₈H₃₆O₂      | 168.2328 |
| 15.67     | 0.2308  | Xylitol                                                                                          | C₃H₆O₂       | 152.1458 |
| 15.90     | 0.3185  | Dimethylamine, N-(neopentoxy)-                                                                   |              |          |
| 16.72     | 0.2561  | Benzeneacetonitrile, 4-hydroxy-                                                                  | C₈H₇NO       | 133.1473 |
| 16.99     | 0.1709  | 2-Acetyl-1-phenylhydrazine                                                                       | C₇H₁₁NO₂O     | 150.1778 |
| 17.27     | 0.5003  | Phenol, 2,4-bis[(1,1-dimethylethyl)- OR 2,4-Di-tert-butylphenol                                   | C₈H₁₄O₂      | 206.3239 |
| 17.64     | 0.4174  | Benzoic acid, 4-hydroxy-                                                                          | C₇H₆O₄       | 138.1207 |
| 17.85     | 0.3759  |                                                                                                  |              |          |
| 18.08     | 0.1626  | Dodecanoic acid                                                                                  | C₁₂H₂₄O₂      | 200.3178 |
| 18.30     | 0.2702  | 4-(2-Methoxyphenyl)phenol                                                                         |              |          |
| 18.42     | 0.3107  | Methyl methacrylate                                                                              | C₅H₈O₂       | 100.1158 |
| 18.44     | 0.1744  | 4-Phosphatricycl[6.1.0(2,6)]dec-2(6)-ene, 4,9,9-trimethyl-                                         |              |          |
| 19.62     | 0.135   | D-Gluconic acid, gamma-lactone                                                                   |              |          |
| 20.64     | 0.1429  | Galactitol                                                                                        | C₇H₁₄O₆       | 182.1718 |
| 21.69     | 0.287   |                                                                                                  |              |          |
| 21.29     | 0.5651  | Tetradecanoic acid                                                                                | C₁₄H₂₉O₂      | 228.3709 |
| 21.44     | 0.1386  | L-Arabinol                                                                                        | C₅H₁₀O₅       | 152.1458 |
| 22.43     | 0.1541  |                                                                                                  |              |          |
| 21.54     | 0.1336  | D-Arabinol                                                                                        | C₅H₁₀O₅       | 152.1458 |
| 21.77     | 0.6697  | Tetradecanoic acid, ethyl ester                                                                  | C₁₄H₂₉O₂      | 256.4241 |
| 22.54     | 0.1872  | Ribitol                                                                                            | C₅H₁₀O₅       | 152.1458 |
| 22.75     | 0.158   | Pentadecanoic acid                                                                                | C₁₅H₃₀O₂      | 242.3975 |
| 23.23     | 1.353   | Pentadecanoic acid, ethyl ester                                                                  | C₁₅H₃₀O₂      | 270.4507 |
| 23.92     | 0.1625  | Palmitoleic acid                                                                                  | C₁₅H₃₀O₂      | 254.4082 |
| 24.36     | 4.4729  | n-Hexadecanoic acid                                                                               |              |          |
| 24.52     | 8.6152  |                                                                                                  |              |          |
| 24.56     | 0.3829  | cis-Vaccenic acid                                                                                 | C₁₅H₃₀O₂      | 282.4614 |
| 24.73     | 9.0869  | Hexadecanoic acid, ethyl ester                                                                   | C₁₅H₃₀O₂      | 284.4772 |
| 25.23     | 0.1234  | 9,17-Octadecadienal, (Z)-                                                                        | C₁₆H₃₂O₂      | 264.4461 |
| 25.32     | 0.4109  | cis-10-Heptadecenoic acid                                                                         | C₁₇H₃₂O₂      | 268.4348 |
| 25.43     | 0.3282  | D-glycero-D-gulo-Heptonic acid, .delta.-lactone                                                   |              |          |
| 25.60     | 0.431   | Heptadecanoic acid                                                                                | C₁₇H₃₂O₂      | 270.4507 |
| 25.66     | 0.2891  | E-9-Tetradecenoic acid                                                                            |              |          |
| 25.97     | 0.6586  | Heptadecanoic acid, ethyl ester                                                                   | C₁₇H₃₂O₂      | 298.5038 |
| 26.27     | 3.7508  | Phytol                                                                                            | C₉H₁₈O₂       | 296.5310 |
| 26.94     | 20.525  | 9,12,15-Octadecatrienoic acid, (ZZZ)-                                                              | C₁₈H₃₆O₂      | 278.4296 |
| 27.05     | 2.7351  | 9,12,15-Octadecatrienoic acid, ethyl ester. (ZZZ)-                                                  | C₁₈H₃₆O₂      | 306.4828 |
| 27.30     | 2.7511  | Octadecanoic acid, ethyl ester                                                                   | C₁₈H₃₆O₂      | 312.5304 |
| 27.60     | 0.2372  | [1,1'-Biphenyl]-4,4'-diamine, N,N,N',N'-tetramethyl-Cyclopentane, 1,1'-[3-(2-cyclopentyl)-1,5-pentanediyl]bis-Cholestan-3-ol, 2-methylene-, (3.beta.,5.alpha.)- | C₂₀H₂₆N₂      | 240.3434 |
| 28.09     | 0.2365  |                                                                                                  | C₂₁H₴₀O₂      | 304.5530 |
| 28.35     | 0.1407  |                                                                                                  |              |          |
| 28.48     | 0.1464  | Octanoic acid, 7-oxo-, ethyl ester                                                                 |              |          |
| 29.30     | 0.4923  | Eicosanoic acid                                                                                  | C₂₀H₄₀O₂      | 312.5304 |
| 29.37     | 0.2159  | 2-Hydroxy-(Z)-9-pentadecenyl propanoate                                                           |              |          |
| 29.41     | 0.2925  | Butyl 9,12,15-octadecatrienoate                                                                  |              |          |

(continued on next page)
| Ret. time | Area % | IUPAC name of identified compound | Mol. formula | Mol. wt |
|----------|--------|----------------------------------|--------------|---------|
| 29.65    | 0.6067 | Methyl 19-methyl-eicosanoate      | C_{19}H_{38}O | 280.5316 |
| 30.78    | 0.1517 | Cyclotetradecane, 1,7,11-trimethyl-4-(1-methylethyl)- | C_{20}H_{40} | 280.5316 |
| 30.82    | 0.2786 | Pentacosane                       | C_{25}H_{52} | 352.6804 |
| 30.96    | 0.359  | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C_{19}H_{38}O_{2} | 330.5026 |
| 31.39    | 0.3206 | 2,6,10,14-Tetramethyl-7-(3-methylpent-4-enyldiene) pentadecane | C_{20}H_{40} | 280.5316 |
| 31.55    | 0.1829 | Docosanoic acid                   | C_{22}H_{44}O_{2} | 340.5836 |
| 31.88    | 0.795  | Docosanoic acid, ethyl ester      | C_{24}H_{44}O_{2} | 368.6367 |
| 32.64    | 0.1615 | 1-Bromo-11-iodoundecane           | C_{21}H_{42}I | 294.5582 |
| 32.93    | 1.4567 | 10-Heneicosene (c.t)              | C_{24}H_{50} | 338.6538 |
| 32.97    | 1.1261 | Tetracosane                       | C_{24}H_{50} | 338.6538 |
| 33.00    | 0.8757 | Linolenic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C_{21}H_{36}O_{2} | 352.5081 |
| 33.09    | 0.1778 | (Z,Z,Z)-                          |              |         |
| 33.20    | 0.6995 | Fumaric acid, isohexyl 2,3,5-trichlorophenyl ester | C_{12}H_{14}Cl_{3}O | 250.2574 |
| 33.49    | 0.1266 | Trifluoroacetyl-lavandulol        | C_{12}F_{3}O_{2} | 352.5081 |
| 34.31    | 0.1391 | Squalene                          | C_{29}H_{50} | 410.7180 |
| 34.97    | 3.0446 | Nonacosane                        | C_{29}H_{50} | 408.7867 |
| 35.19    | 0.1607 | 2- Chloropropionic acid, octadecyl ester | C_{21}H_{42}Cl_{2}O_{2} | 361.002 |
| 35.25    | 0.2337 | 1-Eicosene                        | C_{20}H_{40} | 280.5316 |
| 35.91    | 0.1328 | Triacanthan                       | C_{10}H_{62} | 422.8133 |
| 36.14    | 0.1966 | Triacetyl acetate                 | C_{12}H_{22}O_{2} | 480.8494 |
| 37.29    | 0.4897 | Vitamin E                         | C_{29}H_{50}O_{2} | 430.7061 |
| 38.01    | 0.2394 | 2,6,10,14-Tetramethyl-7-(3-methylpent-4-enyldiene) pentadecane | C_{20}H_{40} | 280.5316 |
| 38.36    | 0.3187 | Campesterol                       | C_{28}H_{48}O | 400.6801 |
| 38.74    | 0.5392 | Stigmasterol                      | C_{29}H_{48}O | 412.6908 |
| 38.80    | 0.2678 | 2,3-2H-Indanone, 2-hydroxyimino-3,3,4,5,7-pentamethyl- | C_{18}H_{38} | 254.4943 |
| 38.92    | 1.6734 | Octadecane                        | C_{29}H_{50}O_{2} | 414.7067 |
| 39.45    | 1.2399 | .beta.-Sitosterol                 | C_{29}H_{50}O_{2} | 414.7067 |
| 39.66    | 0.243  | 1-Bromo-11-iodoundecane           | C_{20}H_{42} | 282.5475 |
| 39.97    | 0.7175 | 6-Isopropenyl-4,8a-dimethyl-4a,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one | C_{29}H_{48}O | 410.6749 |
| 40.47    | 0.2618 | 4,22-Stigmastadiene-3-one         | C_{29}H_{48}O | 410.6749 |
| 40.89    | 0.6517 | D:A-Friedoursan-3-one             | C_{29}H_{48}O | 412.6908 |
| 41.36    | 0.2975 | Stigmast-4-en-3-one               | C_{21}H_{30}O_{2} | 314.4617 |
| 41.47    | 0.4222 | Cannabidiol                      | C_{21}H_{30}O_{2} | 314.4617 |
| 41.93    | 0.2541 |                                |              |         |
| 41.72    | 0.7527 | Eicosane                          | C_{20}H_{42} | 282.5475 |
| 43.54    | 0.2541 |                                |              |         |
| 42.65    | 0.2745 | Neoergosterone semicarbazone      |              |         |
| 43.29    | 0.1294 | 2-Ethylacridine                  |              |         |
Table 5
FTIR absorption frequency (cm\(^{-1}\))/intensity for ethanol, water and ethanol-water (1:1) extracts of A. indica, C. indica, M. indica and M. oleifera.

|      | A. indica          |      |      |      |      |      |      |      |      |      |
|------|-------------------|------|------|------|------|------|------|------|------|------|
|      | EtOH              | 881 (m) | 1048 (s) | 1089 (m) | 1383 (w) | 1451 (w) | 1640 (w) | 1652 (w) | 2925 (w) | 2974 (w) | 3361 (m,b) | - | - |
|      | EtOH/H\(_2\)O     | 881 (w) | 1048 (w) | 1089 (w) | - | 1640 (m) | - | - | - | - | 3264 (s,b) | - | - |
| H\(_2\)O | - | - | - | - | 1637 (m) | - | - | - | - | 3331 (s,b) | - | - |

|      | C. indica          |      |      |      |      |      |      |      |      |      |
|------|-------------------|------|------|------|------|------|------|------|------|------|
|      | EtOH              | 881 (m) | 1048 (s) | 1089 (m) | 1383 (w) | 1451 (w) | 1640 (w) | 1652 (w) | 2925 (w) | 2974 (w) | 3361 (m,b) | - | - |
|      | EtOH/H\(_2\)O     | 881 (w) | 1048 (m) | 1089 (w) | - | 1640 (m) | - | - | - | - | 3320 (s,b) | - | - |
| H\(_2\)O | - | - | - | - | 1637 (m) | - | - | - | - | 3331 (s,b) | - | - |

|      | M. oleifera       |      |      |      |      |      |      |      |      |      |
|------|-------------------|------|------|------|------|------|------|------|------|------|
|      | EtOH              | 881 (m) | 1048 (s) | 1089 (m) | 1275 (w) | 1331 (w) | 1383 (w) | 1454 (w) | 1640 (w) | 2895 (w) | 2974 (w) | 3331 (m,b) | - | - |
|      | EtOH:H\(_2\)O (1:1) | 881 (w) | 1048 (w) | 1089 (w) | - | - | - | - | 1640 (m) | - | 2975 (w) | 3330 (s,b) | - | - |
| H\(_2\)O | - | - | - | - | 1637 (m) | - | - | - | - | 3316 (s,b) | - | - |

EtOH – Ethanol; m – medium; s – strong; w – weak; b – broad
Table 6
Phytochemical properties of ethanol, water and ethanol-water (1:1) extracts of A. indica, C. indica, M. indica and M. oleifera.

| Biochemicals/Inference | CHO | TAN | SAP | FLA | ALK | ANTHO | BETA | QUIN | GLY | CARD-GLY | TER | TRI-TERP | PHE | COU | STE | ACIDS |
|------------------------|-----|-----|-----|-----|-----|--------|------|------|-----|-----------|-----|----------|-----|-----|-----|-------|
| **EtOH extract**       |     |     |     |     |     |        |      |      |     |           |     |          |     |     |     |       |
| M. indica              | +   | +   | +   | +   | -   | +      | -    | -    | +   | +         | -   | -        | -   | -   | -   | -     |
| A. indica              | -   | +++ | +   | ++  | -   | -      | -    | -    | -   | +         | -   | +        | -   | -   | -   | -     |
| C. indica              | -   | +   | +   | +   | -   | -      | -    | -    | -   | +         | -   | +        | -   | -   | -   | -     |
| M. oleifera            | -   | -   | +   | ++  | -   | -      | -    | -    | -   | +         | -   | +        | -   | -   | -   | -     |
| **EtOH/H₂O (1:1) extract** |     |     |     |     |     |        |      |      |     |           |     |          |     |     |     |       |
| M. indica              | +   | +++ | -   | -   | -   | -      | -    | -    | +   | +++       | -   | -        | -   | -   | -   | -     |
| A. indica              | -   | +++ | -   | +   | +   | -      | -    | -    | +   | -         | +   | -        | -   | -   | -   | -     |
| C. indica              | -   | ++  | -   | -   | -   | -      | -    | -    | -   | -         | -   | +        | -   | -   | -   | -     |
| M. oleifera            | -   | ++  | -   | -   | -   | -      | -    | -    | -   | +         | -   | +        | -   | -   | -   | -     |
| **H₂O extract**        |     |     |     |     |     |        |      |      |     |           |     |          |     |     |     |       |
| M. indica              | +   | +++ | -   | -   | -   | -      | -    | -    | +   | +++       | -   | -        | -   | -   | -   | -     |
| A. indica              | -   | +++ | -   | +   | +   | -      | -    | -    | +   | -         | -   | +        | -   | -   | -   | -     |
| C. indica              | -   | ++  | -   | -   | -   | -      | -    | -    | -   | -         | -   | +        | -   | -   | -   | -     |
| M. oleifera            | -   | ++  | -   | -   | -   | -      | -    | -    | -   | +         | -   | +        | -   | -   | -   | -     |

+= trace amount; +++= moderately present; +++= highly present; - = absent

CHO – Carbohydrates, TAN – Tannins, SAP – Saponins, FLA – Flavonoids, ALK – Alkaloids, ANTHO – Anthocyanins, BETA – Betacyanins, QUIN – Quinones, GLY – Glycosides, CARD-GLY – Cardiac Glycosides, TER – Terpenoids, TRI-TERP – Triterpenoids, PHE – Phenols, COU – Coumarins, STE – Steroids
The identified significant phenolics are listed in Table 7 in order of elution based on retention time. The most prominent phenolics found in leaf extracts of A. indica were vitamin E and Cannabidiol, while 4-hydroxy-benzoinic acid and cannabidiol were most abundant in M. oleifera leaf extracts (Table 8). For the M. indica leaves extract, six phenolic phytoconstituents were identified by the GC-MS namely 4-hydroxy-2-methylacetophenone, 1,2,3-benzenetriol, 4-hydroxy-benzoic acid, gamma-tocopherol, vitamin E, delta-8-tetrahydrocannabinol and cannabidiol (Table 9). On the other hand, A. indica had four phenolic constituents identified, representing 2.11% of the total phytochemicals in the ethanolic leaves extract (Table 10). Of these four, namely 2-methoxy-4vinylphenol, gamma tocoherol, vitamin E and cannabidiol, the latter two were the most abundant. The XRD patterns and UV/VIS absorption spectrum of biosynthesized A. indica oxide nanoparticles are presented in Figs. 6 and 7, respectively.

**Fig. 2.** Gas chromatography-mass spectrometry total ion chromatogram of A. indica in ethanolic extract.
2. Experimental Design, Materials and Methods

The present study used A. indica, C. indica, M. indica, and M. oleifera leaves that were sourced locally from Southwestern Nigeria. The leaves were identified and authenticated by botanists at Covenant University and Forest Research Institute of Nigeria (FRIN). To obtain the qualitative and quantitative phytochemical characterization of A. indica, C. indica, M. indica and M. oleifera, 25 g of pre-air-dried ground leaf samples of each plant was extracted separately using EtOH, water, and EtOH:water mix (1:1) for 72 h. The extracts were subsequently concentrated using a rotary evaporator and phytochemical screening was carried out according to reported standard method [1–6]. 10 g of each powdered plant material was extracted in three solvent media for 72 h. The GC-MS analysis was carried out using Agilent 7890A gas chromatograph coupled with a 5977A
**Fig. 4.** Gas chromatography-mass spectrometry total ion chromatogram of *C. indica* in ethanolic extract.

**Table 7**
Structural composition of phenolic constituents of *A. indica* leaf extracts.

| RT  | Area % | IUPAC name of compound | Mol. formula | Mol. weight | Chemical structure |
|-----|--------|------------------------|--------------|-------------|--------------------|
| 13.7| 0.259  | 2-Methoxy-4-vinylphenol| C_9H_10O_2    | 150.175     | ![2-Methoxy-4-vinylphenol](image) |
| 36.5| 0.183  | .gamma.-Tocopherol      | C_{28}H_{46}O_2 | 416.680     | ![.gamma.-Tocopherol](image) |
| 37.3| 0.994  | Vitamin E               | C_{29}H_{50}O_2 | 430.706     | ![Vitamin E](image) |
| 41.9| 0.669  | Cannabidiol             | C_{21}H_{30}O_2 | 314.462     | ![Cannabidiol](image) |
Fig. 5. GC-MS total ion chromatogram of *M. oleifera* ethanolic extract.

Fig. 6. XRD patterns of biosynthesized *A. indica* oxide nanoparticles (1:1) [A] and *A. indica* oxide nanoparticles (2:1) [B].
### Table 8
Structural composition of *M. oleifera* leaf extracts.

| RT  | Area % | IUPAC name of compound               | Mol. formula | Mol. weight | Chemical structure |
|-----|--------|--------------------------------------|--------------|-------------|--------------------|
| 16.7| 0.256  | Benzene acetonitrile, 4-hydroxy-      | C₅H₇NO      | 133.147     | ![Chemical structure](image1) |
| 17.3| 0.500  | Phenol, 2,4-bis(1,1-dimethylethyl)- OR 2,4-Di-tert-butylphenol | C₁₄H₂₂O      | 206.324     | ![Chemical structure](image2) |
| 17.6 | 0.417 | Benzoic acid, 4-hydroxy-             | C₇H₆O₃      | 138.121     | ![Chemical structure](image3) |
| 17.9 | 0.376 | Propylparaben                         | C₁₀H₁₂O₃    | 180.201     | ![Chemical structure](image4) |
|     | 0.250  |                                      |             |             |                    |
| 37.3| 0.490  | Vitamin E                             | C₂₉H₄₅O₂    | 430.706     | ![Chemical structure](image5) |
| 41.5| 0.422  | Cannabidiol                           | C₂₁H₂₀O₂    | 314.462     | ![Chemical structure](image6) |
| 41.9| 0.254  |                                      |             |             |                    |

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 ethanolic extracts of *A. indica*, *C. indica*, *M. indica* and *M. oleifera* were analyzed using gas chromatograph mass spectrometer Agilent 7890A and the phytochemicals were characterized for each plant. The identification of phytoconstituents present in the ethanolic extracts were carried out by comparing and matching the retention times and mass spectral data obtained with the GC mass spectra of the National Institute of Standards and Technology (NIST) library. The matched compounds are presented in Tables 1–4. For the FTIR analysis, each extract was analyzed 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 to 650 cm⁻¹ [4,6].
Table 9
Structural composition of M. indica leaf extracts.

| RT  | Area % | IUPAC name of compound | Mol. formula | Mol. weight | Chemical structure |
|-----|--------|------------------------|--------------|-------------|--------------------|
| 13.7| 0.168  | 4-Hydroxy-2- methylacetophenone | C₉H₁₀O₂ | 150.175     | ![Chemical structure of 4-Hydroxy-2-methylacetophenone](image) |
| 15.0| 0.152  | 1,2,3-Benzenetriol       | C₆H₆O₃  | 126.110     | ![Chemical structure of 1,2,3-Benzenetriol](image) |
| 17.3| 0.108  | Benzoic acid, 4-hydroxy- | C₇H₆O₃  | 138.121     | ![Chemical structure of Benzoic acid, 4-hydroxy-](image) |
| 36.5| 0.259  | .gamma.-Tocopherol       | C₂₉H₄₈O₂ | 416.680     | ![Chemical structure of .gamma.-Tocopherol](image) |
| 37.3| 1.782  | Vitamin E                | C₂₀H₃₀O₂ | 430.706     | ![Chemical structure of Vitamin E](image) |
| 41.5| 0.906  | Cannabidiol              | C₂₁H₂₆O₂ | 314.462     | ![Chemical structure of Cannabidiol](image) |

The synthesis of nanoparticles was performed by mixing dropwise ferric chloride solution (0.1 N) with plant extract at a ratio of 1:1 and 1:2 at a flow rate of 4 – 8 mL/min. After capping vials to prevent oxidation, the solution was constantly agitated for 10 min. Centrifugation at 10,000 rpm for 30 min resulted in the formation of nanoparticles. The nanoparticles were rinsed two times with deionized water and once with anhydrous ethanol. Synthesized nanoparticles were labeled and calcination was carried out at 600 °C. The formation of iron oxide nanoparticles was confirmed using a UV spectrometer (UV-3000 ORI, Germany). The UV-visible spectra of
Table 10
Structural composition of *A. indica* leaf extracts.

| RT  | Area % | IUPAC name of compound                  | Mol. formular | Mol. weight | Chemical structure |
|-----|--------|----------------------------------------|---------------|-------------|--------------------|
| 13.7| 0.259  | 2-Methoxy-4-vinylphenol                | C₉H₁₀O₂       | 150.175     | ![Chemical structure](image1.png) |
| 36.5| 0.183  | gamma.-Tocopherol                      | C₂₈H₄₈O₂      | 416.680     | ![Chemical structure](image2.png) |
| 37.3| 0.994  | Vitamin E                              | C₂₉H₅₀O₂      | 430.706     | ![Chemical structure](image3.png) |
| 41.9| 0.669  | Cannabidiol                            | C₂₁H₃₀O₂      | 314.462     | ![Chemical structure](image4.png) |

Fig. 7. UV/VIS absorption spectrum of biosynthesized iron nanoparticles.
biogenic nanoparticles were measured between 200 and 800 nm spectral range. X-ray diffraction (XRD) study was performed by coating the biosynthesized iron oxide nanoparticles onto a glass slide and analyzing the particles with a high-power CuKα radioactive source \( k = 0.154 \text{ nm} \) at 40 kV/ 40 mA using Empyrean, Malvern PanAnalytical [6].

**Ethics Statement**

This study did not involve human or animal subjects, and no data from social media platforms were used.

**Declaration of Competing Interest**

The authors declare that we have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

**CRediT Author Statement**

Oladotun P. Bolade: Conceptualization, Methodology, Data curation, Writing – original draft, Investigation, Writing – review & editing; Akan B. Williams: Conceptualization, Methodology, Data curation, Writing – original draft, Investigation, Supervision, Writing – review & editing; Nskak U. Benson: Conceptualization, Methodology, Data curation, Writing – original draft, Investigation, Project administration, Supervision, Writing – review & editing.

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