Data Article

Metabolite data of germinated Bambara groundnut flour and starch extracted with two different solvents

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A B S T R A C T

The data presented in this study represents the profile of metabolites of germinated Bambara groundnut flour (GBF) and starch (GBS) extracted using two different extraction solvents. Bambara groundnuts obtained from a local agro market in Minna, Niger State, Nigeria were germinated at 28 ± 1°C for 24, 48 and 72 h, dried and then processed into flour and starch. Raw Bambara groundnuts (0 h) were also processed into flour and starch and served as controls. Samples at the different germination times were extracted using methanol/water (80:20 v/v) and acetonitrile/methanol/water (40:40:20 v/v/v), concentrated, reconstituted and analysed on a gas chromatography-high resolution time of flight-mass spectrometer (GC-HRTOF-MS). Data obtained were classified into compound groups such as acids, alcohols, cyclic compounds, esters, ketones, phytosterols, vitamins and many others, and their characteristics such as the retention time, observed mass, molecular formular and mean peak areas were reported. These data represent the collection of metabolites in GBF and GBS and may be useful for the identification and utilization of functional compounds in foods.

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Specifications Table

| Subject                  | Food Science and Technology |
|--------------------------|-----------------------------|
| Specific subject area    | Germination; Food composition and analysis; Metabolomics |
| Type of data             | Tables |
| How data were acquired   | Flour and starch prepared from previously germinated Bambara groundnut were subjected to two different solvent extraction methods to determine their metabolites composition. The first combination of organic solvents used for extraction was methanol/water (80:20 v/v) while the second combination was acetonitrile/methanol/water (40:40:20 v/v/v). These individual solvent combinations were used to extract metabolites from germinated Bambara groundnut flour (GBF) and germinated Bambara groundnut starch (GBS) which were sprouted between 0-72 h. Analyses of these extracts was done on LECO Pegasus GC-HRTOF-MS system (LECO Corporation, St Joseph, USA) fitted with resolution of 50,000 FWHM (full peak with at one half maximum), with mass accuracies/errors of < 1 ppm and acquisition rates of up to 200 spectra/s. The system is equipped with an Agilent 7890A gas chromatograph (Agilent Technologies, Inc., Wilmington, DE, USA). This GC-HRTOF-MS operates at high resolution and is equipped with a Gerstel MPS multipurpose autosampler (Gerstel Inc., Mülheim an der Ruhr, Germany) and a Rxip®-5ms column (30 m × 0.25 mm ID × 0.25 μm) (Restek, Bellefonte, USA). |
| Data format              | Raw and analyzed data; spectra of identified compounds |
| Parameters for data collection | Samples were extracted in triplicate and data were also obtained from the GC-HRTOF-MS were also collected in triplicate. |
| Description of data collection | Samples were freeze-dried and solvent extraction of metabolites was performed on freeze-dried samples (1 g), using the solvent mixture (10 mL) in each case. Thereafter, samples were concentrated and reconstituted in 1 mL methanol (99.9% pure chromatography grade) and thereafter filtered into dark vials using 0.22 μm syringe filters. For sample analyses in GC-HRTOF-MS machine, 1 μL of samples were auto-injected into the system and metabolite identities were determined using NIST, Mainlib and Feinhab metabolomics databases. |
| Data source location     | Bambara groundnut were sources from a local agro market in Minna, Niger State Nigeria (9.5836° N, 6.5463° E) while Bambara flour and starch samples were produced at the Food Science laboratory of the Federal University of Technology, Minna, Niger State Nigeria (9.6564° N, 6.5278° E). Extraction of metabolites and instrumental analyses were carried out at the University of Johannesburg (Doornfontein Campus), Johannesburg, South Africa (S26°11′32.6″E28°03′28.9″). |
| Data accessibility       | Raw and processed dataset have been deposited in Mendeley repository and is accessible using the link: [https://data.mendeley.com/datasets/3fhfsz5gv9/4](https://data.mendeley.com/datasets/3fhfsz5gv9/4) |

Value of the Data

- The data gives information of the identity of metabolites present in Bambara groundnut flour and starch samples germinated at different times.
- The data represents the effect of germination at different times on the metabolite profile of samples, relative to the ungerminated ones, to understand the progression of germination as a metabolic process and its effect on the production and retention of metabolites at different sprouting times.
- The data gives information about the extractability of metabolites using different mixtures of extraction solvents, to show the efficiency or versatility of each solvent and their applicability in food systems.
• The data represents a cocktail of untargeted metabolites derived from Bambara flour and starch samples as a result of germination at different times, which could lead to the identification and utilization of compounds of functional importance in food production.
• Information provided through this data will be helpful in the determination of germination conditions for Bambara groundnuts and related legumes to produce their flour and starch products to obtain similar or improved production of relevant and functional metabolites.

1. Data Description

The data presented in this study is the information of metabolites obtained from germinated Bambara flour (GBF) and germinated Bambara starch (GBS) using different mixtures of organic solvents for extraction. Table 1 represents the metabolites obtained from GBF and GBS using a mixture of methanol/water (80:20 v/v) as extraction solvent while Table 2 shows the metabolite profile of GBF and GBS using acetonitrile/methanol/water (40:40:20 v/v/v) as extraction solvent. Each table shows information about retention time, observed mass, metabolite name, molecular formula and average peak area for each metabolites in different samples obtained from the peaks generated from GC-HRTOF-MS analysis and comparison of spectra obtained with NIST, Mainlib and Feihn metabolite databases. Subsequent mass spectra of some compounds are presented in supplementary files, deposited in the Mendeley database (https://data.mendeley.com/datasets/3fhfsz5gv9/4).

2. Experimental Design, Materials and Methods

2.1. Germination of Bambara groundnut

Brown variety of Bambara groundnut (Vigna subterranean) were physically cleaned to remove seed broken and extraneous materials. Thereafter, a portion of 250 g was sterilized in 1000 mL of food-grade sodium hypochlorite, blotted dry and soaked in water at 28 ± 1°C for 6 h prior to germination. Hydrated seeds were germinated at 28 ± 1°C for 24, 48 and 72 h and uniformly sprouted seeds were dried at 40°C for 24 h for subsequent processing into flour and starch. Raw Bambara groundnut seeds were equally processed into flour and starch and represents 0 h samples which served as control in each case.

2.2. Production of Bambara groundnut flour and starch

Raw and germinated (dried) seeds were milled (Brook Crompton Series 2000, Christy Hunt Agriculture Ltd., South Humberside, England) and sieved (100 µm mesh-size) to obtain raw and germinated Bambara groundnut flour (GBF) [1]. The method of Oyeyinka et al. [2] was used to extract starch from Bambara groundnut flour samples for each germination time (0-72 h). Flour was dispersed in 0.3% (w/v) NaOH solution at 1:10. The mixture was shaken vigorously, allowed to settle and the supernatant was decanted. Afterwards, distilled water was added to the residue and the slurry was sieved. The suspension was left to stand overnight and the starch obtained was repeatedly washed with distilled water, centrifuged (K24IR, Centurion Scientific Ltd, Stoughton, Chichester, UK) at 10,000 × g for 20 min at 25°C, neutralized with 0.1N HCl and the resulting germinated Bambara starch (GBS) was freeze dried (LGJ-18, SHKY, China) at a set temperature (-40°C) and pressure (40 Pa) for 24 h, and uniformly blended (BLX750RD, Kenwood, Sheffield, UK).
Table 1
Metabolites identified in Bambara groundnut flour (GBF) and starch (GBS) using methanol and water (80:20 v/v) as extraction solvent.

| Rt (mins) | Observed ion m/z | Name | MF | Flour | Starch |
|-----------|------------------|------|----|-------|--------|
|           |                  |      | MF | 0GBF  | 24GBF  | 48GBF  | 72GBF  | 0GBS  | 24GBS  | 48GBS  | 72GBS  |
| **Alcohol** |                  |      |    |       |        |        |        |       |        |        |        |
| 6.83      | 87.0439          | Glycerol | C₃H₆O₃ | ND | ND | ND | 307634 | ND | ND | ND | ND |
| **Amides** |                  |      |    |       |        |        |        |       |        |        |        |
| 19.12     | 154.1225         | Dodecanamide, N-(2-hydroxyethyl)- | C₁₆H₃₀NO₂ | ND | ND | ND | 246097 | ND | ND | ND | ND |
| 19.80     | 212.2011         | Dodecanamide | C₁₂H₂₂NO | ND | ND | 229538 | ND | ND | ND | 272443 | ND |
| 20.32     | 161.0963         | 3-Cyclopentylpropionamide, N,N-dimethyl- | C₁₀H₁₈NO | ND | ND | 356253 | ND | ND | ND | ND |
| 21.27     | 140.1075         | Nonanamide | C₈H₁₀NO | ND | ND | ND | 356772 | ND | ND | ND | ND |
| 21.84     | 100.0326         | Bis(2-(Dimethylamino)ethyl) ether | C₁₈H₃₆NO₃ | ND | ND | 161840 | 212288 | 118436 | 148731 | 207178 | 201073 |
| 22.80     | 126.0910         | Hexadecanamide | C₁₆H₃₂NO | ND | ND | 347814 | ND | ND | ND | ND |
| 22.81     | 140.1067         | Benzeneethanamine | C₁₁H₁₆NO₃ | ND | ND | 161840 | 212288 | 118436 | 148731 | 207178 | 201073 |
| 24.34     | 294.2779         | 9-Octadecenamide, (Z)- | C₁₈H₃₆NO | 1354600 | ND | 2055194 | 4063967 | ND | ND | ND | 3197280 |
| **Cyclic compounds** |                  |      |    |       |        |        |        |       |        |        |        |
| 18.75     | 108.0932         | E.Z-3-Ethylidenecyclohexene | C₆H₁₂ | ND | ND | 687948 | ND | ND | ND | ND |
| 22.28     | 227.0701         | Benzenehexanenitrile | C₁₆H₁₈N₂O | 191620 | ND | ND | ND | ND | ND | ND |
| 24.17     | 279.2317         | Benzene, 2-methoxy-1-(2-nitroethenyl)-3-(phenylmethoxy)- | C₁₆H₁₈NO₄ | ND | ND | 657003 | ND | ND | ND | ND |
| **Esters** |                  |      |    |       |        |        |        |       |        |        |        |
| 12.73     | 177.0547         | Diethyl Phthalate | C₁₂H₂₄O₄ | ND | ND | 102107 | ND | ND | ND | ND |
| 16.32     | 223.0961         | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | C₁₆H₂₄O₄ | ND | ND | 296119 | ND | ND | ND | ND |
| 16.32     | 223.0960         | 1,2-Benzenedicarboxylic acid, butyl octyl ester | C₂₀H₃₂O₄ | ND | ND | 449868 | ND | ND | ND | ND |
| 16.33     | 223.0959         | Phthalic acid, butyl oct-3-yl ester | C₂₀H₂₄O₄ | ND | ND | 130139 | ND | ND | ND | ND |
| 17.36     | 224.0995         | Dibutyl phthalate | C₁₂H₂₄O₄ | ND | ND | 1365627 | 280866 | 302235 | 170104 | 830621 | ND |
| 17.38     | 150.0265         | 1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl ester | C₁₆H₂₄O₄ | 158769 | ND | 129430 | ND | ND | ND | ND |

(continued on next page)
Table 1 (continued)

| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|-----------|------------------|------|----|------|-------|-------|-------|------|-------|-------|-------|
| 17.38     | 223.0959         | 1,2-Benzenedicarboxylic acid, dipropyl ester | C_{14}H_{18}O_{4} | ND   | ND    | ND    | 352860 | ND   | ND    | ND    | ND    |
| 18.69     | 294.2546         | Ethyl 9,12-hexadecadienoate | C_{18}H_{22}O_{2} | ND   | ND    | 5252360 | 8018935 | ND   | ND    | ND    | ND    |
| 19.19     | 174.0936         | 2,2',2''-Nitrilotriethanol, triethyl ether | C_{12}H_{27}NO_{3} | ND   | ND    | ND    | 662787 | ND   | ND    | ND    | ND    |
| 19.33     | 213.0752         | 1-Propene-1,2,3-tricarboxylic acid | C_{18}H_{26}O_{6} | ND   | ND    | 107599 | 107436 | ND   | ND    | ND    | ND    |
| 20.20     | 273.0963         | 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ether | C_{20}H_{34}O_{8} | 249357 | ND    | 280433 | 8018935 | 222530 | 242690 | 764578 | 260777 |
| 20.38     | 144.1019         | Carbonic acid, 2-dimethylaminoethyl isobutyl ester | C_{9}H_{19}NO_{3} | 348980 | ND    | 698929 | ND    | ND    | ND    | ND    |
| 20.48     | 283.2628         | Succinic acid, 3,4-dimethylphenyl 2-(dimethylamino)ethyl ester | C_{16}H_{23}NO_{4} | ND   | ND    | 1466928 | ND    | ND    | ND    | ND    |
| 21.85     | 152.1196         | Carbonic acid, 2-dimethylaminoethyl 2-methoxyethyl ester | C_{8}H_{17}NO_{4} | 331038 | ND    | ND    | ND    | ND    | ND    | ND    |
| 21.91     | 144.1017         | Carbonic acid, 2-dimethylaminoethyl ethyl ester | C_{7}H_{15}NO_{3} | ND   | ND    | 500886 | ND    | ND    | ND    | ND    |
| 22.57     | 280.1631         | Bis(2-ethylhexyl) phthalate | C_{22}H_{26}O_{4} | ND   | ND    | 1000108 | 668139 | ND    | ND    | ND    | ND    |
| 22.58     | 280.0729         | Dicyclohexyl phthalate | C_{20}H_{26}O_{4} | ND   | ND    | 495234 | ND    | ND    | ND    | ND    |
| 22.62     | 279.1580         | 1,2-Benzenedicarboxylic acid, monononyl ester | C_{17}H_{24}O_{4} | ND   | ND    | 368535 | 202911 | ND    | ND    | ND    | ND    |
| 22.64     | 279.1590         | 1,2-Benzenedicarboxylic acid, dicyclohexyl ester | C_{20}H_{26}O_{4} | ND   | ND    | ND    | 202911 | ND    | ND    | ND    | ND    |
| 24.87     | 280.2392         | Oxalic acid, di(1-menthyl) ester | C_{15}H_{20}O_{4} | ND   | ND    | ND    | 288311 | ND    | ND    | ND    | ND    |
| 29.87     | 530.4706         | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadeyl ester | C_{35}H_{62}O_{3} | 120035 | ND    | 592440 | ND    | ND    | ND    | ND    |

FAEEs

| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|-----------|------------------|------|----|------|-------|-------|-------|------|-------|-------|-------|
| 17.61     | 241.2157         | Dodecanoic acid, ethyl ester | C_{14}H_{26}O_{2} | ND   | ND    | ND    | 233196 | ND   | ND    | ND    | ND    |
| 20.60     | 131.0950         | Octanoic acid, 2-dimethylaminoethyl ester | C_{12}H_{25}NO_{2} | ND   | ND    | ND    | 352802 | ND   | ND    | ND    | ND    |
| 22.29     | 299.2574         | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C_{16}H_{29}O_{4} | ND   | ND    | 1415101 | ND    | ND    | 4688360 | 2053117 |

(continued on next page)
| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 23.74     | 336.2648         | 9,12-Octadecadienoic acid (Z,Z)-2-hydroxy-1-(hydroxymethyl) ethyl ester | C\text{_{21}}H\text{_{36}}O\text{_{4}} |
|           |                   |      | ND | ND | 7924939 | 4287462 | ND | ND | ND | ND |

**FAMEs**

| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 16.90     | 228.2038         | Tridecanoic acid, methyl ester | C\text{_{14}}H\text{_{20}}O\text{_{2}} |
|           |                   |      | 4940778 | ND | ND | ND | ND | 330722 | ND | 850485 |
| 16.91     | 270.2551         | Hexadecanoic acid, methyl ester | C\text{_{17}}H\text{_{24}}O\text{_{2}} |
|           |                   |      | 10471598 | ND | ND | ND | ND | 11366836 | 8939116 | 4237592 |
| 18.65     | 263.2357         | 16-Octadecadienoic acid, methyl ester, (E,E)- | C\text{_{19}}H\text{_{34}}O\text{_{2}} |
|           |                   |      | ND | ND | 865286 | 0 | ND | ND | ND | ND |

| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 16.90     | 228.2038         | Tridecanoic acid, methyl ester | C\text{_{14}}H\text{_{20}}O\text{_{2}} |
|           |                   |      | 4940778 | ND | ND | ND | ND | 330722 | ND | 850485 |
| 16.91     | 270.2551         | Hexadecanoic acid, methyl ester | C\text{_{17}}H\text{_{24}}O\text{_{2}} |
|           |                   |      | 10471598 | ND | ND | ND | ND | 11366836 | 8939116 | 4237592 |
| 18.65     | 263.2357         | 16-Octadecadienoic acid, methyl ester, (E,E)- | C\text{_{19}}H\text{_{34}}O\text{_{2}} |
|           |                   |      | ND | ND | 865286 | 0 | ND | ND | ND | ND |

| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 23.74     | 336.2648         | 9,12-Octadecadienoic acid (Z,Z)-2-hydroxy-1-(hydroxymethyl) ethyl ester | C\text{_{21}}H\text{_{36}}O\text{_{4}} |
|           |                   |      | ND | ND | 7924939 | 4287462 | ND | ND | ND | ND |

**Furan**

| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 12.69     | 111.1168         | Furan, 2-butyltetrahydro- | C\text{_{4}}H\text{_{16}}O |
|           |                   |      | ND | ND | 301109 | ND | ND | ND | ND | ND |

**Ketones**

| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 14.21     | 105.0335         | Methanone, (1-hydroxy cyclohexyl)phenyl-7,9-di-tert-butyl-1-oxaspiro(4,5)decadiene-2,8-dione | C\text{_{13}}H\text{_{16}}O\text{_{2}} |
|           |                   |      | 101939 | 164821 | 187249 | 149732 | 146197 | 159302 | ND |
| 16.91     | 232.1823         | Methanone, (1-hydroxy cyclohexyl)phenyl-7,9-di-tert-butyl-1-oxaspiro(4,5)decadiene-2,8-dione | C\text{_{17}}H\text{_{24}}O\text{_{3}} |
|           |                   |      | ND | ND | 32318 | ND | ND | ND | ND | ND |

**Miscellaneous**

| Rt (mins) | Observed ion m/z | Name |
|-----------|------------------|------|
| 3.98      | 60.0208          | 2H-1,2-Oxazine, 6-(4-chlorophenyl)tetrahydro-2-methylcyclooctasiloxane, hexadecamethyl- | C\text{_{11}}H\text{_{14}}C\text{_{NO}} |
|           |                   |      | ND | 1400596 | ND | ND | ND | ND | ND | ND |
| 13.67     | 501.9715         | 2H-1,2-Oxazine, 6-(4-chlorophenyl)tetrahydro-2-methylcyclooctasiloxane, hexadecamethyl- | C\text{_{16}}H\text{_{46}}O\text{_{3}}Si\text{_{8}} |
|           |                   |      | 3282594 | 2169153 | ND | ND | ND | ND | ND | ND |
| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|------|----|-------|--------|--------|--------|------|-------|--------|-------|
| 17.45    | 534.9914         | Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl- | C_{16}H_{30}O_{5}Si_{8} | ND | 2779445 | 2701270 | ND | ND | 1915391 | 928470 | ND |
| 17.46    | 533.9926         | 3-Isopropoxy-1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane | C_{18}H_{32}O_{5}Si_{7} | ND | ND | ND | ND | ND | 2360859 | ND | ND |
| 18.65    | 219.9887         | 1,8,11-Heptadecatriene, (Z,Z)- | C_{17}H_{30} | ND | 667023 | 770836 | ND | ND | 482944 | 854367 | ND |
| 19.07    | 210.2212         | 2,8,9-Trioxa-5-aza-1-silabicyclo(3.3.3)undecane, 1-methoxy- | C_{11}H_{40}O_{5}Si_{6} | ND | 2660774 | 3284057 | ND | ND | ND | ND | ND |
| 20.27    | 434.0867         | 1,1,5,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane | C_{20}H_{23}F_{2}N_{2}O_{3} | ND | ND | ND | ND | ND | 739228 | ND | ND |
| 22.07    | 372.2636         | 3-Methylbutyl N-heptafluorobutyryltryptophanate | C_{25}H_{42} | ND | 1998765 | 887750 | ND | ND | 1698458 | ND | ND |
| 22.23    | 313.2550         | 1H-Indene, 1-hexadecyl-2,3-dihydro-Heptasiloxane, hexadecamethyl- | C_{25}H_{42}O_{6}Si_{7} | ND | ND | ND | ND | ND | ND | ND | ND |

**Phenols**

| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|------|----|-------|--------|--------|--------|------|-------|--------|-------|
| 11.32    | 206.1663         | 2,4-Di-tert-butylphenol | C_{14}H_{22}O | 417837 | 626608 | 707602 | 563806 | 580774 | 701221 | 579501 | 651064 | 279502 |
| 21.61    | 340.2389         | Phenol, 2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl-(Z)-3-(Heptadec-10-en-1-yl)phenol | C_{22}H_{30}O | ND | 230841 | 209691 | ND | ND | ND | ND | 482973 | 439076 |
| 22.07    | 161.0948         | Stigmasterol | C_{23}H_{30}O | ND | ND | ND | ND | 167128 | ND | ND | ND | ND |

**Phytosterols**

| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|------|----|-------|--------|--------|--------|------|-------|--------|-------|
| 27.75    | 412.3692         | d-Tocopherol | C_{29}H_{50}O | ND | ND | ND | 390128 | ND | ND | 482973 | 439076 |
| 28.13    | 414.3854         | β-Sitosterol | C_{29}H_{50}O | ND | 230841 | 209691 | ND | ND | ND | ND | ND |
| 24.62    | 340.0400         | Squalene | C_{29}H_{50} | ND | ND | ND | 395205 | ND | ND | ND | ND |
| 24.62    | 430.0896         | Supraene | C_{29}H_{50} | ND | 757222 | ND | ND | 745590 | 833629 |

**Vitamin**

| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|------|----|-------|--------|--------|--------|------|-------|--------|-------|
| 25.54    | 402.3484         | d-Tocopherol | C_{27}H_{46}O_{2} | ND | ND | ND | 768559 | 1228631 | ND | ND | ND |

MF: Molecular formula; FAEE: Fatty acid ethyl ester; FAME: Fatty acid methyl ester; OGBF: Flour from Bambara groundnut germinated for 0 h; 24GBF: Flour from Bambara groundnut germinated for 24 h; 48GBF: Flour from Bambara groundnut germinated for 48 h; 72GBF: Flour from Bambara groundnut germinated for 72 h OGBS: Starch from Bambara groundnut germinated for 0 h; 24GBS: Starch from Bambara groundnut germinated for 24 h; 48GBS: Starch from Bambara groundnut germinated for 48 h; 72GBS: Starch from Bambara groundnut germinated for 72 h.
Table 2
Metabolites identified in Bambara groundnut flour (GBF) and starch (GBS) using acetonitrile/methanol/water (40:20:20 v/v/v) extraction solvent.

| Rt (mins) | Observed ion m/z | Name                                | MF          | 0GBF | 24GBF | 48GBF | 72GBF | OGBS | 24GBS | 48GBS | 72GBS |
|-----------|------------------|-------------------------------------|-------------|------|-------|-------|-------|------|-------|-------|-------|
| Acids     |                  |                                     |             |      |       |       |       |      |       |       |       |
| 3.26      | 104.0293         | Butanoic acid, 4-hydroxy-           | C₁₀H₁₂O₁Si  | ND   | ND    | ND    | 1379146 | ND   | ND    | ND    | ND    |
| 4.06      | 102.0090         | Pentanoic acid                      | C₈H₁₀O₂     | ND   | ND    | ND    | 850250  | ND   | ND    | 1599442 | 420330 |
| 15.20     | 228.2077         | Tetradecanoic acid                  | C₁₄H₂₂O₂    | ND   | ND    | ND    | 747974  | ND   | ND    | ND    | ND    |
| 17.51     | 256.2398         | n-Hexadecanoic acid                 | C₁₆H₃₂O₂    | 5839377 | 4563896 | ND | ND    | ND | 6469462 | 67444726 |
| 19.73     | 284.2714         | Octadecanoic acid                   | C₁₈H₃₆O₂    | ND   | ND    | ND    | 13076604 | 14514438 | ND  | ND    | ND    | ND    |
| Alcohols  |                  |                                     |             |      |       |       |       |      |       |       |       |
| 5.26      | 92.0213          | Glycerol                            | C₃H₆O₃      | ND   | ND    | ND    | 83692530 | 27609 | ND    | ND    | ND    |
| 5.66      | 126.0311         | Maltol                              | C₄H₆O₃      | ND   | ND    | ND    | 5053284  | ND   | ND    | ND    | ND    |
| 26.65     | 394.3588         | Cholesta-4,6-dien-3-ol, (3β)-      | C₂₇H₄₄O     | 218602 | ND  | ND    | ND    | ND   | ND    | ND    | ND    |
| Aldehyde  |                  |                                     |             |      |       |       |       |      |       |       |       |
| 4.73      | 120.0570         | Benzeneacetaldehyde                 | C₅H₅O      | ND   | ND    | ND    | 559553  | 1873781 | ND  | ND    | 1278347 | ND    |
| Amide     |                  |                                     |             |      |       |       |       |      |       |       |       |
| 4.83      | 114.0312         | Pentanamide                         | C₄H₆N₂O₃    | ND   | 547511 | ND    | ND    | ND    | ND    | ND    | ND    |
| 19.21     | 262.2290         | Octadecanamide, N-(2-hydroxyethyl)- | C₂₇H₃₈N₂O₂  | 247931 | ND  | ND    | ND    | 1637175 | ND   | ND    | ND    | ND    |
| 19.74     | 221.3520         | Decanamide, N-(2-hydroxyethyl)-     | C₂₃H₄₀NO    | 189552 | ND  | ND    | ND    | 864547  | ND   | ND    | ND    | ND    |
| 21.24     | 229.1615         | Tetradecanamide                     | C₂₇H₃₈NO    | 1042090 | ND  | ND    | ND    | 1402093 | ND   | ND    | ND    | ND    |
| 24.48     | 281.2666         | Hexadecanamide                      | C₂₉H₅₂NO    | 208553 | ND  | 560386 | ND    | 194632  | ND   | ND    | ND    | ND    |
| 21.97     | 139.0402         | 9-Octadecanamide, (Z)-              | C₂₅H₄₄NO    | 208553 | ND  | 560386 | ND    | 194632  | ND   | ND    | ND    | ND    |
| 22.90     | 187.1137         | Benzeneethanamine, 2-fluoro-ß,3,4-trihydroxy-N-isopropyl- | C₁₁H₁₆FNO₄ | ND   | ND    | ND    | 1402093 | ND   | ND    | ND    | ND    |
| Cyclic compound |                |                                     |             |      |       |       |       |      |       |       |       |
| 29.06     | 268.0389         | Benzenehexanenitrile, ß,ß-dimethyl-e-oxo- | C₁₄H₁₇NO | ND   | ND    | ND    | 140204  | ND   | ND    | ND    | ND    |
| Esters    |                  |                                     |             |      |       |       |       |      |       |       |       |
| 5.30      | 239.0847         | Tetrahydropyran Z-10-dodecenoate    | C₁₀H₇O₃     | ND   | ND    | ND    | 3652891 | ND   | ND    | ND    | ND    |
| 5.43      | 161.9902         | 1,2-Ethanediol, dipropanoate        | C₇H₁₄O₄     | ND   | ND    | ND    | 4801138 | ND   | ND    | ND    | ND    | (continued on next page)
| Rt (mins) | Observed ion m/z | Name                                                                 | MF         | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|----------------------------------------------------------------------|------------|------|-------|-------|-------|------|-------|-------|-------|
| 9.09     | 210.0302         | 2-t-Butyl-cyclopropene-2-carboxylic acid, 2,6-di-t-butyl-4-methyl-phenyl ester | C_{23}H_{30}O_{2} | ND   | ND    | ND    | ND    | ND   | ND    | ND    | ND    |
| 12.83    | 173.1176         | Butyric acid, thio-, S-hexyl ester                                   | C_{10}H_{20}OS | ND   | ND    | 386699 | ND    | ND    | ND    | ND    | ND    |
| 12.84    | 178.0599         | Diethyl Phthalate                                                    | C_{12}H_{16}O_{4} | 364436 | 519366 | 766294 | 848101 | ND   | ND    | 426673 | 303655 |
| 13.71    | 226.1560         | Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester              | C_{13}H_{22}O_{3} | ND   | ND    | 330280 | ND    | ND    | ND    | ND    | ND    |
| 16.44    | 224.1005         | 1,2-Benzene dicarboxylic acid, bis(2-methylpropyl) ester            | C_{16}H_{22}O_{4} | ND   | ND    | 2147598 | 1318726 | ND   | ND    | ND    | ND    |
| 16.96    | 227.0695         | Phthalic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester                 | C_{22}H_{18}O_{4} | ND   | ND    | 213001 | ND    | ND    | ND    | ND    | ND    |
| 17.26    | 292.2034         | Benzenepropanoic acid, 3,5-bis(1,1-dimethyl-4-hydroxy-, methyl ester | C_{18}H_{26}O_{3} | ND   | ND    | 120184 | 154149 | 67957 | ND    | 137645 | 149942 |
| 17.41    | 243.2109         | Palmitic acid vinyl ester                                           | C_{16}H_{34}O_{2} | ND   | 804464 | 775420 | 651709 | ND   | ND    | ND    | ND    |
| 17.48    | 278.1511         | Phthalic acid, hex-2-yn-4-yl nonyl ester                            | C_{22}H_{22}O_{4} | ND   | ND    | 8078090 | ND    | ND    | ND    | ND    | ND    |
| 17.48    | 279.1548         | Phthalic acid, 8-chloro octyl heptyl ester                          | C_{22}H_{26}ClO_{4} | ND   | ND    | 5363168 | ND    | ND    | ND    | ND    | ND    |
| 17.48    | 223.0967         | Diethyl phthalate                                                   | C_{6}H_{12}O_{4}  | 2222962 | 157059 | 2315416 | ND    | ND    | ND    | ND    | 4389732 |
| 18.54    | 177.9567         | Hexanoic acid, 2-ethyl-, vinyl ester                                | C_{16}H_{10}O_{2} | 197316 | ND    | ND    | ND    | ND    | ND    | ND    | ND    |
| 19.41    | 214.0798         | 1-Propene-1,2,3-tricarboxylic acid, tributyl ester                  | C_{18}H_{18}O_{6} | 129008 | 141974 | 385389 | ND    | ND    | ND    | ND    | ND    |
| 20.32    | 330.1635         | 1,2,3-Propanetricarboxylic acid, 2-(acetyl oxy)-, tributyl ester    | C_{20}H_{34}O_{8} | 1055443 | 482794 | 903051 | 95014 | 800796 | 742288 | 1494626 | 1524229 |
| 20.52    | 219.0957         | Octanoic acid, 2-dimethylaminoethyl ester                          | C_{12}H_{22}NO_{2} | ND   | ND    | ND    | 1115602 | ND   | ND    | ND    | ND    |
| 21.98    | 197.1527         | Carbonic acid, 2-dimethylaminoethyl 2-methoxyethyl ester            | C_{6}H_{17}NO_{4} | ND   | ND    | 17984410 | 3536432 | 1095483 | ND    | 17481691 | 21767625 |
| 22.16    | 185.0817         | Carbonic acid, 2-dimethylaminoethyl isobutyl ester                 | C_{18}H_{19}NO_{3} | 571722 | 1548371 | 3164765 | 274955 | ND    | ND    | 3164986 | 290625 |
| 22.70    | 339.0385         | Bis(2-ethylhexyl) phthalate                                        | C_{24}H_{36}O_{4} | ND   | ND    | 3584849 | ND    | ND    | ND    | ND    | ND    |
| 22.70    | 386.9516         | Diisooctyl phthalate                                                | C_{24}H_{38}O_{4} | 1983617 | ND    | ND    | ND    | ND    | ND    | ND    | ND    |
| 22.70    | 326.9852         | Dicyclohexyl phthalate                                             | C_{26}H_{36}O_{4} | 1790400 | 1212827 | 1113310 | ND    | ND    | ND    | ND    | ND    |
| 22.71    | 358.0683         | Phthalic acid, di(hept-2-yl) ester                                 | C_{22}H_{24}O_{4} | ND   | ND    | 1263691 | ND    | ND    | ND    | ND    | ND    |
| 24.21    | 287.9999         | Terephthalic acid, di(4-octyl) ester                                | C_{24}H_{34}O_{4} | ND   | ND    | 85444 | ND    | ND    | ND    | ND    | ND    |
| 25.04    | 173.0630         | cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(phenethyl) ester        | C_{24}H_{28}O_{4} | ND   | ND    | 305523 | ND    | ND    | ND    | ND    | ND    |

(continued on next page)
| Rt (mins) | Observed ion m/z | Name                                                                 | MF                | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|----------------------------------------------------------------------|-------------------|------|-------|-------|-------|------|-------|-------|-------|
| 28.87    | 426.3870         | Urs-12-en-24-oic acid, 3-oxo-, methyl ester, (+)-                   | C_{31}H_{48}O_{3} | ND   | ND    | ND    | 209859| ND   | ND    | ND    | ND    |
| 30.05    | 530.4690         | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester | C_{35}H_{62}O_{3} | 123534| ND    | ND    | 67852 | 1106099| 3286798| ND    | ND    |

**FAEE**

| Rt (mins) | Observed ion m/z | Name                                                                 | MF                | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|----------------------------------------------------------------------|-------------------|------|-------|-------|-------|------|-------|-------|-------|
| 22.44    | 312.2648         | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester           | C_{19}H_{38}O_{4} | ND   | ND    | 8701469| 11891657| ND   | ND    | ND    | ND    |

**FAMEs**

| Rt (mins) | Observed ion m/z | Name                                                                 | MF                | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|----------------------------------------------------------------------|-------------------|------|-------|-------|-------|------|-------|-------|-------|
| 17.02    | 270.2556         | Hexadecanoic acid, methyl ester                                      | C_{17}H_{34}O_{2} | ND   | 13693362| 35747181| 33880749| 18186155| 4686779| 35059912| 54595941|
| 17.02    | 270.2552         | Pentadecanoic acid, 14-methyl-, methyl ester                         | C_{17}H_{34}O_{2} | ND   | ND    | ND    | ND    | ND   | ND    | ND    | ND    |
| 18.79    | 266.2227         | 9,12-Hexadecadienoic acid, methyl ester                             | C_{17}H_{36}O_{2} | ND   | ND    | ND    | ND    | ND   | ND    | ND    | ND    |
| 18.79    | 294.2544         | 9,12-Octadecadienoic acid, methyl ester                             | C_{19}H_{38}O_{2} | ND   | ND    | ND    | ND    | ND   | ND    | ND    | ND    |
| 18.82    | 296.2714         | trans-13-Octadecenoic acid, methyl ester                            | C_{19}H_{38}O_{2} | 3255171| ND    | ND    | 1152194| 2341413| ND   | ND    | ND    | ND    |
| 19.05    | 298.2860         | Methyl stearate                                                     | C_{19}H_{38}O_{2} | ND   | 4471317| 17709835| 5259746| 3046077| 14396244| ND    | ND    |
| 20.85    | 227.2010         | Tridecanoic acid, methyl ester                                      | C_{13}H_{28}O_{2} | 1025025| 713908| 1152194| 2341413| ND   | ND    | ND    | ND    |
| 20.86    | 200.1731         | Undecanoic acid, methyl ester                                       | C_{11}H_{22}O_{2} | ND   | ND    | ND    | 697166| ND   | ND    | ND    | ND    |
| 22.50    | 356.3561         | Hexacosanoic acid, methyl ester                                     | C_{24}H_{40}O_{2} | ND   | ND    | ND    | 5563687| ND   | ND    | ND    | ND    |
| 25.01    | 282.2511         | Oxalic, di(1-menthyl) ester                                         | C_{10}H_{16}O_{2} | ND   | ND    | ND    | 943438 | ND   | ND    | ND    | ND    |

**Ketones**

| Rt (mins) | Observed ion m/z | Name                                                                 | MF                | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|----------|------------------|----------------------------------------------------------------------|-------------------|------|-------|-------|-------|------|-------|-------|-------|
| 3.25     | 108.0683         | Imidazo[4,5-d]imidazole, 1,6-dihydro-1,2-Cyclopentanedione            | C_{4}H_{4}N_{4} | ND   | ND    | ND    | 17682 | ND   | ND    | ND    | ND    |
| 3.41     | 98.0364          | 7-Chloro-1,3,4,10-tetrahydro-10-hydroxy-1-[2-[1-pyrrolidinyl]ethyl]imin]-3-[3-(trifluoromethyl)phenyl]-9(2H)-acridinone | C_{14}H_{10}O_{2} | ND   | ND    | ND    | 1169975| 2802233| ND    | ND    | ND    |
| 3.68     | 375.9799         | Imidazo[4,5-d]imidazole, 1,6-dihydro-1,2-Cyclopentanedione            | C_{14}H_{10}O_{2} | ND   | ND    | ND    | 1169975| 2802233| ND    | ND    | ND    |

(continued on next page)
| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|-----------|------------------|------|----|------|------|------|------|------|------|------|------|
| 3.94      | 191.0011         | 1-Pentanone, 1-(2-thienyl)-   | C₄H₁₂OS | ND   | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 5.40      | 85.0523          | 2-Pyrrolidinone               | C₄H₈N    | ND   | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 8.34      | 150.0676         | Ethanone, 1-(2-hydroxy-5-methylphenyl)- | C₄H₁₀O₂ | ND   | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 10.95     | 170.0398         | Ethanone, 1-[4-[1-hydroxy-1-methylthyl]phenyl]- | C₁₁H₴O₂ | ND   | ND   | 1021014 | 582086 | ND   | ND   | 325492 | ND   |
| 12.41     | 180.0781         | 2′,4′-Dimethoxyacetophenone   | C₈H₁₂O₃ | ND   | ND   | 1613696 | ND   | ND   | ND   | ND   | ND   |
| 12.41     | 180.0781         | Ethanone, 1-(3,4-dimethoxyphenyl)- | C₁₀H₁₃O₃ | ND   | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 13.00     | 189.1515         | 2-Butanone, 4-(2,3-dihydro-1H-indol-1-yl)- | C₁₁H₁₄O₂ | 85005 | 53880 | ND   | ND   | ND   | ND   | ND   | ND   |
| 13.44     | 182.0727         | Benzenophenone                | C₁₃H₁₀O   | ND   | ND   | ND   | 282691 | ND   | 138491 | 163689 | ND   |
| 14.34     | 188.1198         | Methanone, (1-hydroxycyclohexyl)phenyl- | C₁₃H₁₆O₂ | 386301 | 595229 | 885838 | 1073775 | ND   | 415036 | 347436 | 788474 | 584284 |
| 16.63     | 269.0482         | 2-Morpholin-4-ylmethyl-5-phenoxymethyl-4-phenyl-2,4-dihydro-[1,2,4]triazole-3-thione | C₁₂H₁₅NO | 133625 | ND   | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 17.05     | 262.1520         | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | C₁₇H₂₄O₃ | 165132 | 292457 | 202831 | ND   | ND   | ND   | ND   | ND   | ND   |
| 24.44     | 158.0821         | 2-Octen-4-one, 2-methoxy- | C₉H₁₆O₂ | ND   | ND   | 236995 | ND   | ND   | ND   | ND   | ND   |
| 28.80     | 410.3543         | 4,22-Stigmastadiene-3-one   | C₂₀H₄₀O | ND   | ND   | ND   | 533139 | ND   | ND   | ND   | ND   | ND   |

**Miscellaneous**

| 4.00      | 138.1040         | Furan, 2-pentyl-               | C₅H₁₄O   | 911826 | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 4.40      | 123.0680         | 4(H)-Pyridine, N-acetyl-       | C₇H₅NO   | ND   | ND   | ND   | 391733 | ND   | ND   | ND   | ND   |
| 5.53      | 120.0684         | 1,3,5,7-Tetraoxane            | C₄H₂₀O₄ | ND   | ND   | ND   | ND   | ND   | 99462₉₃₆ | ND   | ND   |
| 5.58      | 120.0683         | 3-Pyridinecarbonitrile, 1,4-dihydro-1-methyl- | C₇H₅N₂ | ND   | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 5.98      | 359.0650         | Cyclopentasiloxane, decamethyl- | C₁₀H₂₀O₅Si₅ | 2178743 | ND   | ND   | ND   | ND   | ND   | ND   | ND   |
| 6.88      | 143.0860         | 1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl- | C₆H₁₂O₄ | ND   | ND   | 4276079 | ND   | ND   | ND   | ND   | ND   |
| 8.30      | 431.0862         | Cyclohexasiloxane, dodecamethyl- | C₁₂H₁₆O₅Si₆ | 5186795 | 724478 | ND   | 9273629 | 192507 | 315644 | 778968 | ND   |

(continued on next page)
| Rt (mins) | Observed ion m/z | Name                                                                 | MF                          | Flour          | Starch          |
|----------|------------------|----------------------------------------------------------------------|-----------------------------|----------------|-----------------|
| 11.06    | 504.1074         | 3-Isoproxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane | C_{18}H_{22}O_{12}Si_{7}   | ND             | ND              |
| 11.07    | 504.1062         | 3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane | C_{19}H_{34}O_{12}Si_{7}   | 432330         | ND              |
| 11.35    | 186.0257         | Tetraglyme                                                            | C_{10}H_{22}O_{5}           | ND             | ND              |
| 12.35    | 219.1747         | (4S,5S)-(+)5-Amino-2,2-dimethyl-4-phenyl-1,3-dioxane                  | C_{12}H_{17}NO_{2}          | ND             | ND              |
| 11.93    | 183.0446         | 6-Hepteno-2-one, 5,7,7-trichloro-                                      | C_{19}H_{42}O_{7}Si_{7}     | ND             | ND              |
| 12.72    | 157.0885         | 3-Methyl-4-phenyl-1H-pyrrole                                          | C_{11}H_{11}N               | ND             | ND              |
| 13.35    | 179.0680         | Thiazolo[3,2-a]pyridinium, 8-hydroxy-2,5-dimethyl-                     | C_{9}H_{9}NOS               | ND             | ND              |
| 13.81    | 416.0373         | Cyclooctasiloxane, hexadecamethyl-                                     | C_{16}H_{40}O_{8}Si_{8}     | ND             | ND              |
| 14.57    | 168.0782         | Thiophene, 2-buty1-5-ethyl-                                            | C_{10}H_{18}S               | ND             | ND              |
| 15.88    | 433.0855         | 1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane          | C_{15}H_{40}O_{5}Si_{6}     | ND             | ND              |
| 17.36    | 154.0738         | Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-         | C_{11}H_{18}N_{2}O_{2}      | ND             | ND              |
| 17.58    | 533.9922         | Octasiloxane, 1,1,3,3,5,5,7,7,9,11,11,13,13,15,15-hexadecamethyl-      | C_{16}H_{30}O_{8}Si_{8}     | ND             | ND              |
| 18.85    | 145.1009         | Cyclopropene, 1-ethenyl-2-hexenyl-[1a,2ß(E)](-)-                       | C_{11}H_{18}                  | ND             | ND              |
| 19.23    | 201.1132         | 2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane, 1-ethenyl-            | C_{8}H_{15}NO_{3}Si          | ND             | ND              |
| 21.13    | 220.2181         | 4,8,12,16-Tetramethylenptadecan-4-olide                               | C_{21}H_{40}O_{2}           | ND             | ND              |
| 21.14    | 167.1431         | 2H-Pyran-2-one, tetrahydro-6-pentyl-Indoline, 2-(hydroxydipheny1methyl)- | C_{16}H_{18}O_{2}           | ND             | ND              |
| 22.19    | 267.2684         | 2-Octen-4-one, 2-methoxy-                                             | C_{16}H_{16}O_{2}           | ND             | ND              |
| 24.45    | 156.9946         | Heptasiloxane, hexadecamethyl-                                        | C_{16}H_{40}O_{6}Si_{7}     | 3291323        | ND              |
| 25.69    | 532.9916         |                                                                      |                             |                |                 |

(continued on next page)
| Rt (mins) | Observed ion m/z | Name | MF | 0GBF | 24GBF | 48GBF | 72GBF | 0GBS | 24GBS | 48GBS | 72GBS |
|-----------|-----------------|------|----|------|-------|-------|-------|------|-------|-------|-------|
| 25.79     | 309.2793        | Propanedinitrile, 2-(1-methyl-2,6-di phenyl-1H-pyrindilidene)-1'-Oxocannabinol | C$_{31}$H$_{35}$N$_{3}$ | ND    | ND    | 47194 | ND    | ND    | ND    | ND    | ND    |
| 25.80     | 310.2833        | Stigmastan-6,22-dien, 3,5-dedihydro-| C$_{28}$H$_{46}$ | ND    | ND    | ND    | ND    | ND    | ND    | ND    | ND    |
| 27.89     | 394.3603        | Pyidine, 3-phenyl- | C$_{11}$H$_{14}$N | ND    | ND    | ND    | 150868 | ND    | ND    | ND    | ND    |
| 28.21     | 155.0859        | Methylenbis(2,4,6-trisopropylphenolphosphine) | C$_{31}$H$_{50}$P$_{2}$ | ND    | 94708 | ND    | ND    | ND    | ND    | ND    | ND    |
| 28.79     | 453.0684        | Methyl 38-hydroxyolean-18-en-28-oate | C$_{31}$H$_{50}$O$_{3}$ | ND    | ND    | 696769 | ND    | ND    | ND    | ND    | ND    |

**Phenolic compounds**

| 8.83      | 154.0625        | Phenol, 2,6-dimethoxy- | C$_{6}$H$_{10}$O$_{3}$ | ND    | ND    | ND    | 288311 | ND    | ND    | ND    | ND    |
| 9.57      | 164.1196        | Phenol, 4-(1,1-dimethylpropyl)- | C$_{11}$H$_{20}$O | ND    | ND    | 332332 | ND    | ND    | ND    | ND    |
| 11.48     | 220.1823        | Butylated Hydroxytoluene | C$_{10}$H$_{24}$O | 95604 | ND    | ND    | ND    | ND    | ND    | ND    |
| 11.49     | 206.1665        | 2,4-Di-tert-butylphenol | C$_{14}$H$_{22}$O | ND    | 167604 | ND    | 78267  | ND    | ND    | ND    |
| 14.12     | 234.1980        | Phenol, 2,4-bis(1,1-dimethylpropyl)- | C$_{16}$H$_{26}$O | ND    | ND    | 157473 | ND    | ND    | ND    | ND    |
| 21.74     | 340.2401        | Phenol, 2,2'-methylenebis[6-(1,1-dimethylhexyl)4-methyl- | C$_{23}$H$_{32}$O$_{2}$ | 69972 | 1728704 | ND    | ND    | ND    | ND    | ND    |
| 28.79     | 646.4521        | Phenol, 2,4-bis[1,1-dimethylhexyl]-phosphite (3:1) | C$_{42}$H$_{60}$O$_{3}$P | 216841 | ND    | ND    | ND    | ND    | ND    | ND    | ND    |

**Phytosterols**

| 27.69     | 400.3700        | Campesterol | C$_{26}$H$_{48}$O | ND    | ND    | 265916 | ND    | ND    | ND    | ND    |
| 27.89     | 412.3710        | Stig masterol | C$_{26}$H$_{48}$O | 753259 | 603033 | 1163792 | ND    | ND    | ND    | 1771221 |
| 28.27     | 414.3861        | β-Sitosterol | C$_{26}$H$_{48}$O | ND    | 345695 | ND    | ND    | ND    | ND    | ND    |
| 28.57     | 409.3783        | β-Am yrin | C$_{10}$H$_{50}$O | ND    | 283324 | ND    | ND    | ND    | ND    | ND    |

**Terpene and Terpenoid**

| 13.90     | 216.1511        | aR-Turmerone | C$_{10}$H$_{20}$O | ND    | ND    | 577405 | ND    | ND    | ND    | ND    |
| 24.78     | 231.2116        | Supraene | C$_{10}$H$_{50}$O | ND    | ND    | 1139640 | ND    | ND    | ND    | ND    |

**Vitamin**

| 25.67     | 402.3495        | d-Tocopherol | C$_{27}$H$_{46}$O$_{2}$ | ND    | ND    | 4693356 | 1276396 | ND    | ND    | 7647813 |

MF: Molecular formula; FAEE: Fatty acid ethyl ester; FAME: Fatty acid methyl ester; 0GBF: Flour from Bambara groundnut germinated for 0 h; 24GBF: Flour from Bambara groundnut germinated for 24 h; 48GBF: Flour from Bambara groundnut germinated for 48 h; 72GBF: Flour from Bambara groundnut germinated for 72 h 0GBS: Starch from Bambara groundnut germinated for 0 h; 24GBS: Starch from Bambara groundnut germinated for 24 h; 48GBS: Starch from Bambara groundnut germinated for 48 h; 72GBS: Starch from Bambara groundnut germinated for 72 h.
2.3. Extraction of metabolites and GC-HRTOF-MS analysis

Two different mixtures of extraction solvents were used to extract GBF and GBS at the different germination times. The first solvent mixture was methanol/water at 80:20 v/v while the second mixture was acetonitrile/methanol/water at 40:40:20 v/v/v. Extraction of metabolites followed the method previously described by Kewuyemi et al. [3]. Briefly, one gram each of the samples (flour and starch), at the different germination times was weighed into 50 mL centrifuge tubes. Then, 10 mL of each extraction solvent was added, the mixture vortexed vigorously to achieve thorough and even mixing. Thereafter, samples were sonicated (Scientech 704, Labotech, South Africa) for 1 h, centrifuged at 3500 rpm for 5 min at 4 °C (Eppendorf 5702R, Merck South Africa). Supernatants from centrifuge tubes where then taken into fresh tubes and concentrated in a vacuum concentrator (Eppendorf Plus, Merck South Africa). Dried extracts were then reconstituted in 1 mL chromatography-grade methanol, vortexed to ensure even dissolution of extracts and filtered through 0.22 μm microfilters into dark amber vials for GC-HRTOF-MS analyses. Extraction was carried out in triplicate in each case.

Reconstituted extracts were analysed on the GC-HRTOF-MS system (LECO Corporation, St. Josheph, MI, USA), having a resolution of 50,000 FWMH (full peak width at one half maximum), with mass accuracies/errors of < 1 ppm and acquisition rates of up to 200 spectra/s. The system is equipped with a multipurpose sampler (Gerstel Inc., Mülheim an der Ruhr Germany) and Rx®-5 ms column (30 m × 0.25 mm ID × 0.25 μm) (Restek, Bellefonte, USA). From the three replicates of each sample, 1 μL of extracts were injected in a spitless mode and pumped at a constant flow rate of 1 mL/min, with helium as the carrier gas. Inlet and transfer line temperature were set at 250 and 225 °C, respectively and the ion source temperature was at 250 °C. The oven temperature cycle used was: initial temperature of 70 °C for 0.5 min; then an increase of 10 °C/min to 150 °C held for 2 min; then ramped at 10 °C/min to 330 °C and held for 3 min for the column to ‘bake-out’. Experiments for solvent blanks were also carried out to observe possible impurities and contamination. To identify metabolites, spectra were matched with NIST1, Mainlib2 and Flehn3 reference library databases, and their identities determined. To process raw data, parameters such as signal to noise ratio of 100, similarity match of above 70% and the occurrence of metabolites at least two times out of the triplicate data were strictly adopted [4]. Therefore, data obtained and reported in Tables 1 and 2 represent the mean of values obtained from triplicate runs of samples after prior processing of raw data.

Ethics Statement

The authors have no competing financial interests or personal relationships that may have influenced the data reported in this work

CRediT Author Statement

Ajibola Bamikole Oyedeji: Sample preparation, Formal data analysis, Methodology, Visualization, Validation, Writing – original draft; Chiemela Enyinaya Chinma: Conceptualization, Project administration, Writing – review & editing; Ezekiel Green: Funding acquisition, Resources, Writing – review & editing; Oluwafemi Ayodeji Adebo: Funding acquisition, Data curation, Methodology, Formal analyses, Project administration, Resources, Software, Validation, Writing – review & editing.

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2 https://www.mainlib.org/
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Declaration of Competing Interest

None.

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