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



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# ABSTRACT

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  $\pm$ 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 (80:20v/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 FWMH (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 atosampler (Gerstel Inc., Mülheim an der Ruhr, Germany) and a Rxi <sup>®</sup> -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	
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 $\mu$ m syringe filters. For sample analyses in GC-HRTOF-MS machine, 1 $\mu$ L of samples were auto-injected into the system and metabolite identities were determined using NIST, Mainlib and Feihn 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

# 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 brokens 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  $28 \pm 1^{\circ}$ C for 6 h prior to germination. Hydrated seeds were germinated at  $28 \pm 1^{\circ}$ 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  $\mu$ m 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  $\times$  g for 20 min at 25°C, neutralized with 0.1N HCI and the resulting germinated Bambara starch (GBS) was freeze dried (LGJ-18, SHKY, China) at a set temperature ( $-40^{\circ}$ 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.

					l	Flour		Starch				
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS	
Alcohol												
6.83	87.0439	Glycerol	$C_3H_8O_3$	ND	ND	ND	307634	ND	ND	ND	ND	
Amides												
19.12	154.1225	Dodecanamide, N-(2-hydroxyethyl)-	C <sub>14</sub> H <sub>29</sub> NO <sub>2</sub>	ND	ND	ND	246097	ND	ND	ND	ND	
19.80	212.2011	Dodecanamide	$C_{12}H_{25}NO$	ND	ND	229538	ND	ND	ND	272443	ND	
20.32	161.0963	3-Cyclopentylpropionamide, N,N-dimethyl-	C <sub>10</sub> H <sub>19</sub> NO	ND	ND	356253	ND	ND	ND	ND	ND	
21.27	140.1075	Nonanamide	C <sub>9</sub> H <sub>19</sub> NO	ND	ND	ND	356772	ND	ND	ND	ND	
21.84	100.0326	Bis(2-(Dimethylamino)ethyl) ether	$C_8H_{20}N_2O$	362197	ND	3373070	ND	ND	ND	6968863	192558	
22.80	126.0910	Hexadecanamide	C <sub>16</sub> H <sub>33</sub> NO	112958	ND	347814	ND	ND	281784	ND	169801	
22.81	140.1067	Benzeneethanamine	$C_{11}H_{16}FNO_3$	ND	ND	161840	212288	1184386	148731	207178	201073	
24.34	294.2779	9-Octadecenamide, (Z)-	C <sub>18</sub> H <sub>35</sub> NO	1354600	ND	2055194	4063967	ND	3053636	2938830	319728	
Cyclic co	mpounds											
18.75	108.0932	E,Z-3-Ethylidenecyclohexene	C <sub>8</sub> H <sub>12</sub>		ND	687948	ND	ND	ND	ND	ND	
22.28	227.0701	Benzenehexanenitrile	C <sub>14</sub> H <sub>17</sub> NO	191620	ND	ND	ND	ND	ND	ND	ND	
24.17	279.2317	Benzene, 2-methoxy-1-(2-nitroethenyl)- 3-(phenylmethoxy)-	C <sub>16</sub> H <sub>15</sub> NO <sub>4</sub>	ND	ND	ND	657003	ND	ND	ND	ND	
Esters												
12.73	177.0547	Diethyl Phthalate	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	ND	ND	102107	ND	ND	ND	ND	ND	
16.32	223.0961	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	$C_{16}H_{22}O_4$	ND	ND	296119	ND	ND	ND	ND	ND	
16.32	223.0960	1,2-Benzenedicarboxylic acid, butyl octyl ester	$C_{20}H_{30}O_4$	ND	ND	449868	ND	ND	ND	ND	ND	
16.33	223.0959	Phthalic acid, butyl oct-3-yl ester	$C_{20}H_{30}O_4$	ND	ND	130139	ND	ND	ND	ND	ND	
17.36	224.0995	Dibutyl phthalate	$C_{16}H_{22}O_4$	ND	ND	1365627	280866	302235	170104	830621	ND	
17.38	150.0265	1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl ester	$C_{20}H_{30}O_4$	158769	ND	ND	129430	ND	ND	ND	ND	

# Table 1 (continued)

					F	lour			5	Starch	
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	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 <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	ND	ND	5252360	8018935	ND	ND	ND	ND
19.19	174.0936	2,2',2''-Nitrilotriethanol, triethyl ether	C <sub>12</sub> H <sub>27</sub> NO <sub>3</sub>	ND	ND	ND	662787	ND	ND	ND	ND
19.33	213.0752	1-Propene-1,2,3-tricarboxylic acid	C <sub>18</sub> H <sub>30</sub> O <sub>6</sub>	ND	ND	107599	107436	ND	ND	ND	ND
20.20	273.0963	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester	$C_{20}H_{34}O_8$	249357	ND	280433	ND	222530	242690	764578	260777
20.38	144.1019	Carbonic acid, 2-dimethylaminoethyl isobutyl ester	$C_9H_{19}NO_3$	348980	ND	698929	ND	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	ND
21.85	152.1196	Carbonic acid, 2-dimethylaminoethyl 2-methoxyethyl ester	$C_8H_{17}NO_4$	331038	ND	ND	ND	ND	ND	ND	ND
21.91	144.1017	Carbonic acid, 2-dimethylaminoethyl ethyl ester	C <sub>7</sub> H <sub>15</sub> NO <sub>3</sub>	ND	ND	ND	5008868	ND	ND	ND	ND
22.57	280.1631	Bis(2-ethylhexyl) phthalate	$C_{24}H_{38}O_4$	ND	1000108	ND	ND	668139	ND	ND	ND
22.58	280.0729	Dicyclohexyl phthalate	$C_{20}H_{26}O_4$	ND	495234	ND	ND	ND	ND	ND	ND
22.62	279.1580	1,2-Benzenedicarboxylic acid, monononyl ester	$C_{17}H_{24}O_4$	ND	ND	368535	ND	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	C22H38O4	ND	ND	ND	592440	ND	ND	ND	ND
29.87	530.4706	Benzenepropanoic acid, 3,5-bis(1,1- dimethylethyl)-4-hydroxy-, octadecyl ester	$C_{35}H_{62}O_3$	120035	288311	ND	ND	ND	ND	ND	ND
FAEEs											
17.61	241.2157	Dodecanoic acid, ethyl ester	$C_{14}H_{28}O_2$	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	$C_{19}H_{38}O_4$	ND	ND	1415101	ND	ND	ND	4688360	2053117

Table 1 (continued)

					Fl	our		Starch				
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS	
23.74	336.2648	9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl) ethyl ester	$C_{21}H_{38}O_4$	ND	ND	7924939	4287462	ND	ND	ND	ND	
FAMEs												
16.90	228.2038	Tridecanoic acid, methyl ester	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	4940778	ND	ND	ND	ND	330722	ND	850485	
16.91	270.2551	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	ND	ND	10471598	ND	ND	ND	11366836	8939116	
18.65	263.2357	9,12-Octadecadienoic acid, methyl ester, (E,E)-	$C_{19}H_{34}O_2$	ND	865286	ND	0	ND	ND	ND	4237592	
18.70	266.2553	9-Octadecenoic acid (Z)-, methyl ester	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>	855686	ND	ND	ND	707676	672492	ND	ND	
18.73	296.2698	trans-13-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	ND	ND	ND	1905757	ND	ND	ND	ND	
18.74	296.2695	cis-13-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	ND	ND	1552481	3409153	ND	ND	ND	ND	
18.93	269.2469	Pentadecanoic acid, 14-methyl-, methyl ester	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	2293504	1557834		4952772	3290367	2076691	ND	ND	
18.95	298.2859	Methyl stearate	$C_{19}H_{38}O_2$	ND	ND	ND	2882498	ND	ND	ND	ND	
20.50	144.1017	Octanoic acid, 2-dimethylaminoethyl ester	$C_{12}H_{25}NO_2$	ND	ND	2401346	1009866	ND	ND	ND	ND	
22.41	354.3488	Hexacosanoic acid, methyl ester	$C_{27}H_{54}O_2$	ND	ND	1270191	ND	ND	ND	ND	ND	
Furan												
12.69	111.1168	Furan, 2-butyltetrahydro-	C <sub>8</sub> H <sub>16</sub> O	ND	ND	301109	ND	ND	ND	ND	ND	
Ketones												
14.21	105.0335	Methanone, (1-hydroxycyclohexyl)phenyl-	$C_{13}H_{16}O_2$	ND	101939	164821	187249	149732	146197	159302	ND	
16.91	232.1823	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca- 6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	ND	ND	32318	ND	ND	ND	ND	ND	
Miscellan	eous											
3.98	60.0208	2H-1,2-Oxazine, 6-(4- chlorophenyl)tetrahydro-2-methyl-	$C_{11}H_{14}C_1NO$	ND	1400596	ND	ND	ND	ND	ND	ND	
13.67	501.9715	Cyclooctasiloxane, hexadecamethyl-	C <sub>16</sub> H <sub>48</sub> O <sub>8</sub> Si <sub>8</sub>	ND	3282594	2169153	ND	ND	ND	ND	ND	
										( t	on novt nago	

Table 1	(continued	)
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					Fl	lour			St	arch	
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	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-	$C_{16}H_{50}O_7Si_8$	ND	2779445	2701270	ND	ND	1915391	928470	ND
17.46	533.9926	3-Isopropoxy-1,1,1,7,7,7-hexamethyl- 3,5,5- tris(trimethylsiloxy)tetrasiloxane	C <sub>18</sub> H <sub>52</sub> O <sub>7</sub> Si <sub>7</sub>	ND	ND	ND	ND	ND	2360859	ND	ND
18.65	219.9887	1,8,11-Heptadecatriene, (Z,Z)-	C <sub>17</sub> H <sub>30</sub>	ND	ND	ND	ND	482944	ND	ND	ND
19.07	210.2212	2,8,9-Trioxa-5-aza-1- silabicyclo(3.3.3)undecane, 1-methoxy-	C <sub>7</sub> H <sub>15</sub> NO <sub>4</sub> Si	667023	770836	ND	ND	854367	ND	ND	ND
20.27	434.0867	1,1,1,5,7,7,7-Heptamethyl-3,3- bis(trimethylsiloxy)tetrasiloxane	$C_{13}H_{40}O_5Si_6$	ND	2660774	3284057	ND	ND	ND	ND	ND
22.07	372.2636	3-Methylbutyl N-heptafluorobutyryltryptophanate	$C_{20}H_{21}F_7N_2O_3$	ND	ND	ND	ND	ND	ND	739228	ND
22.23	313.2550	1H-Indene, 1-hexadecyl-2,3-dihydro-	$C_{25}H_{42}$	ND	ND	ND	1193482	ND	ND	ND	ND
25.56	532.9929	Heptasiloxane, hexadecamethyl-	$C_{16}H_{48}O_6Si_7$	ND	1998765	887750	ND	ND	1698458	ND	ND
Phenols											
11.32	206.1663	2,4-Di-tert-butylphenol	C <sub>14</sub> H <sub>22</sub> O	417837	626608	707602	563806	580774	579501	651064	279502
21.61	340.2389	Phenol, 2,2'-methylenebis[6-(1,1- dimethylethyl)-4-methyl-	$C_{23}H_{32}O_2$	624987	ND	ND	ND	701221	909547	1306974	ND
22.07	161.0948	(Z)-3-(Heptadec-10-en-1-yl)phenol	$C_{23}H_{38}O$	ND	ND	ND	167128	ND	ND	ND	ND
Phytostero	ols										
27.75	412,3692	Stigmasterol	C <sub>29</sub> H <sub>48</sub> O	ND	ND	390128	ND	ND	ND	482973	439076
28.13	414.3854	ß-Sitosterol	C <sub>29</sub> H <sub>50</sub> O	230841	209691	ND	ND	ND	ND	ND	ND
Terpene a	nd Terpenoid										
24.62	340.0400	Squalene	C <sub>30</sub> H <sub>50</sub>	ND	395205	ND	ND	ND	ND	ND	ND
24.62	430.0896	Supraene	C <sub>30</sub> H <sub>50</sub>	757222	ND	ND	ND	ND	ND	ND	ND
Vitamin											
25.54	402.3484	d-Tocopherol	$C_{27}H_{46}O_2$	ND	ND	768559	1228631	ND	ND	745590	833629

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 24 h; 48GBS: Starch from Bambara groundnut germinated for 24 h; 72GBS: Starch from Bambara groundnut germinated for 24 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.

			Fl	our		Starch					
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS
Acids											
3.26	104.0293	Butanoic acid, 4-hydroxy-	C <sub>11</sub> H <sub>22</sub> O <sub>3</sub> Si	ND	ND	ND	1379146	ND	ND	ND	ND
4.06	102.0090	Pentanoic acid	$C_5H_{10}O_2$	ND	ND	ND	850250	ND	ND	1599442	420330
15.20	228.2077	Tetradecanoic acid	$C_{14}H_{28}O_2$	ND	ND	747974	3936087	ND	ND	ND	ND
17.51	256.2398	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	5839377	4563896	ND	ND	ND	6469462	ND	67444726
19.73	284.2714	Octadecanoic acid	$C_{18}H_{36}O_2$	ND	ND	13076604	14514438	ND	ND	ND	ND
Alcohols											
5.26	92.0213	Glycerol	$C_3H_8O_3$	ND	ND	83692530	27609	ND	ND	ND	ND
5.66	126.0311	Maltol	$C_6H_6O_3$	ND	ND	5053284	ND	ND	ND	ND	ND
26.65	394.3588	Cholesta-4,6-dien-3-ol, (3ß)-	$C_{27}H_{44}O$	218602	ND	ND	ND	ND	ND	ND	ND
Aldehyde											
4.73	120.0570	Benzeneacetaldehyde	C <sub>8</sub> H <sub>8</sub> O	ND	ND	559553	1873781	ND	ND	1278347	ND
Amide											
4.83	114.0312	Pentanamide	$C_{36}H_{49}N_5O_5$	ND	547511	ND	ND	ND	ND	ND	ND
19.21	262.2290	Octadecanamide, N-(2-hydroxyethyl)-	C <sub>20</sub> H <sub>41</sub> NO <sub>2</sub>	247931	ND	ND	ND	ND	ND	ND	ND
19.22	210.1848	Decanamide, N-(2-hydroxyethyl)-	$C_{12}H_{25}NO_2$	ND	ND	ND	1637175	ND	ND	ND	ND
19.74	221.3520	Tetradecanamide	C <sub>14</sub> H <sub>29</sub> NO	ND	ND	ND	864457	ND	ND	ND	ND
21.24	229.1615	Hexadecanamide	C <sub>16</sub> H <sub>33</sub> NO	189552	ND	ND	ND	137545	ND	ND	ND
24.48	281.2666	9-Octadecenamide, (Z)-	C <sub>18</sub> H <sub>35</sub> NO	ND	ND	18787957	4012093	8548604	11431519	18472989	18389329
21.97	139.0402	Bis(2-(Dimethylamino)ethyl) ether	$C_8H_{20}N_2O$	1042090	ND	ND	ND	854739	192863	ND	ND
22.90	187.1137	Benzeneethanamine, 2-fluoro-ß,3,4- trihydroxy-N-isopropyl-	C <sub>11</sub> H <sub>16</sub> FNO <sub>3</sub>	ND	208553	560386	194632		471782	571453	1262773
Cyclic co	mpound										
29.06	268.0389	Benzenehexanenitrile, ß,ß-dimethyl-e-oxo-	C <sub>14</sub> H <sub>17</sub> NO	ND	ND	ND	140204	ND	ND	ND	ND
Esters											
5.30	239.0847	Tetrahydropyran Z-10-dodecenoate	C <sub>17</sub> H <sub>30</sub> O <sub>3</sub>	ND	ND	ND	3652891	ND	ND	ND	ND
5.43	161.9902	1,2-Ethanediol, dipropanoate	$C_8H_{14}O_4$	ND	ND	4801138	ND	ND	ND	ND	ND

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# Table 2 (continued)

					Fl	our			St	arch	
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS
9.09	210.0302	2-t-Butyl-cyclopropanecarboxylic acid, 2,6-di-t-butyl-4-methyl-phenyl ester	$C_{23}H_{36}O_2$	ND	ND	ND	ND	ND	ND	ND	ND
12.83	173.1176	Butyric acid, thio-, S-hexyl ester	C <sub>10</sub> H <sub>20</sub> OS	ND	ND	ND	386699	ND	ND	ND	ND
12.84	178.0599	Diethyl Phthalate	$C_{12}H_{14}O_4$	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-Benzenedicarboxylic 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 nonyl ester	$C_{27}H_{38}O_4$	ND	ND	213001	ND	ND	ND	ND	ND
17.26	292.2034	Benzenepropanoic acid, 3,5-bis(1,1- dimethylethyl)-4-hydroxy-, methyl ester	$C_{18}H_{28}O_3$	ND	ND	120184	154149	67957	ND	137645	149942
17.41	243.2109	Palmitic acid vinyl ester	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	ND	804464	775420	651709	ND	ND	ND	ND
17.48	278.1511	Phthalic acid, hex-2-yn-4-yl nonyl ester	$C_{23}H_{32}O_4$	ND	ND	8078090	ND	ND	ND	ND	ND
17.48	279.1548	Phthalic acid, 8-chlorooctyl heptyl ester	C23H35ClO4	ND	ND	ND	5363168	ND	ND	ND	ND
17.48	223.0967	Dibutyl phthalate	$C_{16}H_{22}O_4$	2222962	ND	157059	2315416	ND	775155	ND	4389732
18.54	177.9567	Hexanoic acid, 2-ethyl-, vinyl ester	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	197316	ND	ND	ND	ND	ND	ND	ND
19.41	214.0798	1-Propene-1,2,3-tricarboxylic acid, tributyl ester	$C_{18}H_{30}O_{6}$	129008	141974	385389	ND	ND	ND	ND	ND
20.32	330.1635	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, 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	$C_{12}H_{25}NO_2$	ND	ND	ND	11156024	ND	ND	ND	ND
21.98	197.1527	Carbonic acid, 2-dimethylaminoethyl 2-methoxyethyl ester	$C_8H_{17}NO_4$	ND	ND	17984410	3536432	1095483	ND	17481691	21767625
22.16	185.0817	Carbonic acid, 2-dimethylaminoethyl isobutyl ester	$C_9H_{19}NO_3$	571722	1548371	3164765	274955	ND	ND	3164986	290625
22.70	339.0385	Bis(2-ethylhexyl) phthalate	C24H38O4	ND	3584849	ND	ND	ND	ND	ND	ND
22.70	386.9516	Diisooctyl phthalate	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	1983617	ND	ND	ND	ND	ND	ND	ND
22.70	326.9852	Dicyclohexyl phthalate	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	1790400	1212827	1113310	ND	ND	ND	ND	ND
22.71	358.0683	Phthalic acid, di(hept-2-yl) ester	C <sub>22</sub> H <sub>34</sub> O <sub>4</sub>	ND	ND	ND	1263691	ND	ND	ND	ND
24.21	287.9999	Terephthalic acid, di(4-octyl) ester	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	ND	ND	85444	ND	ND	ND	ND	ND
25.04	173.0630	cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(phenethyl) ester	$C_{24}H_{26}O_4$	ND	ND	ND	305523	ND	ND	ND	ND

9

					Fle	our			S	tarch	
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	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											
22.44	312.2648	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>	ND	ND	8701469	11891657	ND	ND	ND	ND
FAMEs											
17.02	270.2556	Hexadecanoic acid, methyl ester	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	ND	13693362		33880749	18186155	4686779	35059912	54595941
17.02	270.2552	Pentadecanoic acid, 14-methyl-, methyl ester	$C_{17}H_{34}O_2$	3359916	ND	ND		ND	ND	ND	17598151
18.79	266.2227	9,12-Hexadecadienoic acid, methyl ester	$C_{17}H_{30}O_2$	ND	ND	21933465			ND	ND	ND
18.79	294.2544	9,12-Octadecadienoic acid, methyl ester	$C_{19}H_{34}O_2$	ND	ND	ND	ND	3476598	2311803	12037261	ND
18.82	296.2714	trans-13-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	3255171	ND	11609839	14906235	ND	ND	ND	ND
19.05	298.2860	Methyl stearate	$C_{19}H_{38}O_2$	ND	4471317	17709835	ND	5259746	3046077	14396244	ND
20.85	227.2010	Tridecanoic acid, methyl ester	$C_{14}H_{28}O_2$	1025025	713908	1152194	2341413	ND	ND	ND	ND
20.86	200.1731	Undecanoic acid, methyl ester	$C_{12}H_{24}O_2$	ND	ND	ND	6971616	ND	ND	ND	ND
22.50	356.3561	Hexacosanoic acid, methyl ester	C <sub>27</sub> H <sub>54</sub> O <sub>2</sub>	ND	ND	ND	5563687	ND	ND	ND	ND
25.01	282.2511	Oxalic acid, di(1-menthyl) ester	$C_{22}H_{38}O_4$	ND	ND	ND	943438	ND	ND	ND	ND
Ketones											
3.25	108.0683	Imidazo[4,5-d]imidazole, 1,6-dihydro-	C <sub>4</sub> H <sub>4</sub> N <sub>4</sub>	ND	ND	ND	117682	ND	ND	ND	ND
3.41	98.0364	1,2-Cyclopentanedione	$C_5H_6O_2$	ND	ND	ND	ND	ND	ND	ND	ND
3.68	375.9799	7-Chloro-1,3,4,10-tetrahydro-10-		ND	ND	1169975	2802233	ND	ND	ND	ND
		hydroxy-1-[[2-[1- pyrrolidinyl]ethyl]imino]-3-[3- (trifluoromethyl)phenyl]-9(2H)- acridinone	C <sub>26</sub> H <sub>25</sub> ClF <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	2							
										(continued)	on novt na

# Table 2 (continued)

					F	lour			5	Starch	
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS
3.94	191.0011	1-Pentanone, 1-(2-thienyl)-	C <sub>9</sub> H <sub>12</sub> OS	ND	ND	ND	ND	ND	ND	ND	ND
5.40	85.0523	2-Pyrrolidinone	C <sub>9</sub> H <sub>9</sub> N	ND	662123	ND	ND	ND	ND	ND	ND
8.34	150.0676	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	$C_9H_{10}O_2$	ND	ND	ND	1075885	ND	ND	799466	ND
10.95	170.0398	Ethanone, 1-[4-(1-hydroxy-1- methylethyl)phenyl]-	$C_{11}H_{14}O_2$	ND	ND	1021014	582086	ND	ND	325492	ND
12.41	180.0781	2',4'-Dimethoxyacetophenone	$C_{10}H_{12}O_3$	ND	ND	1613696	ND	ND	ND	ND	ND
12.41	180.0781	Ethanone, 1-(3,4-dimethoxyphenyl)-	$C_{10}H_{12}O_3$	ND	ND	ND	2751983	ND	ND	ND	ND
13.00	189.1515	2-Butanone, 4-(2,3-dihydro-1H-indol-1-yl)-	C <sub>12</sub> H <sub>15</sub> NO	85005	53880	ND	ND	ND	ND	ND	ND
13.44	182.0727	Benzophenone	C <sub>13</sub> H <sub>10</sub> O	ND	ND	ND	282691	ND	138491	163689	ND
14.32	188.1198	Methanone, (1-hydroxycyclohexyl)phenyl-	$C_{13}H_{16}O_2$	386301	595229	885838	1073775	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	$C_{20}H_{22}N_4O_2S$	133625	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	$C_{17}H_{24}O_3$	165132	292457	202831	ND	ND	ND	ND	ND
24.44	158.0821	2-Octen-4-one, 2-methoxy-	$C_9H_{16}O_2$	ND	ND	236995	ND	ND	ND	ND	ND
28.80	410.3543	4,22-Stigmastadiene-3-one	$C_{29}H_{46}O$	ND	ND	ND	533139	ND	ND	ND	ND
Miscellan	eous										
4.00	138.1040	Furan, 2-pentyl-	C <sub>9</sub> H <sub>14</sub> O	911826	ND	ND	ND	ND	ND	ND	ND
4.40	123.0680	4(H)-Pyridine, N-acetyl-	C <sub>7</sub> H <sub>9</sub> NO	ND	ND	ND	391733	ND	ND	ND	ND
5.53	120.0684	1,3,5,7-Tetroxane	C4H8O <sub>4</sub>	ND	ND	ND	ND	ND	ND	99462936	ND
5.58	120.0683	3-Pyridinecarbonitrile, 1,4-dihydro-1-methyl-	$C_7H_8N_2$	ND	ND	ND	33385	ND	ND	ND	ND
5.98	359.0650	Cyclopentasiloxane, decamethyl-	C <sub>10</sub> H <sub>30</sub> O <sub>5</sub> Si <sub>5</sub>	2178743	ND	ND	ND	ND	ND	ND	ND
6.88	143.0860	1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-	$C_6H_{12}O_4$	ND	ND	4276079	ND	ND	ND	ND	ND
8.30	431.0862	Cyclohexasiloxane, dodecamethyl-	C12H36O6Si6	5186795	ND	724478	ND	9273629	192507	315644	77896

					F	lour			S	tarch	
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS
11.06	504.1074	3-lsopropoxy-1,1,1,7,7,7-hexamethyl- 3,5,5- tris(trimethylsiloxy)tetrasiloxane	C <sub>18</sub> H <sub>52</sub> O <sub>7</sub> Si <sub>7</sub>	ND	ND	5900698	527949	6713484	435535	658962	832910
11.07	504.1062	3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5- tris(trimethylsiloxy)tetrasiloxane	$C_{19}H_{54}O_7Si_7$	432330	ND	722627	584708	ND	ND	ND	ND
11.35	186.0257	Tetraglyme	C <sub>10</sub> H <sub>22</sub> O <sub>5</sub>	ND	313631	588177	897608	ND	ND	702519	ND
12.35	219.1747	(4S,5S)-(+)-5-Amino-2,2-dimethyl-4- phenyl-1,3-dioxane	C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub>	ND	ND	1469274	ND	ND	ND	ND	ND
11.93	183.0446	6-Hepten-2-one, 5,7,7-trichloro-	$C_7H_9C_{13}O$	ND	ND	ND	11932715	ND	ND	ND	ND
12.72	157.0885	3-Methyl-4-phenyl-1H-pyrrole	$C_{11}H_{11}N$	ND	ND	ND	ND	ND	ND	130634	
13.73	179.0680	Thiazolo[3,2-a]pyridinium, 8-hydroxy-2,5-dimethyl-, hydroxide, inner salt	C <sub>9</sub> H <sub>9</sub> NOS	ND	ND	ND	179883	ND	ND	ND	ND
13.81	416.0373	Cyclooctasiloxane, hexadecamethyl-	C16H48O8Si8	ND	ND	ND	ND	4996853	362566	897430	908938
14.57	168.0782	Thiophene, 2-butyl-5-ethyl-	C <sub>10</sub> H <sub>16</sub> S	ND	ND	ND	799785	ND	ND	ND	ND
15.88	433.0855	1,1,1,5,7,7,7-Heptamethyl-3,3- bis(trimethylsiloxy)tetrasiloxane	$C_{13}H_{40}O_5Si_6$	ND	ND	1098619	ND	ND	ND	1192438	ND
17.36	154.0738	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	$C_{11}H_{18}N_2O_2$	ND	ND	ND	ND	ND	266621	ND	ND
17.58	533.9922	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15- hexadecamethyl-	C <sub>16</sub> H <sub>50</sub> O <sub>7</sub> Si <sub>8</sub>	ND	ND	ND	ND	ND	ND	ND	589423
18.85	145.1009	Cyclopropane, 1-ethenyl-2-hexenyl-, [1a,2ß(E)]-(±)-	C <sub>11</sub> H <sub>18</sub>	ND	ND	ND	ND	ND	ND	3497754	ND
19.23	201.1132	2,8,9-Trioxa-5-aza-1- silabicyclo[3.3.3]undecane, 1-ethenyl-	$C_8H_{15}NO_3Si$	ND	ND	ND	ND	ND	9154266	ND	ND
21.13	220.2181	4,8,12,16-Tetramethylheptadecan-4- olide	$C_{21}H_{40}O_2$	ND	447548	ND	ND	ND	ND	ND	ND
21.14	167.1431	2H-Pyran-2-one, tetrahydro-6-pentyl-	$C_{10}H_{18}O_2$	ND	ND	ND	ND	1072724	460163	ND	ND
22.19	267.2684	Indoline, 2-(hydroxydiphenylmethyl)-	C <sub>21</sub> H <sub>19</sub> NO	ND	ND	ND	ND	ND	ND	50284	ND
24.45	156.9946	2-Octen-4-one, 2-methoxy-	$C_9H_{16}O_2$	ND	ND	141706	ND	ND	ND	ND	ND
25.69	532.9916	Heptasiloxane, hexadecamethyl-	C <sub>16</sub> H <sub>48</sub> O <sub>6</sub> Si <sub>7</sub>	3291323	ND	ND	ND	4761300	ND	ND	ND

Table 2	(continued)
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				Flour				Starch			
Rt (mins)	Observed ion $m/z$	Name	MF	OGBF	24GBF	48GBF	72GBF	OGBS	24GBS	48GBS	72GBS
25.79	309.2793	Propanedinitrile, 2-(1-methyl-2,6- diphenyl-4(1H)-pyridinylidene)-	$C_{21}H_{15}N_3$	ND	ND	47194	ND	ND	ND	ND	ND
25.80	310.2833	1'-Oxocannabinol	$C_{21}H_{24}O_3$	ND	ND		ND	ND	ND	ND	ND
27.89	394.3603	Stigmastan-6,22-dien, 3,5-dedihydro-	C <sub>29</sub> H <sub>46</sub>	ND	ND	ND	ND	778823	931373	ND	ND
28.21	155.0859	Pyridine, 3-phenyl-	$C_{11}H_9N$	ND	ND	ND	150868	ND	ND	ND	ND
28.79	453.0684	Methylenebis(2,4,6- triisopropylphenylphosphine)	$C_{31}H_{50}P_2$	ND	94708	ND	ND	ND	ND	ND	ND
30.02	420.0876	Methyl 3ß-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 <sub>8</sub> H <sub>10</sub> O <sub>3</sub>	ND	ND	ND	288311	ND	ND	ND	ND
9.57	164.1196	Phenol, 4-(1,1-dimethylpropyl)-	C <sub>11</sub> H <sub>16</sub> O	ND	ND	332332	ND	ND	ND	562386	ND
11.48	220.1823	Butylated Hydroxytoluene	C <sub>15</sub> H <sub>24</sub> O	95604	ND						
11.49	206.1665	2,4-Di-tert-butylphenol	$C_{14}H_{22}O$	ND	1676041	ND	ND	2037303	1153076	2870723	2802451
14.12	234.1980	Phenol, 2,4-bis(1,1-dimethylpropyl)-	C <sub>16</sub> H <sub>26</sub> O	ND	ND	157473	78267	ND	ND	ND	ND
21.74	340.2401	Phenol, 2,2'-methylenebis[6-(1,1- dimethylethyl)-4-methyl-	$C_{23}H_{32}O_2$	69972	1728704	ND	ND	ND	ND	ND	ND
28.79	646.4521	Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)	$C_{42}H_{63}O_3P$	216841	ND						
Phytosterols											
27.69	400.3700	Campesterol	C <sub>28</sub> H <sub>48</sub> O	ND	ND	265916	ND	ND	ND	ND	ND
27.89	412.3710	Stigmasterol	C <sub>29</sub> H <sub>48</sub> O	753259	603033	1163792	ND	ND	ND	2283619	1771221
28.27	414.3861	ß-Sitosterol	C <sub>29</sub> H <sub>50</sub> O	ND	345695	ND	ND	ND	ND	ND	ND
28.57	409.3783	ß-Amyrin	$C_{30}H_{50}O$	ND	ND	283324	ND	ND	ND	ND	ND
Terpene and Terpenoid											
13.90	216.1511	aR-Turmerone	C <sub>15</sub> H <sub>20</sub> O	ND	ND	577405	626241	ND	ND	ND	ND
24.78	231.2116	Supraene	$C_{30}H_{50}$	ND	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	7194388

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 24 h; 48GBS: Starch from Bambara groundnut germinated for 24 h; 72GBS: Starch from Bambara groundnut germinated for 24 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 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 a multipurpose sampler (Gerstel Inc., Mülheim an der Ruhr Germany) and Rxi<sup>®</sup>-5 ms column (30 m  $\times$  0.25 mm ID  $\times$  0.25  $\mu$ m) (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 NIST<sup>1</sup>, Mainlib<sup>2</sup> and Feihn<sup>3</sup> 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 Enyinnaya 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.

<sup>&</sup>lt;sup>1</sup> https://www.nist.gov/.

<sup>&</sup>lt;sup>2</sup> https://www.mainlib.org/.

<sup>&</sup>lt;sup>3</sup> https://fiehnlab.ucdavis.edu/projects/softwaredev.

# **Declaration of Competing Interest**

None.

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