Data Article

Dataset on effect of decolourisation on metabolomic profile of *Moringa oleifera* leaf powder

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**ABSTRACT**

Moringa leaf has been widely used in the enrichment of staple foods due to its high nutritional value and hypoglycaemic, immune boosting, antiviral, antioxidant and antimicrobial activities. However, the acceptability of these products is generally low due to the green colour imparted by the colour of Moringa leaf. Decolourisation of the leaves may improve the acceptability of the food products. The decolorisation process may not only change the chlorophyll concentration of the Moringa leaves but also its other chemical components. The data set describes the effect of decolourisation on the metabolites present in Moringa leaf powder. The raw and decolourised samples were extracted with methanol/water (80:20 v/v) and analysed using a gas chromatography-high resolution time of flight-mass spectrometer (GC-HRTOF-MS). The metabolites identified were classified based on their functional group into acids, alcohols, aldehydes, amides hydrocarbons, phenols, phytosterols, vitamins and others. The data presented can be useful in identifying functional compounds available in Moringa-based foods and understanding the effect of decolourisation on the metabolite profile.

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Specifications Table

| Subject                        | Food Science: Food Chemistry |
|--------------------------------|------------------------------|
| Specific subject area          | Processing; Pigment extraction; Metabolomics |
| Type of data                   | Table; Figure; Spectra data |
| How the data were acquired     | *Moringa oleifera* leaf powder (MOLP) was decolourised by homogenising the leaf powder with ethanol (95%) at a powder to solvent ratio of 1:20, placed on an orbital shaker at 150 rpm for 30 min. The samples were later centrifuged, supernatant discarded, and the slurry dried at 40 °C. Metabolites in the raw and decolourised powder were extracted with methanol/water at 80:20 v/v. The extracts were analysed using the 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), Gerstel MPS multipurpose autosampler (Gerstel Inc., Mülheim an der Ruhr, Germany) and a Rxi ®-5ms column (30 m x 0.25 mm ID x 0.25 μm) (Restek, Bellefonte, USA). |
| Data format                    | Raw and analysed data |
| Description of data collection | A single biological *Moringa* leaf powder sample was used in the experiment. The sample was extracted in duplicate, and the duplicate extracts injected in triplicate. Raw and decolourised leaf powder (1 g) was extracted with 10 ml extraction solvent (methanol/water 80:20 v/v). The extract was concentrated, reconstituted in 1 ml methanol (99.9% pure chromatography grade) and filtered into dark vials using 0.22 μm syringe filters. Afterwards, 1 μl of sample was auto-injected to the GC-HRTOF-MS machine and metabolite identities were determined using NIST, Mainlib and Feihlin metabolomics databases. |
| Data source location           | MOLP was sourced from the Agricultural Research Council (ARC), Pretoria, Gauteng, South Africa (S 25° 44’ 55. 8” E 28° 14’ 14. 0”) and analyses were done at the University of Johannesburg (Doornfontein Campus), Johannesburg, South Africa (S 26° 11’ 32. 6” E 28° 03’ 28. 9”). |
| Data accessibility             | Raw and processed dataset have been deposited in Mendeley repository and is accessible using the link: DOI: 10.17632/7mrhxrt9kr.1; https://data.mendeley.com/datasets/7mrhxrt9kr/1 [1] |

Value of the Data

- The data present the effect of decolourisation on the metabolite profile of *Moringa* leaf powder samples and give an insight to metabolite modifications after decolourisation.
- The data reported would be useful to food processors for supplementing staple foods with decolourised *moringa* leaf powder for improved nutrition.
- The data could be useful for comparative analysis of metabolite composition of *moringa* leaf powder grown in different locations and may be useful for selecting *moringa* leaf species for various food and non-food applications.

1. Data Description

The metabolite data obtained from raw and decolourised MOLP are presented. Table 1 represents the metabolites obtained from MOLP. The data in the table includes the following: retention time, observed mass, metabolite name, molecular formula and average peak area for each metabolite identified in the different samples. These were obtained from the peaks generated
### Table 1
Metabolites Identified in Raw and Decolourised Moringa Leaf Powder.

| RT (Min) | Observed Ion m/z | Name                                                                 | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|----------------------------------------------------------------------|-------------------|-------------------|------------------|------------------|
|          |                  |                                                                      |                   |                   |                  |                  |
|          |                  |                                                                      |                   |                   |                  |                  |
|          |                  |                                                                      |                   |                   |                  |                  |
|          |                  |                                                                      |                   |                   |                  |                  |
|          |                  |                                                                      |                   |                   |                  |                  |

#### Acids

| RT (Min) | Observed Ion m/z | Name                                                                 | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|----------------------------------------------------------------------|-------------------|-------------------|------------------|------------------|
| 9:33     | 150.0675         | Hydrocinnamic acid                                                   | C₉H₁₀O₂           | 267444 ± 1677     | ND               | ND               |
| 15:90    | 207.1833         | Tetradecanoic acid                                                   | C₁₄H₂₈O₂          | 870892 ± 1728     | 112615 ± 1544    | ND               |
| 15:85    | 171.1378         | n-Decanoic acid                                                      | C₁₀H₂₀O₂          | ND                | 136420 ± 955     | ND               |
| 18:31    | 256.2399         | n-Hexadecanoic acid                                                 | C₁₆H₃₂O₂          | 20230631 ± 3875   | 4957168 ± 1078   | ND               |
| 20:20    | 178.1343         | 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-                             | C₁₈H₃₀O₂          | ND                | 385144 ± 848     | ND               |

#### Alcohol

| RT (Min) | Observed Ion m/z | Name                        | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|------------------------------|-------------------|-------------------|------------------|------------------|
| 3:50     | 87.0439          | 2-Chloroethanol              | C₂H₅ClO           | ND                | 6540954 ± 381    | ND               |
| 3:10     | 98.0361          | 2-Furanmethanol              | C₅H₆O₂            | 2332645 ± 2154    | ND               | ND               |
| 4:24     | 110.036          | (3-Fluorophenyl) methanol, n-butyl ether                             | C₁₁H₁₅FO          | 2215455 ± 1928    | ND               | ND               |

#### Aldehyde

| RT (Min) | Observed Ion m/z | Name                                                                       | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|---------------------------------------------------------------------------|-------------------|-------------------|------------------|------------------|
| 4:23     | 110.036          | 2-Furancarboxaldehyde, 5-methyl-                                           | C₆H₆O₂            | 4329276 ± 1750    | ND               | ND               |
| 5:29     | 120.0568         | Benzeneacetaldehyde                                                       | C₆H₆O             | 5491177 ± 2096    | ND               | ND               |
| 7:56     | 120.0569         | Benzaldehyde, 3-methyl-                                                   | C₆H₆O             | ND                | 310003 ± 0       | ND               |
| 7:66     | 120.0570         | Benzaldehyde, 2-methyl-                                                   | C₆H₆O             | 709831 ± 691      | ND               | ND               |
| 20:00    | 264.2451         | 9,12,15-Octadecatrienal                                                   | C₁₈H₃₀O₂          | ND                | 3090025 ± 600    | ND               |

#### Amide

| RT (Min) | Observed Ion m/z | Name                        | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|------------------------------|-------------------|-------------------|------------------|------------------|
| 11:23    | 174.0667         | Furmecyclox                  | C₁₄H₂₁NO₃        | 90492 ± 156       | ND               | ND               |
| 12:23    | 193.1693         | Benzamide, 2,6-difluoro-N-heptyl-                                        | C₁₄H₁₅F₂NO        | 548309 ± 1639     | ND               | ND               |
| 14:65    | 197.1204         | Formamide, N-(1,1′-biphenyl)-2-yl-                                       | C₁₃H₁₁NO          | 49904 ± 461       | ND               | ND               |
| 19:65    | 193.0890         | 1-Anthracenamine             | C₁₄H₁₁N          | 63892 ± 187       | ND               | ND               |
| 19:93    | 154.1226         | Dodecanamide, N-(2-hydroxyethyl)-                                         | C₁₄H₂₀NO₂         | ND                | 82268 ± 779      | ND               |
| 25:16    | 172.1561         | 9-Octadecenamide, (Z)-       | C₁₈H₃₅NO          | 297218 ± 1354     | 212162 ± 1040    | ND               |

#### Amines

| RT (Min) | Observed Ion m/z | Name                        | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|------------------------------|-------------------|-------------------|------------------|------------------|
| 12:99    | 143.0730         | 2-Naphthalenamine            | C₁₀H₈N            | ND                | 27586 ± 1359     | ND               |
| 20:07    | 243.2511         | Ethanol, 2,2′-(dodecylimino)bis-                                       | C₁₆H₃₅NO₂         | ND                | 74343 ± 575      | ND               |

#### Diterpenes

| RT (Min) | Observed Ion m/z | Name                        | Molecular Formula | Average Peak Area | Raw               | Decoloured        |
|----------|------------------|------------------------------|-------------------|-------------------|------------------|------------------|
| 17:30    | 207.7144         | Neophytadiene                | C₂₀H₃₈            | 383948 ± 846      | 115003 ± 564     | ND               |
| 19:70    | 279.3006         | Phytol                       | C₂₀H₄₀O           | 2504053 ± 1783    | ND               | ND               |

(continued on next page)
| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Raw | Decolourised |
|---------|-----------------|------|-------------------|-----|-------------|
| 5:97    | 134.0835        | 1,2-Ethanediol, dipropionate | C₆H₁₄O₄ | ND | 1085862 ± 1179 |
| 6:01    | 112.0394        | dl-Alanine ethyl ester | C₆H₁₁NO₂ | 5911350 ± 2645 | ND |
| 6:55    | 168.9881        | Glycine, N-methyl-N-methoxycarbonyl-, undecyl ester | C₁₀H₁₃NO₄ | ND | 435634 ± 690 |
| 7:41    | 149.1073        | Terephthalic acid, 4-fluorophenethyl octyl ester | C₂₄H₂₁NO₄ | 104029 ± 1101 | ND |
| 11:23   | 133.1011        | 4-Fluorobenzoic acid, tridec-2-ynyl ester | C₂₀H₁₂NO₂ | 87384 ± 368 | ND |
| 11:55   | 176.0829        | 3-Butenoic acid, 4-phenyl-, methyl ester | C₁₁H₁₂O₂ | 245772 ± 1255 | 91379 ± 433 |
| 11:69   | 166.0624        | Benzeneacetic acid, 4-hydroxy-, methyl ester | C₈H₁₀O₃ | ND | 183725 ± 496 |
| 12:23   | 161.5899        | 2,4-Difluorobenzoic acid, 2-formyl-4,6-dichlorophenyl ester | C₁₄H₈F₂O₃ | 442533 ± 587 | 106667 ± 943 |
| 12:41   | 178.0623        | 4-Fluorobenzoic acid, tridec-2-ynyl ester | C₂₀H₁₂O₂ | 64013 ± 325 | ND |
| 13:32   | 168.0414        | Fumaric acid, ethyl 3,4,5-trichlorophenyl ester | C₁₂H₇Cl₃O₄ | ND | 74561 ± 613 |
| 13:39   | 139.0377        | Fumaric acid, ethyl 2,3,5-trichlorophenyl ester | C₁₂H₇Cl₃O₄ | 220060 ± 963 | ND |
| 17:19   | 150.0264        | Phthalic acid, monoamide, N-ethyl-N-(3-methylphenyl),-isobutyl ester | C₂₇H₂₅NO₃ | ND | 49831 ± 575 |
| 17:21   | 224.1004        | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | C₁₈H₂₁O₄ | 209387 ± 1458 | ND |
| 18:22   | 223.0960        | Dibutyl phthalate | C₁₆H₂₂O₄ | 237942 ± 909 | ND |
| 21:23   | 157.0838        | Carbonic acid, 2-dimethylaminoethyl isobutyl ester | C₁₈H₂₂NO₃ | 225107 ± 1068 | ND |
| 21:24   | 179.0012        | Octanoic acid, 2-dimethylaminoethyl ester | C₁₂H₂₅NO₂ | 173798 ± 867 | ND |
| 22:74   | 88.0757         | Cyclobutanecarboxylic acid, 2-dimethylaminoethyl ester | C₁₂H₁₇NO₂ | 345374 ± 1472 | ND |
| 23:11   | 300.2600        | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C₁₉H₃₈O₄ | 1227632 ± 1574 | ND |
| 24:67   | 285.2783        | Pentadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C₁₈H₃₆O₄ | 306505 ± 799 | ND |
| 24:67   | 285.2781        | Glycerol 1-palmitate | C₁₉H₃₈O₄ | 414699 ± 1891 | ND |
| 24:67   | 285.2778        | Pentadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C₁₈H₃₆O₄ | 393653 ± 1489 | ND |
| 27:15   | 210.0300        | 2-Amino-3-cyano-4-methyl-4,6-bis-(5-nitrobenzofuran-2-yl)-cyclohexa-1,5-dien-1,3-dicarboxylic acid, diethyl ester | C₁₀H₂₄N₄O₁₀ | 39484 ± 128 | ND |
| 27:16   | 204.1105        | 4′-Cyano-4-biphenyl-p-heptylbenzoate | C₂₇H₂₇NO₂ | 121833 ± 985 | ND |
| 27:16   | 414.3457        | 2-Amino-3-cyano-4-methyl-4,6-bis-(5-nitrobenzofuran-2-yl)-cyclohexa-1,5-dien-1,3-dicarboxylic acid, diethyl ester | C₁₀H₂₄N₄O₁₀ | 137111 ± 568 | ND |

**Fatty Acid Ethyl Esters**

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Raw | Decolourised |
|---------|-----------------|------|-------------------|-----|-------------|
| 18:46   | 241.2156        | Pentadecanoic acid, ethyl ester | C₁₇H₃₄O₂ | ND | 142849 ± 872 |
| 23:12   | 300.2615        | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C₁₉H₃₈O₄ | 652035 ± 1645 | ND |

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### Table 1 (continued)

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Average Peak Area |
|----------|------------------|------|------------------|------------------|
|          |                  |      |                  |                  |
|          |                  | Fatty Acid Methyl Esters |                  |                  |

#### Fatty Acid Methyl Esters

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Average Peak Area |
|----------|------------------|------|------------------|------------------|
| 17:75    | 270.2551         | Pentadecanoic acid, 14-methyl-, methyl ester | C_{17}H_{34}O_{2} | ND               | 452607 ± 1184 |
| 17:76    | 228.2046         | Tridecanoic acid, methyl ester | C_{16}H_{32}O_{2} | 577213 ± 1215 | ND               |
| 17:76    | 213.1850         | Dodecanic acid, methyl ester | C_{15}H_{30}O_{2} | 60741 ± 783 | ND               |
| 19:57    | 236.1769         | 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- | C_{19}H_{32}O_{2} | 523501 ± 964 | ND               |
| 19:77    | 255.2315         | Tridecanoic acid, methyl ester | C_{18}H_{36}O_{2} | ND               | 118000 ± 674 |

#### Heterocyclic organic compounds

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Average Peak Area |
|----------|------------------|------|------------------|------------------|
| 7:91     | 126.0311         | 5-Hydroxymethylfurural\(^\text{a}\) | C_{6}H_{6}O_{3} | 12643146 ± 4287 | 4540831 ± 651 |

#### Hydrocarbons

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Average Peak Area |
|----------|------------------|------|------------------|------------------|
| 5:59     | 95.0332          | Dipivefrine, N.O-bis(pentafluoropropionyl)- | C_{13}H_{17}F_{10}NO_{7} | 488776 ± 1892 | ND               |
| 5:82     | 120.0566         | 1,3,5,7-Tetraoxane | C_{11}H_{14}O_{6} | 28996026 ± 3624 | ND               |
| 10:30    | 126.0467         | 2,2-Dichloroethyl methyl ether | C_{8}H_{8}Cl_{2}O | 3102554 ± 1560 | ND               |
| 10:61    | 172.1245         | (E)-1-(2,3,6-trimethylphenyl)buta-1,3-diene (TPB, 1) | C_{13}H_{16} | 57373 ± 657 | ND               |
| 11:03    | 133.0918         | 5-Trimethylsilylpent-2-ene-4-yne\(^\text{a}\) | C_{8}H_{14}Si | 51869 ± 235 | 30748 ± 464 |

(continued on next page)
| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Raw | Decolourised |
|----------|------------------|------|-------------------|-----|--------------|
| 12:03    | 326.9667         | 3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane | C₁₉H₅₄O₇Si₇ | ND | 60326 ± 837 |
| 14:64    | 401.9880         | Cyclooctasiloxane, hexadecamethyl- | C₁₆H₄₈O₈Si₈ | ND | 107780 ± 553 |
| 20:20    | 173.1325         | 9,12,15-Octadecatrien-1-ol, (2,2,2)- | C₁₈H₃₂O | ND | 285352 ± 848 |

**Indole**

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Raw | Decolourised |
|----------|------------------|------|-------------------|-----|--------------|
| 8:73     | 117.0571         | Indole | C₈H₇N | 187094 ± 961 | 81834 ± 818 |
| 19:62    | 193.0884         | 3-Phenylindole | C₁₄H₁₁N | 26717 ± 561 | ND |
| 19:68    | 278.2972         | Phytol | C₂₀H₄₀O | 1042771 ± 964 | ND |

**Ketones**

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Raw | Decolourised |
|----------|------------------|------|-------------------|-----|--------------|
| 3:38     | 96.0205          | 4-Cyclopentene-1,3-dione | C₅H₈O₂ | 472244 ± 425 | ND |
| 4:39     | 144.0415         | 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-oneᵃ | C₆H₈O₄ | 5669648 ± 3879 | 722966 ± 1181 |
| 5:54     | 128.0468         | Furaneol | C₆H₈O₃ | 1472259 ± 6465 | ND |
| 6:81     | 144.0418         | 4H-Pyran-4-one, 2,3-dihydro-5-dihydroxy-6-methyl-ᵃ | C₆H₈O₄ | 40779689497 | ND |
| 7:58     | 120.0569         | Benzo furan, 2,3-dihydro- | C₆H₈O | ND | 11673960 ± 3650 |
| 7:32     | 142.0261         | 4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-ᵃ | C₆H₈O₄ | 718472 ± 869 | 207912 ± 1452 |
| 8:98     | 150.0675         | Ethanone, 1-(2-hydroxy-5-methylphenyl)- | C₆H₁₀O₂ | 219210 ± 963 | ND |
| 10:43    | 206.1299         | 1-(3,6,8-Trimethyl-1,6,7,7a-tetrahydrocyclopenta[c]pyran-1-yl)ethene n | C₁₃H₁₈O₂ | 25292 ± 563 | ND |
| 10:79    | 120.0679         | 7-Chloro-1,3,4,10-tetrahydro-10-hydroxy-1-[2-[1-pyrrolidiny]ethyl]imino]-3-[3-(trifluoromethyl)phenyl]-9(2H)-acridine | C₂₆H₂₅ClF₃N₃O₂ | 5330994 ± 3056 | ND |
| 11:95    | 190.1355         | 4-(2,6,8-Trimethylcyclohexa-1,3-dienyl)butoxy-2,4-enedione | C₁₃H₁₈O | 1027624 ± 2786 | ND |
| 12:60    | 162.0674         | 5-Hydroxy-3-methyl-1-indanone | C₁₀H₁₀O₂ | 144778 ± 845 | ND |
| 13:65    | 194.0576         | Butyrovanillone | C₁₁H₁₄O₂ | 240775 ± 982 | ND |
| 14:27    | 190.1353         | Megastigmatene | C₁₁H₁₈O | 121488 ± 569 | ND |
| 15:13    | 193.1226         | Methanone, 1-hydroxycyclohexyl]phenyl- | C₁₁H₁₈O₂ | 118337 ± 678 | ND |
| 14:02    | 174.0991         | 4-Phenyl-3-penten-2-one p-toluenesulfonylhydrazone | C₁₈H₂₀N₂O₄S | 61326 ± 323 | ND |
| 15:12    | 175.1116         | Methanone, 1-hydroxycyclohexyl]phenyl- | C₁₁H₁₈O₂ | 85928 ± 476 | ND |
| 29:19    | 379.3343         | Allopregnane-3β,7a,11a-triol-20-one | C₂₁H₂₄O₄ | 1216244 ± 1985 | ND |

**Miscellaneous compounds**

| RT (Min) | Observed Ion m/z | Name | Molecular Formula | Raw | Decolourised |
|----------|------------------|------|-------------------|-----|--------------|
| 7:62     | 154.0625         | 4-tert-Butoxystyrene | C₁₂H₁₆O | 753299 ± 869 | ND |
| 9:16     | 137.0468         | N-(2-Propynyl)-2-methylpiperidine | C₁₇H₁₅N | 33347 ± 155 | ND |

(continued on next page)
Table 1 (continued)

| RT (Min) | Observed Ion m/z | Name                                           | Molecular Formula | Average Peak Area |
|----------|------------------|------------------------------------------------|------------------|-------------------|
|          |                  |                                                |                  | Raw               | Decolourised    |
| 9:68     | 172.1245         | Naphthalene, 1,2-dihydro-1,1,6-trimethyl-      | C_{13}H_{16}      | 106374 ± 563      | ND               |
| 10:21    | 119.0851         | N-Ethyl-2-carbethoxyacetidine                   | C_{5}H_{15}NO_{2} | ND                | 3080824 ± 1883  |
| 10:32    | 172.1245         | 1, 1, 5-Trimethyl-1, 2-dihydronaphthalene     | C_{13}H_{16}      | 22190 ± 209       | ND               |
| 11:35    | 173.0961         | Acetyl eugenol                                 | C_{12}H_{14}O_{3} | 66559 ± 865       | ND               |
| 11:60    | 172.1245         | Naphthalene, 1,2-dihydro-1,4,6-trimethyl-     | C_{13}H_{16}      | 43628 ± 101       | ND               |
| 11:64    | 155.0730         | Pyridine, 3-phenyl-                            | C_{11}H_{8}N      | 106819 ± 1796     | 39467 ± 567     |
| 12:13    | 133.0522         | Benzeneacetonitrile, 4-hydroxy-                | C_{8}H_{6}NO      | 5692313 ± 2058    | 6655507 ± 2504  |
| 12:46    | 169.0881         | Pyridine, 2-(4-methylphenyl)-                  | C_{12}H_{13}N     | 33241 ± 456       | ND               |
| 12:49    | 142.0777         | Piperidine, 1-butyl-                           | C_{13}H_{14}N     | 157108 ± 985      | ND               |
| 14:04    | 183.1193         | 1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene\(^a\) | C_{14}H_{10}O      | 333883 ± 1798     | 56509 ± 306     |
| 16:46    | 166.0625         | 3-Methyl-5-nonylpyrrolizidine                  | C_{17}H_{33}N     | 136101 ± 826      | ND               |
| 17:86    | 194.0771         | Phosphine, cyclohexyl[2-(2-pyridyl)ethyl]-     | C_{13}H_{20}NP    | 105122 ± 1419     | ND               |
| 21:88    | 189.0758         | 4,8,12,16-Tetramethylheptadecan-4-olide        | C_{21}H_{40}O_{2} | 108316 ± 746      | ND               |

**Phenols**

| RT (Min) | Observed Ion m/z | Name                                          | Molecular Formula | Average Peak Area |
|----------|------------------|-----------------------------------------------|------------------|-------------------|
| 8:76     | 138.0674         | Phenol, 4-(methoxymethyl)-                     | C_{6}H_{10}O_{2} | 149528 ± 1432     | ND               |
| 15:80    | 180.0782         | (E)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol\(^a\) | C_{10}H_{12}O_{3} | 148123 ± 979      | 59968 ± 566     |
| 12:35    | 206.1664         | 2,4-Di-tert-butylphenol\(^b\)                 | C_{14}H_{22}O     | 111246 ± 1189     | 91836 ± 684     |
| 12:35    | 206.1657         | Phenol, 2,5-bis(1,1-dimethylethyl)-            | C_{14}H_{22}O     | 125015 ± 1275     | ND               |

**Phytosterol**

| RT (Min) | Observed Ion m/z | Name                                          | Molecular Formula | Average Peak Area |
|----------|------------------|-----------------------------------------------|------------------|-------------------|
| 29:05    | 415.3873         | Cholesterol 3-O-[(2-acetoxy)ethyl]-            | C_{31}H_{32}O_{3} | ND                | 436680 ± 1045   |
| 29:17    | 315.2636         | Cholesta-8,24-dien-3-ol, 4-methyl-, (38,4a)-  | C_{28}H_{46}O     | ND                | 213935 ± 1115   |
| 29:40    | 341.8057         | ß-Amyrin\(^a\)                                | C_{30}H_{50}O     | 487813 ± 1542     | 78184 ± 465     |
| 29:07    | 416.3920         | ß-Sitosterol acetate                          | C_{31}H_{52}O_{2} | ND                | ND               |

**Vitamins**

| RT (Min) | Observed Ion m/z | Name                                          | Molecular Formula | Average Peak Area |
|----------|------------------|-----------------------------------------------|------------------|-------------------|
| 25:75    | 420.3556         | a-Tocopherol B                                 | C_{29}H_{50}O_{4} | 40453 ± 1006      | ND               |
| 25:75    | 420.3552         | a-Tocopherol A                                 | C_{29}H_{50}O_{4} | 37780 ± 77        | ND               |
| 26:38    | 402.3502         | d-Tocopherol                                   | C_{27}H_{46}O_{2} | 150789 ± 1745     | ND               |
| 27:71    | 430.3811         | dl-a-Tocopherol\(^a\)                         | C_{28}H_{50}O_{2} | 8263817 ± 3581    | 804002 ± 1368   |
| 29:71    | 430.3813         | Vitamin E                                      | C_{28}H_{50}O_{2} | ND                | 213437 ± 945    |

Values are reported as mean ± ± SD;
\(^a\) Samples differ significantly \((p < 0.5)\);
\(^b\) No significant difference \((p ≥ 0.5)\); RT - retention time; ND - not detected
Fig. 1. Pie chart indicating the percentage distribution of the compounds in the raw Moringa leaf powder.

Fig. 2. Pie chart indicating the percentage distribution of the compounds in the decolourised Moringa leaf powder.

from GC-HRTOF-MS analysis and comparison of spectra obtained with NIST, Mainlib and Feihn metabolite databases. The raw and analysed data together with the spectra obtained are available as supplementary documents (https://data.mendeley.com/datasets/7mrhxrt9kr/1) [1]. Figs. 1 and 2 summarises the percentage distribution of the compound groups in the raw and decolourised samples, respectively.
2. Experimental Design, Materials and Methods

2.1. Sample Preparation

MOLP was obtained from the ARC, Pretoria, South Africa. The MOLP was decolourised by homogenising the leaf powder with ethanol (95%) at a powder to solvent ratio of 1:20, placed on an orbital shaker (Stuart SSL1, Keison Products, Essex, UK) at 150 rpm for 30 min. The samples were later centrifuged, supernatant discarded, and the slurry dried at 40 °C. Further analysis was conducted on both the raw and the decolourised samples.

2.2. Extraction of Metabolites and GC-HRTOF-MS Analysis

Metabolites were extracted as previously described by Oyediji, Chinma, Green and Adebo [2]. Ten millilitres of the extraction solvent (methanol/water at 80:20 v/v) together with 1 g each of MOLP samples were thoroughly agitated and sonicated in an ultrasonic bath (Scientech 704, Labotech, South Africa) for 1 h at 4 °C. The mixture was then centrifuged at 3500 rpm at 4 °C for 5 min (Eppendorf 5702R, Merck, South Africa). Supernatant obtained after centrifuging was concentrated in a vacuum concentrator (Eppendorf Plus, Merck, South Africa) and made into solution with 1 ml of chromatographic grade methanol (Merck, South Africa). The solution was vortexed and filtered through 0.22 μm microfilters into an amber vial and solvent blanks were also prepared. The extracts were analysed using a GC-HRTOF-MS (LECO Corporation, St Joseph, MI, USA) with a multipurpose sample (Gerstel Inc., Mülheim an der Ruhr Germany) and Rxi®-5 ms column (30 m × 0.25 mm iD × 0.25 μm) (Restek, Bellefonte, USA). Injection of 1 μl extract was done a splitless mode at a flowrate of 1 ml/min and helium used as the carrier gas. The ion source temperature was at 250 °C while the transfer line and inlet temperatures were set at 225 and 250 °C, respectively. 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’. Data obtained were processed using DataPrep Solutions and metabolites were identified by matching the spectra with NIST, Mainlib and Feihn reference library databases, and their identities determined. Table 1 represents the mean of values obtained from triplicate runs of samples after prior processing of raw data.

Ethics Statements

None.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Supplementary data for manuscript ‘Dataset on effect of decolourisation on metabolomic profile of Moringa oleifera leaf powder’ (Original data) (Mendeley Data)

CRediT Author Statement

Adewumi Toyin Oyeyinka: Conceptualization, Methodology, Writing – original draft; Oluwafemi Ayodeji Adebo: Data curation, Software, Writing – review & editing; Muthulisi Si-
**wela**: Funding acquisition, Supervision, Writing – review & editing; **Kirthee Pillay**: Funding acquisition, Supervision, Writing – review & editing.

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