Data Article

LCMS dataset on compounds in Syzygium polyanthum (Wight) Walp. leaves variant from the East coast of Peninsular Malaysia

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ARTICLE INFO

Article history:
Received 11 February 2021
Revised 7 October 2021
Accepted 14 October 2021
Available online 17 October 2021

Keywords:
Syzygium polyanthum
LCMS
Serai kayu
Salam
Traditional plant

ABSTRACT

The data presented here is the liquid chromatography and mass spectrometry (LC-MS) profile of phytochemical compounds in the aqueous extract of Syzygium polyanthum (Wight) Walp. leaves. This plant is consumed raw and sometimes added to local dishes of people in Southeast Asia countries. Most importantly, it has ethnomedicinal values mainly in treating diabetes and hypertension, and at the same time, this plant has anti-microbial, anti-oxidant, anti-cancer, and anti-tumor properties [1]. There are chemical composition variations reported between the same species of different geographical locations, which eventually affect the plant's therapeutic potential [2,3]. This dataset represents the identified compounds for S. polyanthum (Wight) Walp. leaves, a variant collected from Kuantan, a city located in the Pahang state on the East Coast of Peninsular Malaysia. The leaves were then dried in an open-air at room temperature for three weeks, ground, and then macerated in water inside a bath-sonicator,
freeze-dried, and then run using LCMS. The LCMS was run using the ultra-performance liquid chromatography equipped with an electrospray time-of-flight mass spectrometer detector, operated in a negative-ion mode. The mass spectral features from samples raw data were matched with Traditional Medicine (en) and Waters Screening libraries in the Waters UNIFI™ Scientific Information System software version 1.7 (Waters, USA) for compounds identification.

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**Specifications Table**

| Subject | Chemistry |
|---------|-----------|
| Specific subject area | Phytochemicals, Natural product research, Spectrometry |
| Type of data | Tables, Figures |
| How data were acquired | Data on the phytochemical compounds in the aqueous extract of *S. polyanthum* (Wight) Walp. leaves were acquired using liquid chromatography quadrupole-time-of-flight mass spectrometry (Vion IMS LCQTOF MS 2016 model (Waters, USA)) using a reversed-phase column to separate and identify the semipolar to polar compounds. |
| Data format | Raw and Analyzed |
| Parameters for data collection | The data on the phytochemical compounds in *S. polyanthum* (Wight) Walp. leaves were acquired using Vion IMS LCQTOF MS 2016 (Waters, USA) with a reversed-phase column (ACQUITY UPLC HSS 2.1 × 100 mm × 1.8 μm) with the following operating conditions: operation mode (negative), analyzer mode (sensitivity), desolvation gas flow rate (600 L/h), cone gas (50 L/h), desolvation temperature (550 °C), source (electrospray ionization), source temperature (120 °C), capillary voltage (2.50 kV), MS mode (high definition), and scanning range (50–1000 m/z). The Auto MS/MS mode was used to confirm the fragment ions. The mass spectral features from samples raw data were matched with Traditional Medicine (en) and Waters Screening libraries in the Waters UNIFI™ Scientific Information System software version 1.7 (Waters, USA) for compounds identification. |
| Description of data collection | The freeze-dried powder of *S. polyanthum* (Wight) Walp. leaves were extracted in distilled water and then analyzed with Vion IMS LCQTOF MS 2016 model (Waters, USA) and then matched with Traditional Medicine (en) and Waters Screening libraries in the Waters UNIFI™ Scientific Information System software version 1.7 (Waters, USA) for compounds identification. |
| Data source location | *S. polyanthum* (Wight) Walp. leaves were collected from Sultan Haji Ahmad Shah Agricultural Park, Kuantan, Pahang, Malaysia (Latitude: 3.8470088044445445, Longitude: 103.30165631277539), and then extracted at the Natural Product Laboratory, Kulliyyah of Science, International Islamic University Malaysia, Kuantan, Pahang, Malaysia. LC-QTOF-MS/MS analysis and data processing were conducted at Central Laboratory, Universiti Malaysia Pahang, Kuantan, Pahang, Malaysia. |
| Data accessibility | The complete dataset is accessible at the Mendeley Repository: http://dx.doi.org/10.17632/8mt9npzyp8.1 [4]. |
Value of the Data

- This dataset is essential to show the phytochemical constituents in *Syzygium polyanthum* (Wight) Walp. leaves, a variant collected from Kuantan, Pahang, a region in the East Coast of Peninsular Malaysia.
- This dataset provides valuable information to the ethnobotanist, plant chemist, taxonomist, and herbal medicinal plants researchers on this plant variant since there were reported chemical composition variations between the variants of the same plant species with different geographical locations that will affect the therapeutic potential of this plant [2,3].
- The dataset on the plant's chemical profile helps in fostering development of high-quality herbal medicinal products with standardized bioactive compound [5,6].

1. Data Description

Fig. 1 illustrates the total ion chromatogram of the sample. The LC-MS raw datasets were further matched with the Traditional Medicine (en) and Waters Screening libraries in the Waters UNIFI™ Scientific Information System software version 1.7 (Waters, USA) for compounds identification as tabulated in Table 1. The raw data of all identified compounds in the aqueous extract from the leaves of *S. polyanthum* (Wight) Walp. can be found in the Mendeley data repository at: http://dx.doi.org/10.17632/8mt9npzyp8.1 [4]. Supplement 1 shows the complete raw data report as generated by UNIFI. The report contains operating parameters, total ion current (TIC) plot, base peak intensities (BPI) plot, summary table of identified compounds which includes chemical formula, observed neutral mass (Da), observed mass to charge ration (m/z), mass error (in mDa and ppm), observed retention time (min), responses, adducts, observed collision cross-section or CCS (Å²), total fragments found, and the spectral figures for each identified compound. Supplement 2 shows the simplified list of identified compounds in this plant extract. Fig. 2 shows percent distribution of phytochemical groups of identified compounds in this plant extract.

![LCMS Chromatogram of Syzygium polyanthum (Wight) Walp. leaves aqueous extract.](image-url)
Table 1
Chemical compounds identified in *Syzygium polyanthum* (Wight) Walp. leaves aqueous extract using LC-QTOF-MS analysis.

| No | Component name                              | Formula       | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Observed CCS (Å²) | Observed Response | Adducts | Phytochemical Groups |
|----|---------------------------------------------|---------------|-----------------------|---------------------------|--------------|------------------|------------------|-------------------|-------------------|-------------------|----------|----------------------|
| 1  | 2,6-Di-O-galloyl-β-D-glucose               | C20H20O14     | Identified            | 484.0824                  | 483.0752     | −2.9             | −5.9             | 0.59              | 165               | 1110              | −H       | Gallotannin           |
| 2  | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0749                  | 331.0676     | 0.6              | 1.7              | 0.73              | 172.73            | 2695              | −H       | Gallotannin           |
| 3  | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0746                  | 331.0673     | 0.3              | 0.8              | 0.99              | 216.32            | 1060              | −H       | Gallotannin           |
| 4  | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0746                  | 331.0673     | 0.2              | 0.7              | 0.99              | 172.42            | 8288               | −H       | Gallotannin           |
| 5  | 2,3-(S)-Hexahydroxydiphenoyl-D-glucose    | C20H18O14     | Identified            | 482.0705                  | 481.0632     | 0.8              | 1.7              | 1.01              | 200.74            | 2209              | −H       | Hydro-lyzable tannin  |
| 6  | Gemin D                                    | C27H22O18     | Identified            | 634.0814                  | 633.0741     | 0.8              | 1.2              | 1.12              | 222.57            | 2639               | −H       | Ellagitannin          |
| 7  | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0748                  | 331.0675     | 0.4              | 1.3              | 1.25              | 175.04            | 10088              | −H       | Gallotannin           |
| 8  | Pyrogallic                                  | C6H6O3        | Identified            | 126.0318                  | 125.0245     | 0.1              | 0.7              | 1.3               | 130.77            | 3260               | −H       | Phenolic Acid         |
|    | acid                                       |               |                       |                           |              |                  |                  |                   |                   |                   |          | Derivative            |
| 9  | Polyaceto-phenoside                        | C14H18O10     | Identified            | 346.0905                  | 345.0832     | 0.5              | 1.3              | 1.42              | 173.81            | 2846               | −H       | Glucoside             |
| 10 | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0747                  | 331.0674     | 0.4              | 1.1              | 1.47              | 172.23            | 2168               | −H       | Gallotannin           |
| 11 | Norbergenin                                 | C13H14O9      | Identified            | 314.064                   | 359.0622     | 0.2              | 0.6              | 1.58              | 178.19            | 1424               | +HCOO    | Glycoside             |
| 12 | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0744                  | 331.0672     | 0.1              | 0.3              | 1.83              | 177               | 1366               | −H       | Gallotannin           |
| 13 | 5-Desgalloylstachyurin                     | C34H24O22     | Identified            | 784.0755                  | 783.0682     | −0.5             | −0.6             | 2.02              | 254.89            | 4623               | −H       | Ellagitannin          |
| 14 | 1-Galloyl-glucose                          | C13H16O10     | Identified            | 332.0749                  | 331.0674     | 0.3              | 1.1              | 2.24              | 168.93            | 1366               | −H       | Gallotannin           |
| 15 | 5-Desgalloylstachyurin                     | C34H24O22     | Identified            | 784.0759                  | 783.0686     | −0.1             | −0.1             | 2.45              | 256.87            | 1555               | −H       | Gallotannin           |
| 16 | 2,6-Di-O-galloyl-β-D-glucose               | C20H20O14     | Identified            | 484.0854                  | 483.0782     | 0.1              | 0.3              | 3.19              | 196.43            | 3851               | −H       | Gallotannin           |
| 17 | 2,4,5-Tribhydroxybenzaldehyde             | C7H6O4        | Identified            | 154.0265                  | 153.0192     | −0.1             | −0.9             | 3.46              | 171.96            | 1230               | −H       | Simple phenol         |
| 18 | 5-Desgalloylstachyurin                     | C34H24O22     | Identified            | 784.0753                  | 783.0686     | −0.7             | −0.8             | 3.59              | 257.26            | 1216               | −H       | Ellagitannin          |
| 19 | Haematoxylin                               | C16H14O6      | Identified            | 302.079                   | 347.0772     | 0.0              | −0.1             | 3.87              | 179.52            | 1141               | +HCOO    | Phenocyanin          |
| 20 | 2,6-Di-O-galloyl-β-D-glucose               | C20H20O14     | Identified            | 484.0855                  | 483.0782     | 0.2              | 0.4              | 4.2               | 195.97            | 4799               | −H       | Gallotannin           |
| 21 | 2,6-Di-O-galloyl-β-D-glucose               | C20H20O14     | Identified            | 484.0855                  | 483.0782     | 0.2              | 0.3              | 4.29              | 193.82            | 3329               | −H       | Gallotannin           |
| 22 | Mulberroforan C                            | C34H28O9      | Identified            | 580.1742                  | 579.1669     | 0.8              | 1.4              | 4.42              | 223.24            | 1802               | −H       | Benzofuran            |
| 23 | 1-O-Galloylpedun-culagin                   | C41H28O26     | Identified            | 936.0862                  | 935.0789     | −0.7             | −0.7             | 4.83              | 295.29            | 8312               | −H       | Ellagitannin          |
| 24 | Darendoside A                              | C19H28O11     | Identified            | 432.1631                  | 431.1558     | 0.0              | −0.1             | 5.14              | 211.06            | 1402               | −H       | Phenethyl alcohol     |
|    | glycoside                                  |               |                       |                           |              |                  |                  |                   |                   |                   |          | glycoside            |

(continued on next page)
| No | Component name                                      | Formula       | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Observed CCS (Å²) | Response | Adducts | Phytochemical Groups |
|----|-----------------------------------------------------|---------------|-----------------------|---------------------------|--------------|------------------|------------------|------------------|------------------|----------|---------|---------------------|
| 25 | Aspidinol                                           | C12H16O4      | Identified            | 224.1046                  | 269.1028     | −0.3             | −1               | 5.44             | 203.8            | 1138     | +HCOO   | Simple phenol        |
| 26 | Feroxin A                                           | C17H24O8      | Identified            | 356.1472                  | 401.1454     | 0.1              | 0.1              | 5.44             | 202.21           | 15156    | +HCOO   | 3-O Glucoside        |
| 27 | Dendrocandin D                                      | C17H20O5      | Identified            | 304.1289                  | 349.1271     | −2.2             | −6.3             | 5.71             | 182.04           | 2016     | +HCOO   | Bibenzyl phenols     |
| 28 | Brazillein                                          | C16H12O5      | Identified            | 284.069                   | 329.0672     | −0.6             | −1.7             | 5.91             | 169.26           | 1333     | +HCOO   | Phenocyanin          |
| 29 | 2,3-(S)-Hexahydroxydiphenoyl-D-glucose              | C20H18O14     | Identified            | 482.0702                  | 527.0684     | 0.5              | 1                | 6.49             | 210.74           | 1336     | +HCOO   | Ellagitannin          |
| 30 | Isotachioside                                       | C13H18O8      | Identified            | 302.1                     | 301.0928     | −0.1             | −0.5             | 7.91             | 195.15           | 1637     | −H      | Phenolic            |
| 31 | Tachioside                                          | C13H18O8      | Identified            | 302.1                     | 301.0928     | −0.1             | −0.5             | 7.91             | 195.15           | 1637     | −H      | Phenolic Glycoside   |
| 32 | Thannilignan                                        | C19H22O5      | Identified            | 330.1464                  | 329.1391     | −0.3             | −1               | 8.03             | 186.08           | 1238     | −H      | Phenolic Glycoside   |
| 33 | 2,3,5,4′-Tetrahydroxystilbene-2-O-(6′-O-α-D-glucopyranosyl)-β-D-glucopyranoside | C26H32O14 | Identified            | 568.1792                  | 567.1719     | 0                | −0.1             | 11.59            | 224.46           | 1544     | −H      | Lignan               |
| 34 | 2′-Hydroxy-3′,4′-dimethoxy-isoflavan-7-O-β-D-glucoside | C23H28O10 | Identified            | 464.164                   | 509.1622     | −4.2             | −8.3             | 16.58            | 221.66           | 1885     | +HCOO   | Glucoside            |
| 35 | Aspidinol                                           | C12H16O4      | Identified            | 224.1048                  | 223.0975     | −0.1             | −0.4             | 12.34            | 200.45           | 1323     | −H      | Simple phenol        |
| 36 | Nisoldipine                                         | C20H24N206    | Identified            | 388.1645                  | 387.1572     | 1                | 2.7              | 16.99            | 205.15           | 1353     | −H      | Alkaloid             |
| 37 | Yakuchinone A                                       | C20H24O3      | Identified            | 312.1757                  | 311.1684     | 3.1              | 10               | 18.56            | 189.48           | 6985     | −H      | Bibenzyl phenol      |
| 38 | 2,7-Dihydroxy-4′-methoxyphenanthrene-2-O-glucoside   | C21H22O8      | Identified            | 402.1354                  | 447.1336     | 3.9              | 8.7              | 18.64            | 214.4            | 1064     | +HCOO   | Phenanthrene phenol  |
2. Experimental Design, Materials and Methods

2.1. Plant collection, authentication, and preparation of plant material

*S. polyanthum* (Wight) Walp. leaves were collected from Sultan Haji Ahmad Shah Agricultural Park, Kuantan, Pahang, Malaysia in May, 2019. The dried leaves samples were deposited into Kulliyyah of Pharmacy Herbarium, International Islamic University Malaysia, with the voucher number of PIIUM-0282-1 and were identified as *Syzygium polyanthum* (Wight) Walp. For the plant's extraction, the leaves were allowed to dry for three weeks at room temperature. The dried leaves were then grinded into powder, macerated in distilled water at 80 °C for 30 min in a bath-sonicator (WiseClean, Switzerland) with the wavelength range of 40–80 λ. The macerated leaves were then filtered using Whatmann filter paper No. 1, and then the filtrate was freeze-dried for a week in a freeze-dryer (CHRIST Model Beta 1-8 LO, Germany) before LC-MS analysis.

2.2. Phytochemical profiling of the aqueous extract of *S. polyanthum* (Wight) Walp

Phytochemical profiling of the aqueous extract of *S. polyanthum* (Wight) Walp. leaves was conducted using an LC-MS instrument, VION Ion Mobility QTOF-MS (Waters, USA) based on the method adopted from our previous study [7]. The crude extract (1 mg) was firstly dissolved in 1 mL distilled water before being filtered using a filter membrane (25 mm diameter, 0.45 μm pore size). 10 μL of sample was then injected into a reversed-phase ACQUITY UPLC HSS (2.1 × 100 mm × 1.8 μm) column system with a binary pump of two different solvents comprising Solvent A and B with the compositions as shown in Table 2. The operating parameters used in the analysis are presented in Table 3.
Table 2
Gradient flow profiles of the mobile phase.

| Time (min) | Flow (μL/min) | Solvent A (Water with 0.1% Formic acid) | Solvent B (Acetonitrile with 0.1% Formic acid) |
|------------|---------------|----------------------------------------|-----------------------------------------------|
| 0          | 0.5           | 99%                                    | 1%                                            |
| 0.5        | 0.5           | 99%                                    | 1%                                            |
| 16         | 0.5           | 65%                                    | 35%                                           |
| 18         | 0.5           | 0%                                     | 100%                                          |
| 20         | 0.5           | 99%                                    | 1%                                            |

Table 3
Operating parameters of Vion IMS QToF analyzer.

| Operating parameters         | Values                                      |
|------------------------------|---------------------------------------------|
| Operation mode (Polarity)    | Negative (–ve)                              |
| Analyzer Mode                | Sensitivity                                 |
| Source type                  | Electrospray ionization (ESI)               |
| Source temperature           | 120 °C                                      |
| Desolvation temperature      | 550 °C                                      |
| Desolvation gas flow rate    | 600 L/h                                     |
| Cone gas                     | 50 L/h                                      |
| Capillary voltage            | 2.50 kV                                     |
| Scan time                    | 0.200 s                                     |
| MS mode                      | High-definition MS                          |
| Scanning range               | 50–1000 m/z                                 |
| Column type                  | ACQUITY UPLC-BEH (Waters, USA)              |
| Dimension                    | C18, 2.1 × 100 mm                            |

2.3. Data acquisition, processing, and reporting

In this study, the Waters® UNIFI [1,7] Scientific Information System with embedded Traditional Medicine library as well as Waters® Screening library databases were utilized for data acquisition, data mining, library searching and report generation. This system utilized the raw data including individual chromatographic peaks, retention time, mass-to-charge ration (m/z), and spectral resolution to match with the library and then generated the summary of identified compounds along with data for its chemical formula, observed neutral mass (Da), observed mass to charge ration (m/z), mass error (in mDa and ppm), observed retention time (min), responses, adducts, observed collision cross-section or CCS (Å²), total fragments found, and the spectral figures for each identified compound. Only identified components with mass error of less than 5 mDa were included in the list http://dx.doi.org/10.17632/8mt9npzyp8.1.

Data Availability

Phytochemical Compounds in Syzygium polyanthum (Wight) Walp. Leaves Collected from Kuantan, Pahang, Malaysia: LCMS dataset (Original data) (Mendeley Data).

Ethics Statement

This research work does not require ethical approval.
Declaration of Competing Interest

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

CRediT Author Statement

T.A. Faiz T. Anuar: Writing – original draft, Formal analysis; Azlini Ismail: Conceptualization, Methodology, Writing – original draft; Izzat Fahimuddin Mohamed Suffian: Supervision, Validation; Azzmer Azzar Abdul Hamid: Writing – review & editing; Mohd Hafiz Arzmi: Writing – review & editing; Muhammad Nor Omar: Supervision, Validation, Writing – review & editing.

Acknowledgments

This project was funded by Minister of Higher Education, Malaysia with grant number FRGS/1/2018/SKK10/UIAM/02/1. The authors would like to acknowledge the staff at Central Laboratory, University Malaysia Pahang and Natural Product Laboratory, Kulliyyah of Science, International Islamic University Malaysia for their technical supports in completing this study. The authors also would like to acknowledge Nurul Alia Risma Rismayuddin for her assistance in drafting the paper.

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