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Data Article

Qualitative dataset on UPLC-QTOF/MS tentative identification of phytochemicals from bioactive extract of *Ipomoea mauritiana* Jacq.

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ABSTRACT

The current data report describes the predictive identification of phytochemical constituents in the bioactive extract of *Ipomoea mauritiana* (IM) whole plant. For several formulations this plant was commonly used as 'Vidari' for Ayurvedic medicine. Traditionally, IM tubers are used to alleviate spinal cord pain, improve breast milk, as a tonic, increase sperm count and treating jaundice. The methanol extract can potentially scavenge free radicals and possess antibacterial activity that could be correlated with its chemical composition. So it is crucial to identify the major compounds of IM. An ultra-performance liquid chromatography coupled electrospray ionization quadrupole time-of-flight mass spectrometry (UPLC-ESI-QTOF/MS) method was adopted to detect the flavonoids, saponins, alkaloids, terpenoids in IM methanol extract. Data presented here is related to a published work Antioxidant and antibacterial activity of *Ipomoea mauritiana* Jacq.: A traditionally used medicinal plant in Bangladesh (Alam et al., 2020). Secondary metabolites were analyzed by the comparison of the mass fragmentation arrangements with Waters UNIFI library that enables for positive identification of the compounds based on the spectral match.

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Specifications Table

Subject area	Pharmacy, Chemistry
Specific subject area	Natural products, analytical chemistry
Type of data	Table and Figures
How data were acquired	The acquired data was from an Ultra-performance liquid chromatography coupled with electrospray ionization quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS) and controlled by Waters® UNIFI Software 1.0.0
Data format	Raw, analyzed
Parameters for data collection	*Ipomoea mauritiana* was obtained from Taingail, Bangladesh and authenticated. The whole plant material was dried and ground to powder to be extracted with MeOH and membrane filtered (0.22 mm) before injecting into the UPLC-QTOF/MS system.
Description of data collection	Identification of different flavonoids, saponins, alkaloids, and terpenoids in the IM extract was accomplished with the help of UPLC-QTOF/MS system. The extract was passed through a C18 UPLC column. A gradient elution of mobile phases comprising solvent A (water + 0.1% formic acid) and solvent B (acetonitrile + 0.1% formic acid) were used. The compounds were detected by a diodaray detector (DAD).
Data source location	Faculty of Industrial Science and Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300, Gambang, Pahang, Malaysia.
Data accessibility	Provided with this article
Related research article	Alam I, Forid SM, Roney M, Aluwi MFFM, Huq M. Antioxidant and antibacterial activity of *Ipomoea mauritiana* Jacq.: A traditionally used medicinal plant in Bangladesh. Clin. Phytoscience (2020) 6:35. (https://doi.org/10.1186/s40816-020-00185-w)

Value of the Data

- Data presented here can be utilized to identify natural flavonoids, saponins, alkaloid and terpenoids by UPLC-ESI-QTOF/MS.
- IM methanol extract has been reported to show antioxidant and anti-microbial activity against varieties of bacteria and fungi in our previous study [1]. It is very important to know the type of compounds responsible for the activity of this extract.
- This data provides researchers with information about the phytochemical compounds of IM that will be of guidance in drug discovery for new clinical application of compounds from this plant.
- This mass spectrometric data can be referred in future studies on IM and comparison will serve as a benchmark for the elucidation of compounds.
- The flavonoids, saponins, alkaloid and terpenoids data would be a valuable reference for any study comparing the phytochemical and biological effects of IM.

1. Data Description

Data represents the UPLC-QTOF/MS base peak frequency characteristics of the positive ionization of different saponins, flavonoid compounds, terpenoids, alkaloids, and glycosides obtained

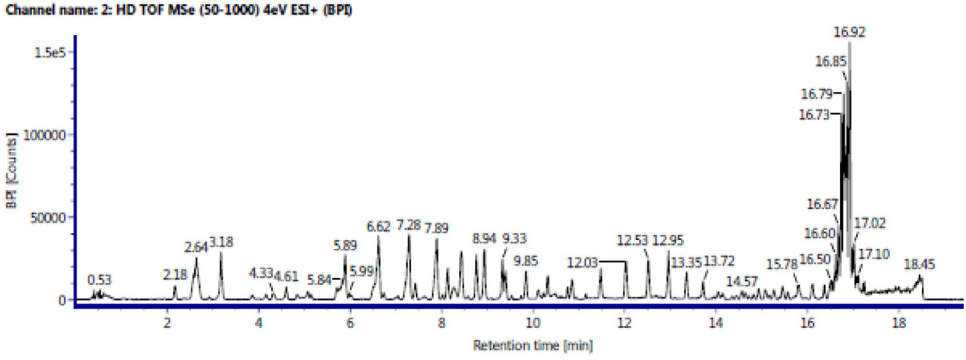

Fig. 1. Base peak chromatogram (BPC) of the crude whole plant methanol extract of *Ipomoea mauritiana*.

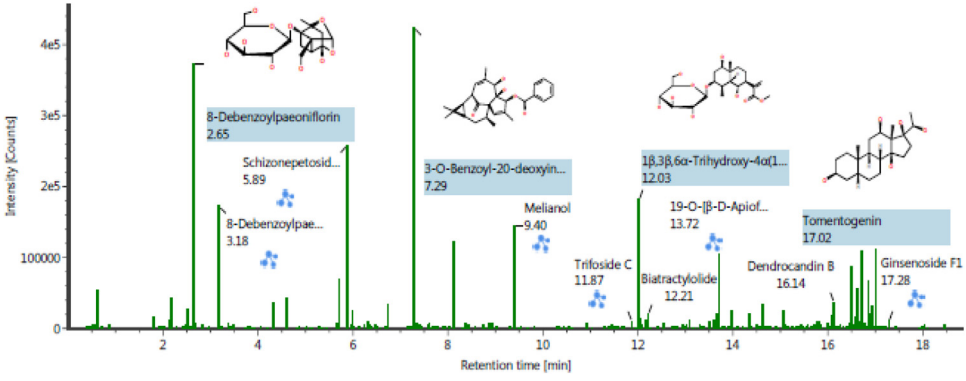

Fig. 2. Identified compounds (B) of methanolic extract of *Ipomoea mauritiana*.

from the methanol extract of IM whole plant comparing with the Waters UNIFI library in the positive ionization mode (Figs. 1 and 2). All the predictive compounds are tabulated in the supplementary table 1.

2. Material, Method Sample Preparation

The powder of IM was taken for extraction and phytochemical analysis. The dry plant material were passed through a grinder to ground into a fine powder (Miyako 3 in one blender, Model No: DL-718, China). As previously mentioned [1], simple maceration technique was applied to prepare the extract. About 50 g of powder was taken in amber glass container and 500 mL methanol was added to soak the powder completely. Occasional shaking and stirring was applied and kept overnight. The following day, the extractive was then filtered using Whatman filter paper number 1. The same process were continued for 3 days until a clear filtrate was obtained. The filtrate was vacuum-dried by a rotary evaporator at 40 °C (RE 200, Sterling, UK) and kept at 4 °C for further analysis.

The profiling of phytochemicals in IM methanol extract was carried out using Vion IMS LCQTOF/MS (Waters, USA). The instrument was equipped with a binary pump, an auto sampler, a degasser and a diodearray detector (DAD). The phytocamicals were tentatively assigned using Waters® UNIFI Software 1.0.0. An ACQUITY UPLC HSS T3 C_{18} (2.1 mm × 100 mm, 1.8 µm) chromatography column was used. A combined mobile phase was prepared comprising solvent system A (water with 0.1% formic acid) and solvent system B (acetonitrile with 0.1% formic acid).

A gradient elution system was obtained from previous works [2,3]. Briefly, 90% solvent A and 10% solvent B (0.00 min), 90% solvent A and 10% solvent B (0.00–1.25 min), 45% solvent A and 55% solvent B (1.25–4.17 min), 10% solvent A and 90% solvent B (4.17–6.25 min) and lastly 90% solvent A and 10% solvent B (6.25–8.34 min). The flow rate was 0.5 mL/min with an injection volume of 20 mL keeping column temperature at 40 °C. For the operating conditions, low and high collision energy were 4.00 eV and 40.00 eV respectively, sample temperature desolvation temperature were 15 and 550 °C respectively. The flow rate of gas was 0.5 mL/min with the cone gas of 50 L/h was maintained. A 2.0 kV of capillary voltage and a 800 L/h of desolvation gas flow rate were set. The mass range was 50–1000 m/z.

Declaration of Competing Interest

Authors declare no conflict of interest.

Acknowledgement

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2021.106839.

References

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[2] OR. Alara, NH. Abdurahman, CI. Ukaegbu, NH. Azhari, *Vernonia cinerea* leaves as the source of phenolic compounds, antioxidants, andanti-diabetic activity using microwave-assisted extraction technique, Ind. Crop. Prod. 122 (2018) 533–544.
[3] OR. Alara, NH. Abdurahman, Ukaegbu, Soxhlet extraction of phenolic compounds from *Vernonia cinerea* leaves and its antioxidant activity, J. Appl. Res. Med. Aromat. Plants 11 (2018) 12–17.