Data Article

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Metabolomics data of *Mitragyna speciosa* leaf using LC-ESI-TOF-MS

Rubashiny Veeramohan [a], Kamalrul Azlan Azizan [a],
Wan Mohd Aizat [a], Hoe-Han Goh [a], Sharif Mahsufi Mansor [b],
Nur Sabrina Mohd Yusof [b], Syarul Nataqain Baharum [a],
Chyan Leong Ng [a,*]

[a] *Institute of Systems Biology (INBIOSIS), Universiti Kebangsaan Malaysia UKM, 43600 Bangi, Selangor, Malaysia*

Q2 [b] *Centre for Drug Research, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia*

ARTICLE INFO

ABSTRACT

Mitragyna speciosa is a psychoactive plant known as "ketum" in Malaysia and "kratom" in Thailand. This plant is distinctly known to produce two important alkaloids, namely mitragynine (MG) and 7-hydroxymitragynine (7-OH-MG) that can bind to opioid receptors (Kruegel et al., 2016) [1]. MG was reported to exhibit antidepressant properties in animal studies (Hamid et al., 2017) [2]. Hence, these compounds were proposed to have the potential to replace morphine with much lower risks of side effects (Raffa, 2015) [3]. To date, there are only over 40 metabolites identified in *M. speciosa* (Adkins et al., 2011; Yearsley, 2016) [4,5]. To obtain a more complete profile of secondary metabolites in ketum, we performed metabolomics study using mature leaves of the green *M. speciosa* variety. The leaf samples were extracted using methanol prior to liquid chromatography-electrospray ionization-time of flight-mass spectrometry (LC-ESI-TOF-MS) analysis. This data can be useful to for the identification of unknown metabolites that are associated with alkaloid biosynthesis pathway in *M. speciosa*.

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* Corresponding author.
  E-mail addresses: nataqain@ukm.edu.my (S.N. Baharum), clng@ukm.edu.my (C.L. Ng).

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Specifications Table

Subject area	Biology
More specific subject area	Metabolomics
Type of data	Analyzed LC-ESI-TOF-MS Data
How data was acquired	Raw data attained from MicroTOF-Q III (Bruker Daltonic) using an ESI positive ionization coupled with Ultimate 3000 UHPLC system (Dionex)
Data format	Analyzed data in the form of.xlsx file
Experimental factors	Methanolic extracts from mature leaves of *M. speciosa* of the green variety
Experimental features	Data was processed using ProfileAnalysis 2.1
Data source location	Bangi, Malaysia
Data accessibility	Supplementary Table 1

Value of the data

- LC-MS data allow metabolite profiling and the identification of target metabolite compounds present in *M. speciosa* leaf.
- The data will also be useful in the reconstruction of secondary metabolite biosynthesis pathway in *M. speciosa*.
- Metabolomics analysis will provide insights on the metabolite expression in mature leaf of *M. speciosa*.

1. Data

This dataset shows the retention time (RT), mass-to-charge (*m/z*) values of compounds detected in mature leaves of the green variety of *Mitragyna speciosa*, and normalized peak intensity values of five biological replicates, each with five technical replicates. The raw data was obtained from mass spectrometry (MS) analysis and was processed using ProfileAnalysis 2.1 (Bruker). The processed data is provided in Microsoft Excel (.xlsx) file (Supplementary Table 1).

2. Experimental design, materials and methods

2.1. Chemicals and reagents

Analytical-grade methanol (CH_3OH) was purchased from Merck, Germany. Umbelliferone ($C_9H_6O_3$, purity 99%) was purchased from Sigma-Aldrich, USA.

2.2. Sample preparation

Mature leaf samples of *M. speciosa* were flash frozen using liquid nitrogen, supplied by Universiti Sains Malaysia. The frozen leaves were stored in $-80\,°C$ freezer prior to metabolite extraction.

2.3. Metabolite extraction

Sample extraction was done based on [6] with slight modifications. Mature leaves were individually ground with mortar and pestle in liquid nitrogen, weighed and transferred into respective