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Data Article

LC-MS data for metabolomics analysis of *Garcinia mangostana* L. seed germination

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ABSTRACT

Metabolic regulation is important during seed germination for the establishment of seedling. The germination strategy of mangosteen (*Garcinia mangostana* L.) seed is thought to be unique due to its recalcitrant characteristic (sensitive to coldness and drying). To investigate the metabolic changes during seed germination, we performed metabolomics analysis on germinating mangosteen seed sown after zero, one, three, five, seven and nine days. Sampled mangosteen seeds were subjected to methanol extraction prior analysis using Liquid Chromatography-Time of Flight-Mass Spectrometry (LC-TOF-MS). MS data were further analyzed using ProfileAnalysis (version 2.1). This is one of the earliest reports in metabolite identification and profiling of mangosteen seed at different germination stages. This data article refers to the article entitled "Metabolite profiling of mangosteen seed germination highlights metabolic changes related to carbon utilization and seed protection" (Mazlan et al., 2019) [1].

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Specifications table

Subject area	Biology
More specific subject area	Metabolomics
Type of data	Table
How data was acquired	Dionex liquid chromatography platform (Ultimate 3000 UHPLC+, Thermo Scientific) coupled with a MicroTOF-QIII (Bruker, Germany) MS system with electrospray ionization (ESI) in positive mode was used to obtain mass spectrometry data.
Data format	Analyzed data in XLSX format.
Experimental factors	Mangosteen seed at different germination stages (seed sown after zero, one, three, five, seven and nine days) extracted using methanol solvent.
Experimental features	LC-TOF-MS was used to analyze methanol extract of seed samples and acquired raw data were processed using ProfileAnalysis (version 2.1) and MS Excel 2016 for tabulation.
Data source location	UKM Bangi, Malaysia (2.922662 °N, 101.786690 °E)
Data accessibility	Data is within this article
Related research article	O. Mazlan, W.M. Aizat, N. S. A. Zuddin, S.N. Baharum, N.M. Noor, Metabolite profiling of mangosteen seed germination highlights metabolic changes related to carbon utilization and seed protection [1]

Value of the data

- The LC-MS platform enables a comprehensive metabolite profiling for mangosteen seed germination at different stages (zero, one, three, five, seven and nine days after sowing).
- This permits the identification of metabolites or potential biomarkers during the germination of mangosteen seed which is known to be recalcitrant (sensitive to cold and dry conditions).
- Understanding metabolic expression and regulation in mangosteen seed germination may provide valuable insights towards developing better preservation strategy for this recalcitrant seed.
- Furthermore, this data can be analyzed in conjunction with the transcriptome data [2] for an integrated examination of metabolic pathways of recalcitrant seed germination in mangosteen.

1. Data

Data presented in this manuscript are related to the earlier report entitled “Metabolite profiling of mangosteen seed germination highlights metabolic changes related to carbon utilization and seed protection” [1]. It consists of retention time (RT) to molecular ions’ mass over charge ratio (m/z) listed as table in XLSX format. To create the table, raw LC-MS data of six mangosteen seed germination stages (zero, one, three, five, seven and nine days after sowing) with three biological replicates per stage were analyzed using ProfileAnalysis and tabulated using MS Excel as per [3].

2. Experimental design, materials and methods

2.1. Plant materials

Mature fruits were picked from mangosteen tree plots at Universiti Kebangsaan Malaysia, Bangi, Malaysia. Preparation for seed de-pulping, cleaning, planting and selecting seeds for extraction followed Mazlan et al. [1].

2.2. Metabolite extraction

Methanol extraction of seed employed methods detailed by Roessner et al. [4] with modifications [1,5].

2.3. Liquid Chromatography-Mass Spectrometry (LC-MS) protocol

Dried samples were resolubilized in methanol. This study adheres to Glauser et al. [6] method with adjustments as detailed in [1] and [5]. Separation of compound utilizing liquid chromatography system (Ultimate 3000 UHPLC+, Thermo Scientific, USA) outfitted with a C18 column was performed as per Mamat et al. [7].

2.4. Mass spectrometry data treatment and handling

MS raw data (*.d* format) were imported into ProfileAnalysis 2.1 (Bruker, Germany) for bucketing using Find Molecular Features settings as per Mamat et al. [7] with smoothing width: 2 [3]. Bucket generation was set as follows: advanced bucketing feature calculated using parameters from time alignment, time range 2.00 minutes until 30.00 minutes, mass range 50 *m/z* to 1000 *m/z*, normalization is by sum of bucket values in analysis. Then, the data were exported to Microsoft Excel 2016 for tabulation.

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Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.072.

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.072.

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