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Data Article

A comprehensive metabolomic data set of date palm fruit

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ARTICLE INFO

Article history: Received 4 February 2018 Received in revised form 22 March 2018 Accepted 4 April 2018 Available online 10 April 2018

ABSTRACT

This article provides detailed information on the phenotypes and the metabolic profiles of 196 date fruits from 123 unique date fruit varieties. These date fruits are extensively diverse in their country of origin, variety and post harvesting conditions. We used a nontargeted mass-spectrometry based metabolomics approach to metabolically characterize date fruits, and measured 427 metabolites from a wide range of metabolic pathways.

The metabolomics data for all the date fruit samples are available at the NIH Common Fund's Data Repository and Coordinating Center (supported by NIH grant, U01-DK097430) website, http://www.metabolomicsworkbench.org), under Metabolomics Workbench StudyID: ST000867. The data are directly accessible at http://www.metabolomicsworkbench.org/data/DRCCMetadata. php?Mod

e = Study & Study ID = ST000867 & Study Type = MS & Result Type = 1.

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https://doi.org/10.1016/j.dib.2018.04.012

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| Subject area | Plant Biology |
|----------------------------|---|
| More specific subject area | Plant physiology, Metabolomics |
| Type of data | Tables, Figures, images |
| How data was acquired | non-targeted mass-spectrometry based metabolomics |
| Data format | Raw data, image files |
| Experimental factors | Samples were frozen at $-$ 80 °C without any treatment |
| Experimental features | Samples were preprocessed and the metabolite measurement was done |
| | on Gas Chromatography Mass Spectrometry (GC-MS) and the Orbi- |
| | trap Elite Accurate Liquid Chromatography Mass Spectrometry (LC– |
| | MS/MS) platforms |
| Data source location | Samples were collected from 14 different countries, including Qatar, |
| | UAE, Iran, Saudi Arabia, Egypt, Pakistan, Libya, Tunisia, USA, Morocco, |
| | Jordan, Sudan, Oman and Spain and metabolomics analysis was done |
| | by Metabolon Inc. |
| Data accessibility | The data is deposited to data repository, Metabolomics Workbench under |
| | StudyID: ST000867. Also available with this article. |

Specifications Table

Value of the data

- This data presents the metabolic variation in date fruits and can be used to identify healthiest varieties.
- Since the data includes fresh and processed samples, the impact of date fruit processing can be investigated.
- Fruits from all collected varieties are available at our Bio-bank for future collaborative research.

1. Data

Here we describe a freely available non-targeted metabolomics data set together with phenotypic information of 196 date fruit samples. To provide wide geographical coverage, we collected dates from 14 different countries including Qatar, United Arab Emirates (UAE), Iran, Saudi Arabia, Egypt, Pakistan, Libya, Tunisia, United States of America (USA), Morocco, Jordan, Sudan, Oman and Spain. Since developmental stage can impact the metabolic profile, we included date fruits at different ripening stages from ten different varieties. Additionally, biological replicates from forty varieties were included.

2. Experimental design, materials and methods

2.1. Sample collection

The samples were collected in two separate batches. A first collection was performed in 2012 followed by a second collection in 2013. The first batch contained only mature dates, whereas in the second batch included both mature dates and dates at different ripening stages. Dates were mostly acquired from commercial sources such as shops, markets and date festivals. Depending on availability, up to ten individual dates from same date variety were collected.

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