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Data Article

Data from identification of diagnostic biomarkers and metabolic pathway shifts of heat-stressed lactating dairy cows

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ABSTRACT

Controlling heat stress (HS) is a global challenge for the dairy industry. In this work, an integrated metabolomics and lipidomics approach using ^{1}H nuclear magnetic resonance (NMR) and ultra-fast LC–MS in combination with multivariate analyses was employed to investigate the discrimination of plasma metabolic profiles between HS-free and HS lactating dairy cows. Here we provide the information about the acquiring and processing of raw data obtained by ^{1}H NMR and LC–MS techniques. The data of present study are related to the research article "Identification of diagnostic biomarkers and metabolic pathway shifts of heat-stressed lactating dairy cows" in the Journal of Proteomics (Tian et al., J. Proteomics, (2015), doi:10.1016/j.jprot.2015.04.014).

Specifications table

Subject area	Biology
More specific subject area	Plasma metabolomics

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Type of data	Table, figure, excel file
How data was acquired	^{1}H NMR and UFLC–MS (Bruker Biospin Billerica) Ultra-fast LC(Shimadzu) 5600 Triple TOF mass spectrometer(Applied Biosystems/MDS Sciex) QTRAP 5500 (Applied Biosystems/MDS Sciex) TopSpin software (version 3.0; Bruker Biospin) AMIX software package (version 3.8.3, Bruker Biospin) MATLAB R2012a software (MathWorks, Natick, MA, USA) SIMCA-P 12.0 software package (Umetrics AB, Umeå, Sweden) Analyst® TF 1.6 Software (Applied Biosystems/MDS Sciex) open-source XCMS package (version 1.20.1) Human Metabolome database and METLIN database
Data format	Analyzed
Experimental factors	Plasma samples from Chinese Holstein cows with and without heat stress were collected to characterize the metabolic changes induced by heat stress (HS)
Experimental features	Integrated metabolomics and lipidomics using ^{1}H nuclear magnetic resonance (NMR) and UFLC–MS techniques
Data source location	Beijing, China
Data accessibility	Programs of data transformation are directly provided with this article

Value of the data

The data of multivariate analysis highlight the significant differences of plasma metabolic profiling between HS and HS-free dairy cows.

The data point out the potential biomarkers of HS dairy cows.

The data provide insights into shifted pathways of dairy cows induced by HS.

1. Data, experimental design, materials and methods

1.1. Sample collection and experimental design

All experiments involving animals were conducted according to the principles of the Chinese Academy of Agricultural Sciences Animal Care and Use Committee (Beijing, China). Fasting blood samples were collected before morning feeding from the caudal veins of Holstein dairy cows, put into K2 EDTA anti-coagulation vacuum tubes, and centrifuged at 1600*g* for 10 min at 4 °C. The supernatants were transferred to tubes, frozen quickly, and stored at −80 °C until use. An overview of the experimental design to acquire the data in present article is shown Fig. 1.

1.2. Sample preparation

For LC–MS metabolomics analysis, 150 μL aliquots of each thawed plasma sample were mixed with 600 μL ice-cold acetonitrile, vortexed, and centrifuged for 10 min at 10,000 rpm and 4 °C. The 650 μL supernatant of each sample was transferred to another tube, and concentrated to dryness with a SpeedVac Concentrator (SPD121P, Thermo Savant, Waltham, MA, USA). Each dried sample was reconstituted in 100 μL ACN/H_2O (1:99 v/v), and filtered through a Captiva 96-well filter plate (Agilent, Santa Clara, CA, USA) for analysis.

For analyses of the plasma lipidome, a modified preparation method was used [2]. Briefly, a 30 μL aliquot of each plasma sample was mixed with 200 μL methanol, followed by the addition of 660 μL methyl *tert*-butyl ether, and vortexing of the sample. Subsequently, 150 μL water were added to each tube, the samples were vortexed for 5 min, incubated for 5 min, and centrifuged for 5 min at 10,000 rpm and 4 °C. The upper layers (500 μL) were collected, evaporated to dryness using a SpeedVac SPD121P concentrator, and re-dissolved in 500 μL of ACN/isopropanol/H_2O (65:30:5 v/v/v). The corresponding solvents were filtered through a Captiva 96-well filter plate for LC–MS analysis.

For NMR analysis, the plasma samples were centrifuged for 10 min at 1600*g* and 4 °C. The supernatants (20 μL) were collected, mixed with 40 μL of deuterium oxide containing 1 mM 3-(trimethylsilyl) propionic-2,2,3,3,d4 acid sodium salt, and transferred to 1.7 mm NMR tubes for analysis.