Data Article

Data on coffee composition and mass spectrometry analysis of mixtures of coffee related carbohydrates, phenolic compounds and peptides

Ana S.P. Moreira [a], Fernando M. Nunes [b], Cristiana Simões [b], Elisabete Maciel [a,c], Pedro Domingues [a], M. Rosário M. Domingues [a], Manuel A. Coimbra [a,*]

[a] QOPNA, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal
[b] CQ-VR, Chemistry Research Centre, Department of Chemistry, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal
[c] CESAM, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal

A B S T R A C T

The data presented here are related to the research paper entitled "Transglycosylation reactions, a main mechanism of phenolics incorporation in coffee melanoidins: inhibition by Maillard reaction" (Moreira et al., 2017) [1]. Methanolysis was applied in coffee fractions to quantify glycosidically-linked phenolics in melanoidins. Moreover, model mixtures mimicking coffee beans composition were roasted and analyzed using mass spectrometry-based approaches to disclose the regulatory role of proteins in transglycosylation reactions extension. This article reports the detailed chemical composition of coffee beans and derived fractions. In addition, it provides gas chromatography–mass spectrometry (GC–MS) chromatograms and respective GC–MS spectra of silylated methanolysis products obtained from phenolic compounds standards, as well as the detailed identification of all compounds observed by electrospray mass spectrometry (ESI-MS) analysis of

roasted model mixtures, paving the way for the identification of the same type of compounds in other samples.

Specifications Table

Subject area	*Chemistry*
More specific subject area	*Composition of coffee and mass spectrometry analyses of coffee related carbohydrates, phenolic compounds and peptides*
Type of data	*Tables and figures*
How data was acquired	*Methanolysis products were analyzed by GC–MS (Trace-GC with Polaris Q MS, Thermo-Finnnigan, San Jose, CA)*
	Content of chlorogenic acids, caffeine, adsorbed phenolics, and phenolics released by alkaline saponification and alkaline fusion was obtained by HPLC (Dionex Ultimate 3000, Thermo, Waltham, MA);
	Content of sucrose, glucose and fructose was determined by anion exchange chromatography (ICS 3000, Dionex);
	Total sugars were determined by GC-FID (Trace GC, Thermo-Finnigan);
	Protein content was determined using a carbon-nitrogen/protein analyzer (PRIMACS, Skalar Analytical B.V., Breda, The Netherlands);
	Roasted coffee powder colors were measured with a CR-300 Minolta chroma meter (Tokyo, Japan);
	HPLC-ESI-MS analysis used a Waters Alliance 2690 HPLC system (Milford, MA) coupled to the LXQ linear ion trap (LIT) mass spectrometer (Thermo Fisher Scientific Inc., Waltham, MA);
	Direct ESI-MS analyses were also performed using LIT mass spectrometer;
	High resolution and high mass accuracy measurements were performed on a LTQ-Orbitrap XL mass spectrometer (ThermoFisher Scientific, Germany).
Data format	*Analyzed*
Experimental factors	*Roasted model mixtures and coffee beans*
Experimental features	*Chemical characterization and identification of the changes induced by roasting*
Data source location	*Robusta coffee beans from India*
	Arabica coffee beans from Honduras
	Commercial standards of carbohydrates, phenolic compounds and peptides
Data accessibility	*Data is provided with this article*

Value of the data

- Detailed chemical characterization of Arabica and Robusta coffee beans and derived fractions is able to be compared with data from other authors when profiling the phenolic compounds incorporated in melanoidins.