Quantitative lipidomics in green robusta coffees from the Brazilian Amazon by LC-HRMS

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Coffea arabica L. (arabica coffee) and *Coffea canephora* (robusta coffee) are the two economically relevant coffee species commercialized worldwide. Although arabica coffee is more reveleant economically than robusta coffee, an effort has been made to improve the quality of robusta coffees. Brazil is the second largest robusta coffee producer in the world, and its production is concentrated in the states of Espirito Santo and Rondônia. In 2003, the Brazilian Agricultural Research Corporation (Embrapa) located in Rondônia developed ten hybrid cultivars with high yield potential and agronomic characteristics typical of the conilon and robusta botanical varieties The state of Rondônia (located in the Amazon Region of Brazil) is known for the development of specialty robusta coffees with high productivity and disease resistance Lipids play an important role in coffee bean development and impact the coffee brew quality. The lipid fraction of raw coffee beans is mainly composed of triacylglycerols (TG) and other minor constituents, such as diterpenes, sterols, phospholipids (PL), and $^{?}$*N*-alkanoyl-5-hydroxytryptamides (C_n-5HT). Despite these classes of compounds having been previously characterized by lipidomics, this approach was limited to semi-quantitative analysis. In this work, we developed a multiclass quantitative approach using liquid chromatography-high resolution mass spectrometry to quantify lipids in raw robusta coffees from different producers of the Brazilian Amazon region. The quantitative method for LPC, PC, PI, PG, DG, TG, and C_n-5HT classes was successfully developed and validated. The total lipid content in the robusta coffees ranged from 17.13-29.03 g $100g^{-1}$ for TG, 1.44-2.10 g $100g^{-1}$ for DG, 0.27-0.53 g $100g^{-1}$ for PC, 0.34-0.36 g $100g^{-1}$ for FI, 0.10 – 0.19 g 100 g^{-1} for C_n-5HT, and 0.01 g $100g^{-1}$ for LPC. In addition, individual components from the C_n-5HT class were analyzed. PC, PI, TG, DG, and C_n-5HTs were relevant factors in discriminating the coffee samples according to their origin. Therefore, these results can help to further understand how the lipid composition of coffee beans is related to the place of harvest and the development of origin certificates of Amazon robusta coffees.

Agradecimentos: The authors thank Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Coordenação de Aperfeiçoamento de Nível Superior – Brasil (CAPES) Finance code 001, Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ), and EMBRAPA Café for financial support.