

[P.FC.69]

Screening for emerging metabolites by ESI-QTOF in arabica coffee under different roasting levels

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Brazil is the world largest coffee producer but its performance as roasted and ground coffee exporter still needs investments in order to boost exports. The objective of this work was qualitatively comparing Arabica coffee ions profile in different levels of roasting in order to found potential roasting markers. Samples of Arabica coffee from Minas Gerais state were roasted at light, medium, dark and very dark roastings. Green beans were also evaluated. Extracts of 1 g of whole beans were treated in ultrasound bath during 1 minute with a solution of methanol and 0.1% formic acid. A QTOF Waters Synapt[®] G1 mass spectrometer was used. ESI (+) source temperature: 80 °C; Desolvation: 40 °C; Capillary 3.0 kV; Cone: 22V; Cone extraction: 7,0V; N₂ flow: cone: 60mL/min; desolvation: 300mL/min and default energy in collision cell. Screenings were performed during five minutes in direct infusion mode. Ions profiles were reproducible despite possible ion suppression problems in the ESI source and also the lower sensitivity of QTOF as a high-resolution equipment. In the relatively low molecular region of spectra characteristic ions of coffee matrix and/or its sodium/potassium adducts were found. Sucrose and chlorogenic acid were found in green and soft roast only. Trigonelline levels appeared even in very dark roasts, which is in according to the literature. Since its degradation occurs at about 80% to niacin. Other roast dependent species found were fatty acid tryptamides (serotonin derivatives), substances also responsible for coffee stomach irritation. As the roasting level arises other ions with good relative intensity presented the same behavior, but they were not fully identified yet. Nevertheless, ions with high molecular mass (800-900 Da) were produced in higher roasting levels. Results obtained with this work support additional investigations using bean surface analysis with an EASI source.

Keywords: roast, ESI-QTOF, mass spectrometer