Quality control of *Coffea canephora* genotypes cultivated in the state of Espírito Santo (Brazil) by ESI-FT-ICR MS

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Introduction: The quality of coffee is related to good production practices in agriculture, among these factors are genetic improvement. Cloning influences the final product and therefore, sensory and analytical analyzes are extremely important for quality control. The aim of this study was to analyze the results obtained by the ESI($\pm$)FT-ICR MS and compare them with the data from the sensory analysis.

Materials/Methods: The 42 coffee genotypes in northern Espírito Santo were sent for sensory analysis, performed by Q-Graders. Subsequently, the samples were also analyzed by ESI($\pm$)FT-FT MS. Based on the results obtained, chemometric models were constructed by principal component analysis (PCA). Pre-treatment optimization was carried out in order to obtain the excellent models.

Table 1. Sensory analysis results

CLASS	SAMPLE	SENSORY RANGE
1	8	58
2	28, 29	70-72,5
3	1, 11, 12, 9, 24, 33, 37, 39	72,5-75
4	2, 3, 4, 5, 6, 10, 13, 19, 21, 25, 27, 30, 31, 32, 34, 35, 38, 41, 42	75-77,5
5	7, 14, 15, 16, 17, 18, 20, 22, 23, 26, 40, 43	77,5-80
6	36	80-82,5

Results/Discussion: Sensory analysis data resulted in low values for sample 8, 28 and 29. In contrast, sample 36 has the highest score in the assessment (**Table 1**). In the analysis of main components taking into account the best separation of the samples and the explained variance values, after the pretreatments of the models, it was possible to notice that the ESI(+), Fig. 1, shows that in PC1>0 there is the sample 36, while in PC1<0, samples 28 and 29.However, through ESI(-), Fig. 2, it was possible to notice better clusters. PC3 separated the samples with the lowest/highest score in the sensory evaluation. The loads graph identifies that at PC3<0 the ions of *m/z* 255, 367, 353 and 361, respectively, palmitic acid, feruloylquinic acid, caffeoylquinic acid and internal standard, are the main ones for discrimination.
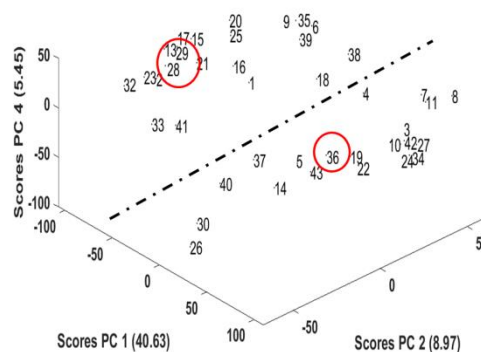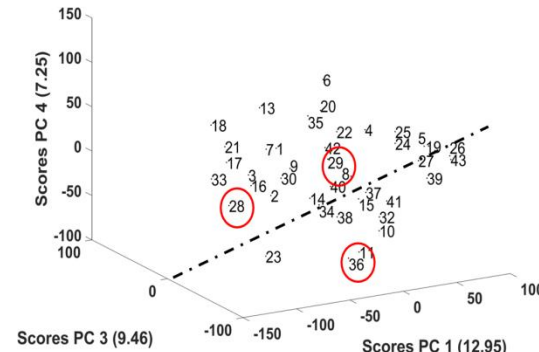

Figure 1. ESI(+) FT-ICR MS results.

Figure 2. ESI(-) FT-ICR MS results.

Conclusion/Perspectives: The ESI-FT-ICR MS proved to be an appropriate technique for classification in the quality control of genetically modified Conilon coffees.