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METABOLOMIC PROFILING OF GREEN AND MATURE BEANS OF COFFEA ARABICA GENOTYPES BY GC-MS: INSIGHTS INTO QUALITY MARKERS

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The metabolomic profiling of coffee beans provides valuable insights into the biochemical factors that determine beverage quality, particularly for *Coffea arabica*, the most widely cultivated species for specialty coffees. In this study, green and mature beans from three *C. arabica* genotypes (Arara, Catucaí 785-15, and Catuaí 62), collected in experimental fields located in Brejetuba, Espírito Santo, Brazil, were subjected to gas chromatography coupled to mass spectrometry (GC-MS) to characterize their chemical composition, followed by multivariate statistical analysis. A total of 28 metabolites were identified, comprising sugars, organic acids, phenolic compounds, and alkaloids. Clear biochemical shifts were observed during ripening, with mature beans enriched in sucrose, fructose, and chlorogenic acids, while green beans exhibited higher levels of trigonelline, caffeine, and certain amino acids. Principal Component Analysis (PCA) revealed a distinct separation between green and mature beans and a partial exploration among genotypes. Arara was characterized by higher accumulation of reducing sugars and a sweeter chemical profile, Catucaí 785-15 by balanced levels of phenolics contributing to acidity and aromatic complexity, and Catuaí 62 by elevated caffeine and chlorogenic acid levels, associated with stronger body and bitterness. Hierarchical clustering and heatmap analyses confirmed that maturation stage was the primary discriminant factor, although genotypic differences remained evident, suggesting a strong genetic control of metabolite accumulation. These findings highlight key metabolic markers for maturation and genotype, providing valuable tools for selecting superior *C. arabica* cultivars with enhanced sensory quality. This work reinforces metabolomics as a powerful strategy for the research and valorization of Brazilian specialty coffee.

Keywords: *PCA, Multivariate analysis, Specialty coffee, Espirito Santo, Chlorogenic acid, Maturation stage.*