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Beyond the First Cup: Untargeted Metabolomics Reveals Metabolite Depletion and Persistence Across Multiple Coffee Brewing Cycles

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Abstract

Coffee brewing is a dynamic solid–liquid extraction process, yet the fate of metabolites beyond the conventional single brewing cycle remains unclear. Here, untargeted UPLC-QTOF-MS/MS–based metabolomics was applied to systematically profile metabolites depleted and retained across multiple brewing cycles under three roasting levels. The results showed that brewing cycle exerted a stronger influence on metabolite features than roasting level, with over 98% of features significantly affected. Multivariate analysis indicated that the first cycle differed most distinctly from subsequent cycles. A total of 1030 negative and 360 positive features were identified as significantly different between the first and subsequent cycles. Key depleted metabolites were confirmed using authentic standards as phloretic acid, shikimic acid, quinic acid, and caffeine, each decreasing over tenfold from the first to the second cycle. Notably, the second cycle retained the highest intensities of several bioactive compounds, including caffeoylquinic acid and its derivatives (dimer, lactone, and methyl ester), along with caffeine, cysteinesulfenic acid, and levoglucosan. This study provides scientific evidence supporting the effectiveness of conventional single-cycle brewing. Meanwhile, by revealing the retention of bioactive compounds beyond the initial brew, it highlights the potential of their targeted recovery from coffee by-products, thereby contributing to sustainable waste valorization and functional ingredient development.

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