Upcycling Coffee Waste: Sustainable Oil Recovery and Lipidomic Profiling of Spent Coffee Grounds

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Spent coffee grounds (SCG), a major by-product of the global coffee industry, represent an underexploited source of bioactive lipids with promising applications in cosmetics, nutraceuticals, and functional foods. This study presents a novel, integrative approach that combines green extraction techniques with advanced multi-omics profiling to sustainably recover and characterize high-value oil from SCG.

Three green extraction methods, ultrasonic-assisted extraction (UAE), supercritical CO_2 (SC-CO_2), and ethanol maceration, were evaluated alongside conventional Soxhlet hexane extraction. The oil yield ranged from 8.3% (SC-CO2) to 10.5% (UAE), with green techniques demonstrating superior efficiency and compound preservation. Untargeted lipidomics was conducted using LC-QTOF-MS with reversed-phase chromatography to comprehensively profile triacylglycerols, ceramides, Fatty Acid esters of Hydroxy Fatty Acids (FAHFAs), and oxidized lipids. Targeted LC-MS/MS quantified oxidized phosphatidylcholines (OxPCs), while HPLC was used to identify and quantify α-, β-, and γ-tocopherols. Volatile compounds of the extracted oil were analyzed via HS-SPME GC-MS, and polar metabolites were profiled using HILIC-LC-QTOF-MS.

Lipidomic data were processed using open-source tools, including MS-DIAL and GNPS, allowing for robust data processing, deconvolution, alignment and identification. Multivariate analysis of PLS-DA models showed clear separation and tight clustering of samples according to extraction method, reflecting distinct lipidomic signatures. Importantly, green extraction techniques led to a 50% increase in FAHFAs and over 80% higher ceramide content compared to Soxhlet extracts. These findings reveal not only greater lipid diversity but also enhanced recovery of functionally important compounds known for anti-inflammatory, skin health, and metabolic benefits.

In contrast, green extraction techniques resulted in a markedly lower contet of OxPC species, which are often associated with lipid degradation and oxidative stress. This suggests that UAE, SC-CO_2, and ethanol maceration provide a milder extraction environment, minimizing lipid oxidation compared to Soxhlet hexane extraction. Additionally, tocopherol content—particularly α-, β-, and γ-tocopherols—was significantly higher in green extracts, indicating better preservation of natural antioxidants.

This work demonstrates the synergistic power of green chemistry and omics-driven analysis for the valorization of agri-food waste. The comprehensive dataset and methodological framework provide a scalable model for transforming SCG into high-value bioactive ingredients, contributing the way for more sustainable and economically viable industrial applications.