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MULTIVARIATE ANALYSIS APPLIED TO CAFFEINE EXTRACTION USING CHOLINE BASED NADES

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Coffee, a raw material rich in bioactive molecules, has a long-standing history of consumption in Brazil and worldwide. Among these molecules, caffeine (1,3,7-trimethylxanthine) stands out due to its stimulant, anti-inflammatory, and diuretic properties. With the growing interest in environmentally sustainable practices, several programs have been developed to encourage the adoption of less environmentally harmful extraction processes. Over the past decade, Deep Eutectic Solvents (DES) and their natural counterparts (Natural Deep Eutectic Solvents – NADES) have gained increasing prominence. These solvents are biodegradable, biocompatible, exhibit low flammability, high dissolution capacity, and are cost-effective. In the search for optimal extraction conditions using DES or NADES, mathematical modeling has been successfully employed to optimize the overall process. In this context, the present study aimed to optimize caffeine extraction from roasted and ground coffee powder, evaluating which choline-based NADES formulation (Choline Chloride:Lactic Acid – ChCl:LA, Choline Chloride:Oxalic Acid – ChCl:OA, Choline Chloride:Citric Acid – ChCl:CA, Choline Chloride:Urea – ChCl:U, or Choline Chloride:Tartaric Acid – ChCl:TA) yielded the best caffeine extraction using the water bath extraction method. Furthermore, the study evaluated which variables (extraction time, temperature, water volume, and NADES mass) exerted the greatest influence on the extraction efficiency. Caffeine quantification was performed using the standard addition method. Based on previously developed studies (Grise et al., 2025), multivariate analysis revealed that the use of ChCl:LA in a 1:1.5 molar ratio resulted in the extraction of 56.1 mg/g of caffeine under optimized extraction conditions (15 minutes, 90 °C, 5 mL of water, and 10 g of NADES). The most influential variables identified were the amount of NADES and the extraction temperature. Regarding the analysis of the most effective extracting solvent, the following combinations were identified as the most efficient (in descending order): ChCl:OA, ChCl:LA, and ChCl:U. Moreover, ATR-FT-IR spectroscopy enabled the identification of bonds and interactions among the constituents of the selected NADES. Further studies focusing on optimizing caffeine extraction using ChCl:OA, as well as the development and optimization of a ternary system, are currently underway.
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