SIMPLEX CENTROID MIXTURE DESIGN AS A STATISTICAL TOOL TO OPTIMIZE TOTAL SOLUBLE PHENOLIC COMPOUNDS EXTRACTION FROM UMBU PEEL

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RESUMO

Phenolic compounds are powerful antioxidants naturally present in nature and are subdivided into three groups: phenolic acids (benzoic and cinnamic acids and their derivatives), flavonoids (anthocyanins, isoflavones, catechins, and flavones), and non-flavonoids (tannins, stilbenes, and lignans). Among the most employed techniques for extracting these phytochemicals, solid-liquid, liquid-liquid or supercritical fluid extraction stand out, which can be assisted by emerging techniques such as microwave or ultrasound. The solvents frequently mentioned in the literature for extraction include water, acetone, acetic acid, methanol, and ethanol due to their differing polarities. However, it is worth noting that there is no standardized set of solvents, as their combinations vary according to the evaluated food matrix and class of phytochemicals. This study aimed to optimize the extracting solution for total soluble phenolic compounds (TSPC) in the natural umbu peel using a Simplex-Centroid Mixture Design, employing solvents with relative polarities of 1.0, 0.762, 0.355, and 0.648 for water, methanol, acetone, and acetic acid, respectively. Next, 10 cycles for exhaustive extraction were performed. An aliquot of 400 mg of the sample and 1500 µL of extracting solution were subjected to low-frequency ultrasound-assisted leaching (40 Hz, 100 W) at 20°C for 30 minutes, followed by a 20 min rest period and an additional 30 min extraction. Subsequently, the phases were separated by centrifugation (5000g/10min/20°C), the final volume adjusted to 2000 µL, and the absorbance values determined by the Folin-Ciocalteau colorimetric method (750nm). The absorbance values ranged from 0.0100±0.003 to 0.2604±0.002, with the highest extraction of TSPC promoted by binary interactions between water and acetic acid (β14=0.596, P<0.001) and water and acetone (β13=0.252, P=0.021). Additionally, the mixture of acetone with acetic acid (β34=0.233, P=0.031) and water with methanol (β12=0.219, P=0.041) showed prominence. Among the pseudo-components, acetone provided the highest extraction (β3=0.236, P<0.001). The predictive mathematical model was explained by 90.40% (P<0.001). The optimized point was determined by maximizing the absorbance, achieved by the maximum extraction of TSPC, composed of 27% water and 73% acetone, with a

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desirability of 98.50%. The optimum point was performed in true triplicate and exhibited an absorbance of 0.333±0.010, with a relative standard deviation of 30.25%. Exhaustive extraction was achieved with 6 cycles, with over 95% of TSPC. The total quantification of TSPC was 4.17g GAE.100g^{-1} (d.b.). Although the mathematical model was not validated, the extracting solution defined in the experimental design was capable of extracting a higher quantity of TSPC than indicated. Acknowledgment: CAPES, CNPq.

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