

Modelling the Influence of Extraction Temperature on the Ellagitannin and Antioxidant Profiles of “Wonderful” Pomegranate Peel Using Advanced Chemometrics Analysis

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Abstract

Pomegranate peel contains ellagitannins as antioxidant principles but the aqueous extraction temperature for optimum ellagitannins recovery and antioxidant profile remains elusive. This study employed advanced chemometrics models, including principal component analysis (PCA) and orthogonal projections to latent structures (OPLS) to determine the influence of extraction temperatures (25 – 95 °C) during a 1 h period on the antioxidant profile of "Wonderful" pomegranate peel's aqueous extract, as well as the profile of the constituent ellagitannins recovered using Amberlite® XAD16N resin and characterized by LC-MS. Extraction at 78 °C had the most potent radical scavenging potency, oxygen radical absorbance capacity (ORAC) and anti-lipid peroxidative activity, which was consistent with the high constituent of ellagitannins. Pearson's bivariate correlation depicted strong positive correlations ($r = 0.7 - 0.9$) between the ellagitannins and the anti-lipid peroxidative profile of the extracts. PCA and OPLS models adequately characterized and predicted the variation and patterns in the antioxidant and phytochemical datasets (up to 93.6%). OPLS biplot showed a distinct clustering pattern of the antioxidant and ellagitannins variables around 78 °C extraction temperature, suggesting the observable influence of the ellagitannins on the potent antioxidant profile of the extraction done 78 °C. The variable contribution plots, as well as the obtained antioxidant data suggest punicalagins, granatin A and ellagic acid as notable influencing ellagitannins. It is safe to speculate that extraction at 78 °C optimally influenced the ellagitannin and antioxidant profiles of pomegranate fruit peel. Thus, this aqueous extraction temperature may be promising for optimally recovering the ellagitannins from pomegranate peel, without sacrificing the antioxidant capacity.