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Estimation of Proximate Composition of Quinoa (*Chenopodium quinoa* Wild.) Flour by Near-Infrared Transmission Spectroscopy Models

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Abstract

The aim of this study was to develop chemometric models for protein, fat, moisture, ashes and carbohydrates contents of quinoa flour using Near-Infrared Transmission (NIT) spectroscopy. Spectra of quinoa flour originated from grains of 77 different cultivars were scanned while dietary constituents were determined in duplicate by reference AOAC methods. As a pre-treatment, spectra were subjected to extended multiplicative signal correction (EMSC) with polynomial degree 0, 1 or 2. The performance of two algorithms, partial least squares regression (PLSR) and Canonical Powered Partial Least Squares (CPPLS), was compared in terms ofaccuracy and predictability. For all dietary constituents,as opposed to PLSR, the CPPLS regression produced lower root meat square errors of cross-validation (RMSECV), lower root meat square errors of prediction (RMSEP) and higher coefficient of correlation of cross-validation (RCV) while retaining fewer number of components. More robust models were obtained

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when quinoa flour spectra were pre-processed using EMSC of polynomial degree 2 for moisture (RMSECV: 0.564 and RMSEP: 0.648), fat (RMSECV: 0.268 and RMSEP: 0.256) and carbohydrates (RMSECV: 0.641 and RMSEP: 0.643) following extraction of five CPPLS latent variables. High coefficients of correlation of prediction (RP: 0.7-0.8) were found when models were validated on a test data set consisting of 15 quinoa flour spectra. Thus, good predictions of the dietary constituents of quinoa flour could be achieved by using NIT technology, as implied by the low coefficient of variation of prediction (CVP): 6.1% for moisture, 5.6% for protein, 3.9% for fat 7.4% for ashes and 0.8% for carbohydrates contents.

Keywords: Quinoa, spectra, PLS, calibration,chemometrics