Classification and determination of total protein in mussel *Mytella Falcata* collected in river estuary Brazilian using NIR and multivariate calibration

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Introduction:

Mussel is the term used to name the various species of bivalve mollusks of the family Mytilidae (Mytella).The seafood (mussel) are commonly consumed foods in coastal regions and are of significant nutritional importance because they constitute sources of dietary protein and minerals. The Kjeldahl method is has been used for decades to determine protein levels in sample matrices, such as mussels. This procedure is time-consuming and tedious due to various analytical steps: digestion, distillation and titration. Thus, the aim of this study was classification and determination total protein content of mussels samples collected in five river estuary presents in the coast Brazilian using NIR and multivariate calibration methods (PCR, PLS, MLR-SPA and SIMCA).

Materials and Methods:

Initially, a portion of mussel powder samples was analyzed to determine protein content using the Kjeldahl method, performed in triplicate. After, the spectra were recorded in triplicate using an MB-160 D FT-NIR spectrophotometer (Bomem), with spectral resolution of 8 cm^{-1} and 50 scans in the near infrared range of 714 – 2500 nm. The calibration and validation samples were used to model the procedures, whereas the predicted samples were only used for final evaluation. Spectrum differentiation, Savitzky-Golay smoothing and derivates, principal components analysis (PCA), PCR, PLS, SIMCA were carried out in Unscrambler$^{®}$ 9.8 (CAMO S.A). The *F*-test for SIMCA classification was conducted at a 5% significance level.

Results and Discussion:

Principal component regression (PCR) and partial least squares (PLS) multivariate calibrations were used to predicted total protein. For comparison purposes, the successive projection algorithm for variable selection was applied to the original set. In the prediction stage the MLR-SPA model obtained an R^2 of 0.90 and root mean square error (RMSEP) of 1.56 g/100 g. Soft independent modeling of class analogy (SIMCA) was also used for full-spectrum classification, resulting in almost 100% classification accuracy of according with the estuary localization, regardless of the significance level adopted for the *F*-test.

Conclusion:

NIR spectroscopy combined with chemometric data evaluation is a good tool for determining total protein in mussel powder found in river estuary Brazilian and coupled with SIMCA models to classification 100% accuracy.

Novelty statement:

This work indicating that the NIR diffuse reflectance spectroscopy method coupled with regression and classification methods could be used to analyze of mussels in river estuary Brazilian.

Summary:

This work was investigated the potential of NIR technique to classification and determination total protein in mussels samples.