Simultaneuosly Calibrating Solids, Sugars and Acidity of Tomato Products Using PLS2 and NIR Spectroscopy

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The purpose of this work is to develop a robust calibration model for determining, simultaneously and non-destructively, relevant quality parameters in processed tomato products, namely total and soluble solids, total acidity and sugars. These are key quality parameters once they largely determine sensorial profile and consumer acceptance of tomato products.

Forty-two samples of tomato concentrate products with total solids content ranging from 6.9 to 35.9% were collected from Latin America, the US and Europe. Three spectra of each sample were acquired in the 4000 to 10000 cm^{-1} region using a Büchi NIRLab N-200 spectrometer with a MSC-100 diffuse reflectance cell. Total solids were determined by oven-drying under vacuum (70ºC, ~150 mmHg abs. pressure) until constant weight. Soluble solids were determined with an Abbe refractometer, 0.1° Brix accuracy. Total acidity was potentiometrically determined using a Metrohm 702 automatic titrator and NaOH 0.1 mol L^{-1} Merck standard solution. Sugars were quantified by HPLC using an Shimatzu refractive index detector, a Shodex NH_2P-50 4E column and Shodex NH_2P-50G column-guard. Mobile phase was acetonitrile:water (75:25), isocratic, 1mLmin^{-1}.

Simultaneous Partial Least Squares (PLS2)[1,2] was used to build the calibration models. Original spectra were pre-processed by applying a 50-points mean smoother, followed by multiplicative signal correction (MSC)[1,3]. Alternativelly, a Fourier filter with Gaussian convolution function was applied, followed by MSC and first- or second-derivatives according to Savitsky and Golay[4]. Seven samples were separated for external validation and the others were used in the calibrations. The optimum number of factors was determined by leave-one-out cross validation[1,2]. Comparisons between different models were performed through RMSEP and r_{val}[1,2]. PLS1 models were built for comparison as well[1,2].

Results have shown that PLS2 gave models with better prediction abilities and/or with a smaller number of factors than PLS1. The best pre-processing strategy was mean smoothing followed by MSC; despite the Fourier filter followed by MSC giving quite similar results, it is a more complex approach. The RMSEP for each property was: total solids, 0.6294; soluble solids: 0.6755; total acidity: 0.2189, total sugar: 1.9648; glucose: 0.5365 and fructose: 0.8802. The final model required only 4 factors, much less than PLS1 models previously reported[5].

As conclusion, PLS2 gave a good model for predicting the levels of important properties of concentrate tomato products. Despite its usage not being widely reported in the literature, this application clearly shows the advantages of PLS2 over PLS1 for some applications, as a better and simpler model was obtained.

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