Extracting quantitative information from temperature dependent near infrared spectra

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NIR spectra show not only isolated molecular structure and functional groups, but also inter- or intra-molecular hydrogen bonds. Variation of temperature can change the hydrogen bonding, and therefore the NIR spectra measured under different temperatures can reflect these changes. For examples, the dynamic behavior of water was studied using NIR spectra measured under different temperatures, and structural analysis of hydration shell surrounding the proteins was performed based on the effect of temperature on NIR spectra. These studies proved that the technique is helpful to understand the influence of water in biological systems. Aquaphotomics is a new discipline that provides a framework for understanding changes in the structure of water caused by various perturbations, such as variations in temperature or additives. NIR aquaphotomics offers the possibility for extracting the information hidden in NIR spectra. Water was used as a mirror to explore the spectral changes related to saccharide in the aqueous systems, and NIR water spectral patterns were used to discriminate different DNA structures. In our works, a quantitative spectra-temperature relationship (QSTR) model between NIR spectra of water and temperature was established using partial least squares (PLS) regression and applied to the quantitative determination of the compositions in aqueous solutions. Therefore, water can be a probe for sensing the analyets in aqueous solutions, and the temperature dependency of the NIR spectra of water can be regarded as an advantage for the analysis.

For extracting the quantitative information from temperature dependent NIR spectra, chemometric methods were studied. Multilevel simultaneous component analysis (MSCA) was employed to investigate temperature- and concentration-induced spectral variations in NIR spectra. Both the quantitative relationship of the spectra with temperature and concentration can be obtained. Mutual factor analysis (MFA) was proposed to extract quantitative information from temperature dependent NIR spectra. Quantitative model of the analyte in aqueous solutions can be established by the NIR spectra of water.

Quantitative detection of glucose in aqueous solutions and human serum samples was studied. Using the spectral changes of water captured from the temperature dependent NIR spectra using MSCA, two models of the first and second level were obtained to describe the QSTR model and the quantitative spectra-concentration relationship (QSCR) model, i.e., the calibration curve. The correlation coefficients (R^2) of the QSTR model between the score and temperature are higher than 0.99, and that of the calibration model (QSCR) between the spectral features and the concentration of glucose are 0.99 and 0.84 for glucose solutions and serum samples, respectively.

The results obtained by MFA shows that the mutual spectral information can be obtained, and the spectral variation induced by temperature is contained in the extracted signal. A very good linearity between the intensity and temperature (R^2 = 0.9994) was obtained. An acceptable calibration model with a good correlation coefficient (R2 = 0.8639) was obtained for glucose measurement. The relative deviations of the measured concentrations from the calibration model are in the range of –18.7% to 8.52%, which are in a reasonable level for clinical uses. More importantly, the calculations are based on the spectral information of water that has interactions with the analyte. These studies may prove that changes in NIR spectra can be quantitatively analyzed taking the advantage of the temperature effect, and water may be a promising probe for analyzing the changes in aqueous systems.