Abstract

Near infrared transmission spectra of saline solutions: a testing ground for aquaphotomics

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Introduction

Aquaphotomics aims to gain new knowledge on the structure related functions of water in biological systems by observation of the water-light interaction using NIR spectroscopy. However, methods for identification of bands relating to water structure in NIR spectra are hampered due to the overlapping nature of vibrational overtone and combination bands in the NIR wavelength range. Moreover, interfering factors, such as the strong influence of ambient temperature on NIR spectra of water, confound the elucidation of more interesting spectral responses unrelated to the interferents.

Methods and Materials

Saline solutions of different concentrations were prepared by dissolving appropriate masses of NaCl in Millipore water. Transmittance spectra of samples of different concentrations were obtained in random order at three different temperatures (29, 38 and 49°C). An NIRSystems 6500 spectrophotometer (FossNIRSystems, Laurel, USA) fitted with a quartz cuvette of 1 mm optical pathlength was employed. The cuvette was positioned in a cell holder in conjunction with a temperature bath to control sample temperature. Extended multiplicative signal correction (EMSC) was applied to correct for additive and multiplicative scatter as well as other sources of interference in NIR spectra.

Results and Discussion

Correction of saline solution spectra by EMSC enabled extraction of spectral information unrelated to the interferent (in this case the temperature effect) from residual spectral information. Unlike methods such as observation of PC loadings or PLS regression vectors, the residual spectral information after EMSC was more consistent for the different experimental replicates considered. The main features of these spectra were a sharp peak around 1400 nm related to free water and a broader peak around 1530 nm.

Conclusion

EMSC can be employed for alleviating spectral features introduced due to temperature changes in NIR spectroscopy of saline solutions. The residual spectra remaining after correction for the temperature effect, contain analyte specific information which is useful for understanding the effect of the analyte on its watery surroundings, a goal of aquaphotomics.

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