Physiological Properties of Phytoplankton Cells Investigated by Chemometric Analysis of FTIR-Spectra

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Fourier Transform infrared (FTIR) spectroscopy has been proven to be a useful analytical method in the field of algal physiology. Indeed, quantitative/qualitative changes of the organic compounds (i.e. lipids, proteins and carbohydrates) that make up algal cells can be rapidly assessed [1].

Recently has been demonstrated that FTIR-spectra of whole cells contain information related not only to cellular organic compounds, but they can be used by means of multivariate analysis also to model and characterize cell properties like growth rate [2]. In the process of modelling, chemometric analysis like Partial Least Square (PLS) regression play a central role providing useful statistical tools like regression coefficients, component loadings and VIP scores. These can be used for model interpretation, that in physiological terms means to extract information regarding the organic composition of the cells in relation to cell properties (like the growth rate) or to different growing conditions.

In a previous study we modelled the growth rate of phytoplankton algae growing under different nutrient and irradiance conditions on the base of their FTIR-spectra via PLS-regression. In order to further characterize FTIR-spectra dependence on abiotic factors, we cultivated four freshwater algal species (Cyanobacteria and Chlorophyta) over a temperature range between 7 and 35°C. PLS-regression was applied to investigate spectral changes related to the growth temperature. The modelling process has been improved by using the Extended Multiplicative Scatter Correction (EMSC) described in [3] as a pre-processing method. The model interpretation has been simplified by "filtering" the data-set through the Orthogonal Projections to Latent Structures (O-PLS) [4]. That allows to remove all the systematic variations present in the descriptor variables (FTIR-spectra) that are not correlated with the response variable (i.e. growth rate).

We will show that the O-PLS algorithm is able to lead to a sole component model by maintaining almost the same predictive ability as the un-filtered model. Furthermore, the models will be discussed in terms of the physiological information that they can provide.

References
[1] H. Wagner, Z. Liu, U. Langner, K. Stehfest, C. Wilhelm, *Journal of biophotonics* 3(8-9), 557-566 (2010).
[2] C. Jebsen, A. Norici, H. Wagner, M. Palmucci, M. Giordano, C. Wilhelm, *Physiologia Plantarum* 146(4), 427-438 (2012).
[3] A. Kohler, U. Böcker, J. Warringer, A. Blomberg, S. W. Omholt, E. Stark, H. Martens, *Applied spectroscopy* 63(3), 296-305 (2009).
[4] J. Trygg, S. Wold, *Journal of Chemometrics* 16(3), 119-128 (2002).