FTIR spectra interpretation of phytoplankton cell spectra and their implications for physiological traits

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FTIR spectroscopy has been shown to be a useful tool in phytoplankton cell monitoring, especially in response to changing abiotic environmental factors. Cell parameter such as nutrient contents or macromolecular composition have been analyzed with a variety of different methods such as band ratios, band integrals calibration via reference substances and statistical methods (e.g. PCA and PLS regression analysis). All results published so far showed a clear dependency of different vibrational regions to these direct physiological parameters. This raises the question, if statistical methods can also be used to evaluate physiological key features of cells which are not directly correlated with the biochemical composition of a cell, e.g the growth rate. This would be possible only if this indirect parameter is related to some extend to the direct parameter measured by FTIR spectroscopy. We will show how such a method can be established, using more than only one changing external parameter. The application of statistic parameters like VIP vectors and regression coefficients show that PLS regression analysis has the potential for monitoring complex physiological key parameters like the growth rate. Furthermore these parameters indicate which vibrational region is correlated with the monitored trait.