

Evaluating the spectral quality to improve the results of data analysis

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Numerous publications have proven the scientific impact and practical applicability of aquaphotomics, and the field of research has been growing rapidly, opening new horizon for scientists and end-users to gain more information from the recorded near-infrared spectra of liquid or moist samples than ever before. The sophisticated data evaluation techniques make it possible to detect and highlight minor changes of the water spectral pattern among very diverse conditions, but it is crucial to be aware of the nature of the investigated spectra when starting such analyses. The better understanding of the spectra and the recognition of limitations may lead to more accurate results and even more valid theory explanations. This workshop presentation focuses on some basic methods to detect unwanted spectral variations and to evaluate their impact on the data analysis. The presentation summarizes a protocol of reviewing the recorded raw data, but the introduced evaluation methods may also be used individually.