Recent Trend in NIR Spectroscopy including Quantum Chemistry and 2D-COS and its Future Potential for Aquaphotomics

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The field of near-infrared spectroscopy (NIRS) applied to food quality monitoring, mobile healthcare and related discipline is developing dynamically. Mini- and micro-spectrometers are poised to pervade the industrial and consumers´ market. For this type of application compact footprint, integration of powerful chip and extremely low cost (<100$/unit) are required. Currently, miniaturized NIR spectroscopy solutions suffer from limited spectral range, resolution and high costs. Conventional spectrometers can be classified in three broad categories: The first category employs dispersive properties of a prism or a grating to generate the individual wavelengths onto different spatial positions, which are measured in the following by a detector array. The second category is based on tuneable filters and single detectors, the third on Fourier-transform (FTIR) spectrometers which measure the first-order coherence function in a Michelson interferometer. Most commercial miniaturized spectrometers are working with the grating & array concept, but more and more companies are now commercializing micro-spectrometers based on microelectromechanical (MEMS) tuneable filters. Both present fundamental limitations in their size and performance. Applying dispersive elements results in an intrinsic size-resolution trade-off, because long grating-detector distance is needed to achieve high resolution. Spectrometers based on MEMS-tuneable Fabry-Perot resonators have limited spectral range and it is difficult to tune over a wide wavelength range. The integration of FTIR spectrometers is very challenging as the resolution is inversely related to the stroke of the moving mirrors in the range of hundreds of micro-meters. For the critical evaluation of a spectrometer, two-dimensional correlation spectroscopy (2D-COS) has been developed towards a powerful analytical tool for monitoring its dynamics [1], which can be further supported by quantum mechanical calculations, e.g. by calculating a heat map about mode contribution into NIR spectrum [2]. Multivariate determination of lower limits of detection (LOD) and quantitation (LOQ) applying Kennard-Stones and Duplex algorithm can be additional criteria judging the performance of a spectrometer [3]. The most suitable evaluation of a spectrometers performance is its application. For this reason, the suitability of the three different types of micro-spectrometers will be discussed for food quality control and fraud detection, medicinal plant quality analysis and optimisation of harvest time. From this presentation limits and advantages should become much clearer and future potential for Aquaphotomics can be drawn therefrom.

References

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