Future Directions of Near-Infrared Spectroscopy in Food, Phyto and Bioanalysis

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Keywords: at least one of these should be one of the areas that are listed on the website or in the submission guidelines.

The field of near-infrared spectroscopy (NIRS) applied to food, phyto and bioanalysis is developing dynamically. Miniaturized NIR spectrometers 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 show 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 micro-spectrometer´s performance, two-dimensional correlation spectroscopy (2D-COS) has been developed towards a powerful analytical tool for monitoring its dynamics, which can be further supported by quantum mechanical calculations (Figure 1). 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.

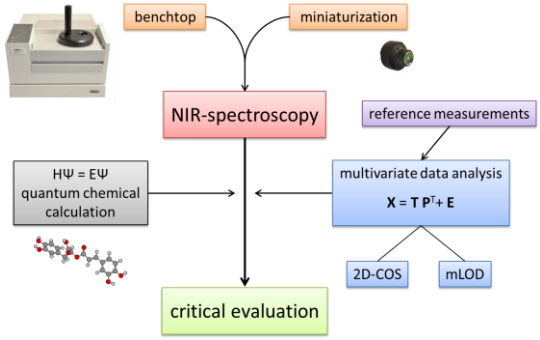

Figure 1. Evaluation workflow

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, phyto and bioanalysis. From this presentation limits and advantages should become clear and future trends can be concluded therefrom.

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