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

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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. The second category is based on tunable filters and single detectors, the third on Fourier-transform (FTIR) spectrometers which measure the first-order coherence function in a Michelson interferometer. More and more companies are now commercializing micro-spectrometers based on microelectromechanical (MEMS) tunable filters. For the critical evaluation of a micro-spectrometer's performance, two-dimensional correlation spectroscopy (2D-COS) has been developed, 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.



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 microspectrometers will be discussed for food, phyto and bioanalysis.

^[1] Henn, R, Krichler CG, Grossgut ME, Huck, CW. Talanta 2017, 166, 109

^[2] Pezzei, CK, Schönbichler, SA, Kirchler, CG, Schmelzer, J, Hussain, S, Huck-Pezzei, VA, Popp, M, Krolitzek, J, Bonn, GK, Huck CW. *Talanta* **2017**, 169, 70.

^[3] Grabska J., Beć K.B., Kirchler C.G., Ozaki Y., Huck C.W. Molecules 2019, 24, 1402