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One Sample, One Worldwide Result – An Interlaboratory Ring Trial

AquaSpec™ Technology revolutionises analytical chemistry worldwide. Using an ultrathin flow cell, aqueous sample MIR spectra are captured within minutes, at low concentrations, and at high reproducibility. And - can then be used across all your labs. Embedded in the fully automated and robust MIRA Analyzer benchtop device, AquaSpec™ is applicable across the pharmaceutical, chemical, and food industries. The exceptionally high accuracy, precision, and interlaboratory reproducibility of the MIRA Analyzer has recently been confirmed in an interlaboratory ring trial, carried out in cooperation with a global leader in the chemical industry.

Application Note: Ring Trial

An aqueous test mixture of acesulfame K (1.714 g/L) and glycerin (33,571 g/L) was measured on twelve MIRA Analyzers of different construction type, distributed over five laboratories, and operated by a single staff member in each laboratory. For quantification, a partial least square (PLS) model was built on one single device, using the concentration range of 1.5 – 3.0 g/L for acesulfame K and 25 - 35 g/L for glycerin. This PLS model was then used by the remaining eleven devices for concentration prediction. It should be noted that other industry techniques currently require time-consuming calibration models to be built on each individual device, due to low device-to-device transferability.

In the current study, accuracy (Figure 1A) was calculated as percentage deviation of the mean predicted concentration from the true concentration of each sample substance. Precision (Figure 1B) was calculated as the standard deviation between the predicted concentrations of six measurements on each device for each sample substance.

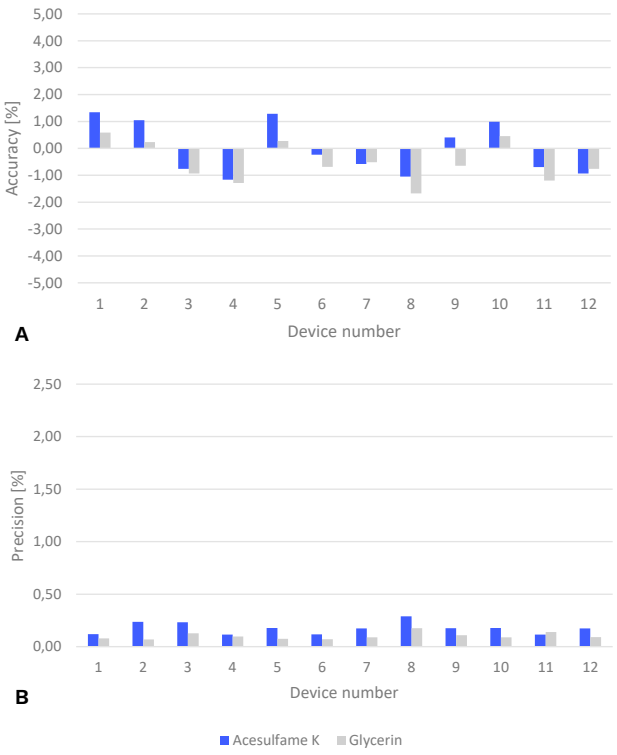

Figure 1. Accuracy (A) and precision (B) of both analytes on each device.

The results confirm the high accuracy and precision of the MIRA Analyzer design, with accuracy values between -1,68 to 1,34%, and precision values between 0,07 to 0,29 % for all twelve devices.

As an index for interlaboratory reproducibility, the Horwitz Ratio (Horrat) is routinely used. This is defined as the ratio of the measured relative standard deviation (RSDM) and the theoretical relative standard deviation after Horwitz (RSDH), as follows:

$$Horrat = \frac{RSD_M[\%]}{RSD_H[\%]}$$

with

$$RSD_M = \sqrt{\frac{\sum(x_i - \bar{x})^2}{n-1}} * \frac{100}{\bar{x}}$$

$$RSD_H = 2^{(1-0.5log_{10}(x_t))}$$

where xt is the true analyte concentration of the test mixture, xi the calculated analyte concentration per device or laboratory, and $\bar{x}$ is the arithmetic mean of the calculated analyte concentrations. A Horrat value of 1.5 or below indicates a satisfactory interlaboratory reproducibility [1]. In this study, the Horrat values obtained for both analytes were clearly below this limit (Table 1), with 0.19 for acesulfame K and 0.23 for glycerin. For comparison, Horrat values generally reported for other spectroscopic techniques for the quantification of organic acids (such as 1H-NMR spectroscopy) lie between 0.6 and 1.5, which are higher [1].

Table 1. The Horrat value obtained for acesulfame K and glycerin as index for interlaboratory reproducibility.

	Acesulfame K	Glycerin
Horrat value	0.19	0.23

This study is a clear demonstration of MIRA Analyzer's excellent performance for quantitative analysis. The robust and fully automated design allows highly accurate, precise, and reproducible analytical results within global and distributed laboratories, independent of the operator, the laboratory, or the instrument construction type. With its high device-to-device reliability and its flexible application in numerous industrial processes, the MIRA Analyzer delivers as a true Industry 4.0 technology with fast and transferable analysis.

[1] R. Godelmann, C. Kost, C.-D. Patz, R. Ristow, H. Wachter, Quantitation of Compounds in Wine Using 1H NMR Spectroscopy: Description of the Method and Collaborative Study, J. AOAC Int., 99, 5, 2016, 1295–1304.