Technical Note

Quantification Calculations on accroma® samplePrep Systems

Per definition, concentration is the abundance of a constituent divided by the total volume of a mixture (e.g. mg/ml). This unit originates from the traditional way of preparing samples using volumetric flasks. Volumetric flasks are calibrated at 20°C and are filled to the mark to obtain the total volume. However, if sample matrix components (e.g. excipients) are not or partly soluble, volumetric errors appear. Furthermore, volumes depend on temperature.

accroma samplePrep systems use a different concept as volumes are determined gravimetrically. In the accroLab software, measured masses of solvents are converted into volume by using the solvents density ($\rho_{solvent}$). The general unit is the mass of a component divided by the volume of the solvent, called Mass per solvent (w).

Unit in manual sample preparation

Mass concentration (c)

$$c = \frac{m_{analyte}}{V_{mixture}} = \frac{mass\ of\ analyte}{total\ volume}$$

Unit in automated sample preparation by accroma

Mass per Solvent (w)

$$w = \frac{\rho_{solvent} * m_{analyte}}{m_{solvent}} = \frac{mass\ of\ analyte}{volume\ solvent}$$

The total volume of a mixture (c) could be also calculated by using mass (m) and density (ρ) of all dissolved components and neglecting volume contractions. However, if some matrix components (e.g. excipients) are partly soluble, it is getting complex.

$$c = \frac{m_{analyte}}{m_{analyte} * \rho_{analyte} + m_{solvent} * \rho_{solvent} + m_{matrix} * \rho_{matrix}}$$

Calculation

The quantification of an analyte is based on the comparison of the signal of the sample (e.g. Area under the Curve, AUC) with the signal of the reference standard.

It is crucial that reference standard and sample are handled with same units. Therefore, reference standards should be also prepared on the accroma system or if done manually, added solvents need to be determined gravimetrically.

In case of one point calibration of the reference standard, the sample concentration can be calculated as followed:

$$c_{sample} = \frac{c_{reference} * Signal_{sample}}{Signal_{reference}}$$

Edition 01/2021

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