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Setting Data Requirements

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A prime requirement for the analytical data is the accurate collection of all the information associated with the sample from its arrival in the laboratory, through the measurement process, to the final report to the customer. A Laboratory Information Management System (LIMS) provides a facility for doing this and, if well designed, eliminates the need for any manual transcription of data. However, it is still necessary to determine what data is required particularly for the measurement process, especially when only a small sample is available and repeat measurements may not be possible.

This presentation concentrates on the measurement data required to ensure that the measurement result is fit for purpose, a requirement that is addressed during measurement procedure validation but should also be checked in routine measurements. A measurement procedure produces fit for purpose results if the reported uncertainty is small enough to allow conclusive decisions for the items studied. A target (i.e. maximum admissible) uncertainty should be defined to allow an objective and transparent decision about the adequacy of the measurements.

Depending on the used approach for estimating the measurement uncertainty, the data that needs to be managed to report and check the magnitude of the measurement uncertainty, varies. Bottom-up assessments requires more data than pragmatic top-down assessments of the measurement uncertainty. This presentation presents some examples of the type of data required to estimate and optimise the measurement uncertainty in order to ensure measurement uncertainty is adequate for compliance assessment.

Additionally, the issue of structuring the data, not only to meet the management needs associated with a particular sample or similar samples, but also to meet possible future needs is discussed.
The above is dealing with specifying the data required by the laboratory to produce a satisfactory result and report. A much wider problem is how to structure this data so that not only can data from a specific sample be retrieved but the data can be used for much wider applications, for example.

- What percentage of samples showed non-compliance, subdivided by types of samples, e.g. food or environment, or even subdivided further by types of matrices or contaminants. This information can be useful, for example, to redefine the target measurement uncertainty.
- Comparison of the uncertainty achieved as a function of the procedure, type of sample, approach used for uncertainty evaluation, cost of analysis et cetera.

The collection, structuring and sharing of data useful for redefining a target uncertainty and for guiding the selection of the methodology to achieve an adequate measurement uncertainty can be extremely useful for laboratories.