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EDITORIAL

What to measure?

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Quality assurance for measurements in chemistry and the biosciences seems to deal at a first look with questions such as 'Did we determine the amount of the requested compound (acrylamide, human growth hormone, etc.) accurately?'. Why should the stakeholders of *this* journal reflect on 'What to measure?'. Remember, most of the measurements are performed in response to a customer demand (which could be also our own scientific curiosity). And quality is about satisfying the customer. One may argue that the analyst in the measurement laboratory obtains the specifications for the 'what to measure' from his/her customer. But according to my experience, even a simple-looking request from a non-measurement expert to the analyst that she/he should just perform a 'routine service' by analysing a provided sample with respect to pre-specified parameters can turn into a fruitful scientific discussion and collaboration about defining together the analytical problem and designing a measurement strategy which could really answer the original question. By that we are focussing on quality, because we ensure the provision of measurement results allowing the customer to take an informed decision. We are not just producing measurement data about a sample, which would comply with the stereotype of an analyst as 'service maid' to other scientists dealing with the 'grand challenges' of society.

Consequently, delivering measurement results of adequate quality includes also 'measuring the right target'. Therefore, the first required step to quality is identifying what is the decision-relevant measurand which is—according to ISO Guide 99 (VIM-3)—the 'quantity intended to be measured'. However, this may not be sufficient for specifying what to measure; as such an 'intended quantity' may not be directly accessible by a measurement. This is, for example, the case for a measurand 'mass fraction of total protein in a foodstuff'. Therefore, the next step requires the intellectual contribution of analysts ('measurement scientists') in the problem-solving exercise to an even greater extent. Namely, one has to specify the (physical, chemical or biological) entity that can represent adequately the identity, sometimes called analyte or target species (here 'total protein'), of the measurand (here mass fraction of total protein in a foodstuff) in the measurement procedure. For example, the nitrogen content in the food sample as measured by using the so-called Kjeldahl method may serve as substituting quantity in the example. But this has to be well thought-out throughout the whole measurement process. For the latter, various operations from taking the analytical subsample via sample preparation, creating and registering the instrumental signal until delivering the quantitative measurement result have to be considered. Otherwise, one may overlook the interference of nitrogen from non-protein sources, such as melamine, in the foodstuff.

Many chemical or biological measurement procedures include transformations of the analyte, for instance, by derivatisation or fragmentation. Consequently, 'measurement' in chemistry and the biosciences can usually not be reduced to a simple one-step attribution of a value to the predefined measurand. It includes also mastering the changes of identity (chemical nature) for the target species during the whole measurement procedure. For instance, getting to know the mass fraction of acrylamide in toasted bread may include the following steps: extraction (accurate knowledge on extraction yield required), bromination (derivatisation yield has to be known), gas chromatography (separation yield has to be checked) and mass spectrometry. Calibration

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for the latter step is straightforward and can also be extended backwards up to the derivatisation step, if well-characterised isotopically labelled acrylamide is available and co-eluted compounds from the bread do not interfere. But a mathematical equation between the mass fraction of acrylamide in the bread sample and the mass spectrometric signal can only stay at an empirical case-to-case level, because the extraction yield cannot be predicted and interferences in the following steps cannot be excluded. For more complex analytical tasks, such as the quantification of human growth hormone in blood, quality assurance for the identification steps ('qualitative analysis') can be critical.

Ensuring the quantitative understanding (i.e. knowing the mathematical equations) of transformations and partial losses of target species during measurement procedures is crucial for establishing metrological traceability. Obviously, calibration strategies have to take into account such transformations (and incomplete phase transfers of the analyte, for instance during chromatographic separation and clean-up steps). This issue is exacerbated even further when one starts to consider some of the additional challenges that analytical chemists face where operationally (or method)-defined measurands, such as mass fraction of total protein in a foodstuff or amount of extractable lead in a sediment, are involved.

Therefore, *Accreditation and Quality Assurance* (ACQUAL) welcomes the submission of manuscripts explaining new ideas and generic concepts for:

- Traceability concepts when the measurand is not directly measurable itself, that is, a substitute target (such as Kjeldahl nitrogen for total protein) is measured;
- Accurate estimation of extraction yields ('recoveries') for analytes embedded in heterogeneous materials such as solid matrices or biological tissues;
- Measures of quality assurance for the identification of chemical or biological species ('qualitative analysis');
- Calibration strategies for operationally defined measurands;
- The demonstration of traceability for measurement results of operationally defined parameters.

The latter two topics are connected with a number of open issues in metrology, which are very much in the scope of ACQUAL. I would also like to encourage the use of ACQUAL's Discussion Forum for corresponding debates.

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