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What developments do you need to work more efficiently?

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Last issue I opened a discussion on what developments we need in the field of spectroscopy which are not being currently provided by our vendors. For those who don't know the English phrase… try using your favourite search engine for "Can of Worms" and you will know what we have opened in this debate. First, thanks for those who took a short break in their working day to submit your comments on the website. I must admit the discussions we have been having did not exactly all go in the direction I had been expecting—which is probably good because it means people were prepared to put some thought into expressing their opinions.

> **Can of Worms**
> *informal*
> "A situation that causes a lot of problems for you when you start to deal with it"
>
> —Definition of "can of worms" from the *Cambridge Advanced Learner's Dictionary & Thesaurus*, © Cambridge University Press

What is "the State of the Art"

First worm!... What exactly is State-of-the-Art? The Cambridge University Press defines it as *"very modern and using the most recent ideas and methods"*. However, if you took time to look at your laboratory, as was suggested in the last issue, how often is that shiny new, freshly installed instrument not much more than an almost like-for-like replacement for a worn-out old friend?

All of us have experienced downsizing, right-sizing, fit-for-purpose activities in one shape or other. Whether in academia or industry, has this reached the point that decision makers are too scared to support innovation? This may be because there are simply not the resources available any more to be able to work on new ideas or to work up new equipment which really does make use of "…the most recent ideas and methods…" without endangering the laboratory's delivery targets?

How does development prioritisation happen?

Wolfgang Bremser, previously of BASF, responded to the question with some good insights. The symbiosis between users and vendors really needs to be active and healthy if our field is to move strongly forward. He looked back at a structure which they had in place to achieve the goals we are striving for now.

His model can easily be copied across different sectors. Despite my comments under State of the Art, I am sure our current generation of Analytical Laboratory Managers would

"What developments do we need in Spectroscopy"—one of the most important if not the most important question.

As Hamlet says: that's the rub.

This evidently leads to the questions "how does prioritisation happen" and "what is the return on investment"—for vendors and buyers equally. We are in a symbiosis.

We initiated an extremely successful meeting together with friends at Shell Amsterdam. The working title was "Industrial NMR Users Meeting". The most prominent and active English representatives were Margret Chippendale and Peter Reagan.

In very open and intense as well as demanding discussions and presentations we opened a dialogue between the most prominent industrial representatives and experts (maximum one per company) and the instrument manufacturers. Most prominent on that side and very open to suggestions was Tony Keller, but also the Varian representatives understood the importance of the dialogue.

In successive meetings, one year after, the manufacturers always gave a survey on whether and how our demands were fulfilled in the year passed.

Thus, the development of industrial spectroscopy and especially NMR was pushed and directed into the desired products. It greatly helped to open our (users and developers) mind for future ideas and created a mutual understanding of problems and solutions. We at BASF profited a great deal from the meeting.

Maybe you know about this annual meeting, maybe not. Anyhow, it was a milestone or better a series of stepping stones in NMR development. And could be a model for your activities.

Good luck and best regards from
Wolfgang Bremser

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see the benefit of getting cross-industry agreement on key priority areas. Our vendors would certainly value independent validated input to steer their developments.

Hardware and software developments

A well thought out request was received directly badly needed targeting hardware developments.

The top instrumentation advancement they would like to see was in the delivery of compact, stable mid-infrared spectrometer for real-time spectral data collection under reaction conditions without the use of expensive, consumable detectors therefore reducing cost of ownership.

At the same time, the available software innovation should include the integration of spectroscopic data from multiple sources, where that data varies in the time domain. Easy alignment of multiple batches of data to allow rapid analysis and feeding of outputs to data analytics platforms.

Further discussions were also had around the actual functional handling of today's software platforms. There has been a steady replacement of dedicated powerful workstations for data processing with more generally applicable and more easily deployable Microsoft Windows-based systems. However, for domain experts, this may have come at the cost to some functionality and sacrificed some useful shortcut features to remain compliant with the overarching "Windows Style Guide".[1] There are also clearly issues around "number of mouse clicks" required to complete any particular task. Although the style guides may well mean that anyone familiar with writing articles using Microsoft Word will know where to find all the functionality to drive an NMR spectrometer, I don't think this really comes very high on anybody's priority list anymore? A good example was discussed of a specific piece of common functionality found in the parameterisation of an NMR experiment which, in the old vendor software, was simply carried out by the selection of a single button. In the new vendor software, this same set-up now requires the writing of a completely new pulse sequence. Hardly any efficiency gains there! On a personal level, I must admit that I was very happy in my own laboratories when Windows-based instrument control software first appeared, as it made it much easier to train staff to operate more flexibly across instrument types and makes. At that time, staff had often tended to be utterly dedicated to single instruments.

Don't forget about sampling!

A long submission hit on a very important, if not key topic. Although dealt with specifically in another column in this journal, sampling should be much better handled in our own data analysis and reporting software solutions. I know this topic will find strong resonance in the activities within my own company and has also started to have a much more higher profile in the topic areas I teach. I have reproduced some of the salient points made here due to the available space.

They would like to see analytical instrument vendors no longer disregarding the preceding sampling contributions to the total measurement uncertainty.

Analytical capabilities are forever on the rise, in some areas faster than in others, but the competition assures progress galore. Allow me one comment in this context—there is an elephant in the room: sampling representativity.

In the total uncertainty budget there are two terms, var(TAE) and var(TSE), the Total Analytical Error and the Total Sampling Error, respectively. Members of this community naturally and overwhelmingly focus on the former. Nothing wrong with this, only it is not complete, and here is the catch: analytical results are only as relevant as the analytical aliquot is representative of the entire target lot. Who was responsible for taking the primary sample? Was this sampling representative? Across the wide swath of target materials that are characterised analytically by NIR, the sampling rate [aliquot/lot] is ranging 3–6 orders of magnitude (m/m), summed up by var(TSE). Var(TSE) is determined exclusively by how well we are able to deal with the lot-to-aliquot sampling path (reduce, suppress or eliminate no less than eight sampling errors at every sampling and subsampling stage).

Since var(TSE) is typically 10–25–50 larger than var(TAE), depending on intrinsic material/lot heterogeneity, the importance of this critical success factor should be abundantly clear.

"What is the meaning of analysing, with ever increasing precision, a smaller and smaller aliquot that cannot be documented to be representative of the original target lot/material?"

It is not only about analytical optimisation, it is just as much about mastering the preceding lot-to-aliquot pathway —TOS to the fore!

So, the challenge is to ensure that the programming of our sampling robots is stronger in the area of the calculation of not only the Total Analytical Error, which is often fairly simple to configure, but to allow and understand the entry of additional data for the errors introduced at the sampling stage prior to the measurements themselves. This may require some standardisation and agreement across vendors as to how to represent sampling information and uncertainty.

Our survey

Our survey is still open, so please add your weight and suggest improvements in your specific area of interest. Please visit our survey at **spectroscopyeurope.com/survey** and answer four simple questions:

1) What is your field of operation?
2) List the top three most important hardware developments you would like to see in your field?
3) List the top three most important software developments you would like to see in your field?
4) Any other aspects that would help your Return of Investment calculations?

And let's see if we can get some (more) movement in our fields.

References

1. https://msdn.microsoft.com/en-us/library/windows/desktop/dn688964(v=vs.85).aspx (accessed 4 December 2017).