What developments do you need in spectroscopy?

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I have been involved recently in quite heated discussions around what developments we need in the field of spectroscopy which are not currently being provided by our vendors. Phrases like "surely it should be capable of…" or "but it is common sense that the instrument must be able to…" and more frequently "in this day and age it is unacceptable that…".

Do YOU recognise this? Anyway, I thought it was time to look at the developments we would all like to see and to get some feedback from the readership which could help our vendors' Product Managers in deciding on development priorities and market justifications in upgrading the technology we are able to purchase. It has also been suggested to me that we should explore what is a reasonable price to pay for such developments!

What is "the State of the Art"

Take a step back and look at your instrument park. How much has it changed since you took on your current role? How much has it changed since your predecessor took on your role? Do you get the feeling that in your specialism time has actually stood still? Now we know there are specialist labs around with seemingly unlimited funding, full of gleaming kit leant as prototypes by the vendors. But I am talking about a standard analytical laboratory. Very important for our suppliers, as they will represent the source of the majority of their turnover.

For example, if you are an infrared spectroscopist, what is the biggest technology development which has helped you in your work? Probably the biggest development seen in the instrument park in this area was the step—resisted by some vendors—to move from dispersive instruments to Fourier transform instruments by adding a Michelson interferometer as the wavelength selection device. Now, there have been advances in the sample handling attachments that you can add to a base spectrometer with better microscopes or optical fibres for somewhat remote measurements. Clearly, significant focus and advances have been made on the use of advanced statistics (chemometrics) to pull information out of the noise or low resolutions and background contamination signals, but the fundamentally low speeds of the instruments (time per sample for good signal-to-noise ratios) remain. There have also been some micro-spectrometer developments, but these make use of the significantly more powerful computing capabilities to deliver acceptable results in some specific areas of activity from significantly worse data sets, and can only be rather specialist. Probably one of the most amazing facts is the widespread acceptance of an energy source for the spectrometers with such poor linearity in the actual energy delivered to the samples giving significantly different signal-to-noise ratios across the range of wavelengths we expect it to operate in. In an age of the rapid development and vast increases in energy efficiency of, for example, LED light sources, why has the promise of the quantum cascade laser technology not resulted in easily available laser-based infrared spectrometers—even if you have to multiplex arrays of the sources.

Mass spectrometrists are somewhat better served than their optical spectroscopy brothers and sisters, with a steady stream of incremental instrumentation improvements leading to fundamentally new ways of approaching their analyses, such as accurate mass approaches to analyte identification and different sample inlet technologies making more difficult samples amenable to a mass spectrometric approach. Nuclear magnetic resonance has seen field strengths increase significantly, although the cost of these restricts their use to a few laboratories.

How does development prioritisation happen?

Money! Pure and simple. I sometimes feel quite sorry for our product managers who have to fight for resources to get new developments to market. If your lab is hanging on to outdated spectrometers for 10–20 years, there are issues for a keen product manager to show where they can produce the required return on the necessary vendor investment. Unlike some other laboratory science areas, spectroscopy usually does not rely on the use of vast amounts of consumables to keep a vendor division's turnover moving. For some of our smaller, innovative start-ups there are lower barriers to get their innovations to market, but much bigger challenges in supporting their innovations on a global stage in the longer term. The necessary overheads of training, deploying and retaining support engineers inevitably start to take up an ever-larger proportion of their precious cash flow, diverting badly needed funding from the work on the next "innovation". This can often lead to their takeover by one of our global multinational vendors with the inevitable corporate culture clash. So, what do we need as a society of spectroscopists to do to break this viscous circle?

Clearly, innovation is possible, we discussed in this column the superb developments in the field of terahertz spectroscopy from the old days of poor weak sources and insensitive detectors in the far-infrared to the latest instruments based on innovative sources and detectors based on completely new technologies.[1]

Return on investment—for us end users and our financial controllers

Evidently, the age of our instrument parks can be one of the issues hindering ongoing innovation? So, what is stopping us from upgrading more frequently? Those of us with strong financial controller guidelines need to produce our own detailed Return on Investment calculations to justify these capital investment decisions. If we look at the full economic costs of the time our expert staff are spending with outdated equipment, it is not hard to find 10–20% improvements in the data acquisition speed. The latest Royal Society of Chemistry staff remuneration survey results will be available for all to see from 1 November, but even without the latest figures it is likely that you should easily be able start with at least 20–30k € in cost savings over the write-down period of the planned investment.[2]

You should next look at the issues brought to our laboratories from Microsoft's policies on stopping legacy operating system support. It is often preferably, in both industrial and academic organisations, to have expensive spectrometers supplying data to several users, and to do this efficiently it is best to carry out the analysis of this data off-spectrometer. The legitimate demands of the IT support police to keep ancient instrument control PCs off the internal networks as potential sources of security vulnerabilities usually means additional loss of efficiency. These demands can result in simply stopping off-spectrometer data analysis or resulting in scientists running backward and forward clutching USB sticks, or USB drives for the instruments delivering hyperspectral high-resolution data sets—that is, of course, if the old computers actually support USB! So, let us add another 10% to the ROI calculation for inefficiencies which have crept in to the data analysis workflows as the spectrometers have aged.

How about considering, for example, the time lost by your internal or external colleagues who may potentially be waiting for your delayed results on their samples before they can work out the most appropriate strategy to handle a key customer's complaint. These may also provide further strong financial leverage for an instrument update policy. Finally, and probably most obviously, more modern instruments tend to be far more efficient in terms of energy consumed, expensive laboratory floor or bench space required and consumables devoured.

Return on Investment—for the instrument and software vendors

OK, so if we manage to revive demand by making it clear to our finance experts how an up-to-date instrument park can bring strong financial sense, let us look at some of the underlying issues hindering our vendor product managers from making the case for more innovation in their spectrometer offerings for "normal" laboratories. First, and quite annoyingly, it may again be worth looking longingly across at our brother and sister chromatographers. They are extremely well served by their vendors providing a range of chromatography data systems which deliver standardised data handling routines for chromatogram processing and results generation. They also provide multi-run and multi-vendor instrument control, greatly simplifying the development of the off-instrument data processing strategy. It also allows for better innovation deployment, as you can buy the best separation science hardware for the desired task without having to deploy another data processing solution for your scientists to have to learn. This capability can only be dreamt of at the moment for the spectroscopy laboratory. Current attempts to integrate hyphenated methods linking chromatography and spectrometry instrumentation into centralised CDS data processing workflows have only been partially successful. So, if our spectroscopy vendors can lower their guards a little and allow access to their control codes, maybe we can look to a future of reduced overall instrument development costs through the use of common CDS-like instrument control capabilities.

It is also worth looking outside our own industry for examples where others have faced similar price pressures. In the automobile industry, we live in an age of common chasses underpinning vehicles addressing vastly differing user needs from sports cars to people carriers. Such an approach could also reduce the cost of introducing innovation where the development can focus on the new ideas whilst relying on stable common components to keep development costs focused where they need to be deployed. This would also deliver further downstream cost savings for our vendors in the area of keeping their support engineers trained and up to speed on their diverse instrument parks.

Our survey

So, in our utopian world we have shown why and how you can justify financing the purchase of innovation from our vendors, and also some ideas as to how vendors can address the stifling ROI demands from corporate financial controllers to even allow innovation to be pursued. So, what do you want to be delivered? Please go to our survey page at https://www.spectroscopyeurope.com/survey and answer three simple questions:

- What field of spectroscopy do you work in?
- Name the top three instrumentation innovations you would like to see available to help in you daily work.
- Name the top three software innovations you would like to see available in coming years.

And let us see if we cannot persuade our suppliers to protect and nurture innovators and our financial controllers to realise the benefits of reinvigorating our instrument parks and working environments. Your staff are, of course, your best assets, but do not underestimate the benefits of targeting investments to ensure your best assets have access to the best tools to support their daily work.

Comments

Perhaps you disagree? Feel free to comment on the online version of this article at https://www.spectroscopyeurope.com/td-column/what-developments-do-you-need-spectroscopy.

References

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2. *The results are in....* Royal Society of Chemistry (2015) [Accessed 15 October 2017]. http://rsc.li/2giFcGc

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