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Another one bites the dust

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On 10 October 2014 the impossible happened. An event which many nuclear magnetic resonance (NMR) spectroscopists and their risk managers had probably assessed as "High Risk—Never Going to Happen" actually occurred. Agilent announced they were exiting the NMR business they had entered with the acquisition of Varian four years earlier for $1.5 billion.[1] Hardest hit were, of course, the 300 people whose jobs are being "eliminated" (in the words of the press release) mostly in Yarnton, UK, and Santa Clara, USA, by the end of this year.

However, the trouble this decision is likely to cause to the NMR user community globally is likely to be immense. There have already been some very illuminating comments around the whole direction of the future of NMR in the Magnetic Resonance Research Network group on LinkedIn initiated by Vanni Piccinotti. Those who wish to delve deeper may find it interesting to review the discussion, but you will need to join the group to gain access.[2] Andy Extance also discussed this development and had gleaned some interesting comments from the academic community on the practicalities of training future analytical chemists and research spectroscopists on outdated equipment and the likelihood of government funding being available to replace such systems.[3]

Why is this development so important?

- NMR capability is a key technology in many analytical laboratories around the world and often represents the largest single investment item.
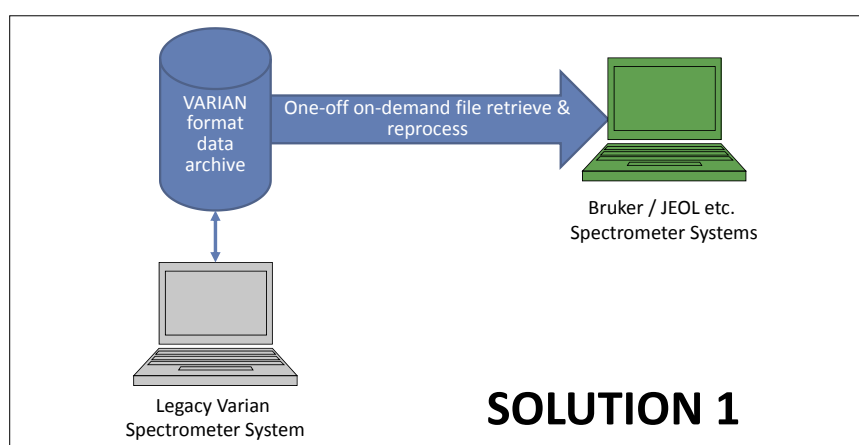

Figure 1. Use of alternative instrument vendor software on an *ad hoc* basis.

Strengths	Weaknesess
■ Low/zero short-term investment required ■ Delays required decisions until more detailed analysis of the available legacy support is available ■ No change to current record retention policy required immediately ■ Allows gradual transition of Varian experts to future NMR systems	■ Relies on Agilent support for Varian hardware/computing for an extended period ■ Limited support for different Varian data formats/pulse sequences/experiments ■ Accelerates need for NMR experts to be conversant in two radically different data processing systems ■ Requires good laboratory networks
Opportunities	**Threats**
■ Deeper understanding of two systems increases compliance ■ Provides a reasonable breathing space for other scientific data processing software vendors to come up with innovative commercial solutions ■ Some data may reach its record retention period allowing deletion thereby avoiding risk of migration	■ Required computer software updates to remain compliant with corporate computing environment ■ Potential for degraded support as system-specific expertise become increasingly rare ■ Support may become even more varied by geography ■ Computer hardware repairs become increasingly difficult/expensive

- Before the announcement there were really only three major instrument vendors left.
- We are losing one of the two vendors that was driving scientific development in the field of NMR systems.

- Often NMR spectroscopists do not store processed result data files but the original raw data free induction decay (FID) files—preferring to reprocess on-the-fly. This practise is only viable if the avail-

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ability of your vendor is ensured in the long term.

- In the regulated laboratory environment, access to the data/results is needed for the length of the record retention period stipulated by regulators and management.

So putting aside speculation about the future of the whole field of NMR, let us look at what we can do to mitigate the impact of the decision on our spectroscopic data handling strategies. This development can actually been seen as a positive trigger to get our house in order with improved overall data processing and storage strategies and more robust "future-safe" NMR data archiving. We have looked at three potential mitigating solutions with differing timescales and carried out a high level SWOT analysis which we hope you will find useful. There is, of course, a fourth solution, to ignore what is going on, but I have never liked what I call taking the Dodo position!

Solution One: Process using another instrument vendor's software

Obviously many laboratories will have made or are in the process of reviewing their position with regard to "preferred vendors" going forward. Some laboratories will be in the useful position of already having NMR spectrometers from different vendors in their environment. Alternatively they may have been contemplating cheaper options such as replacing everything except the expensive superconducting magnet. Either option makes Solution One a viable position to take for legacy data handling.

Solution Two: Central scientific data management systems

For those of us who have been promoting vendor-neutral, long-term data archiving solutions for so many years, the temptation to shout "We Told You So!" at the tops of our voices from tall buildings is, of course, pretty overwhelming.[4] This forms the second solution we have analysed. It is rather complicated in the NMR case, with the community's own preference in many cases to
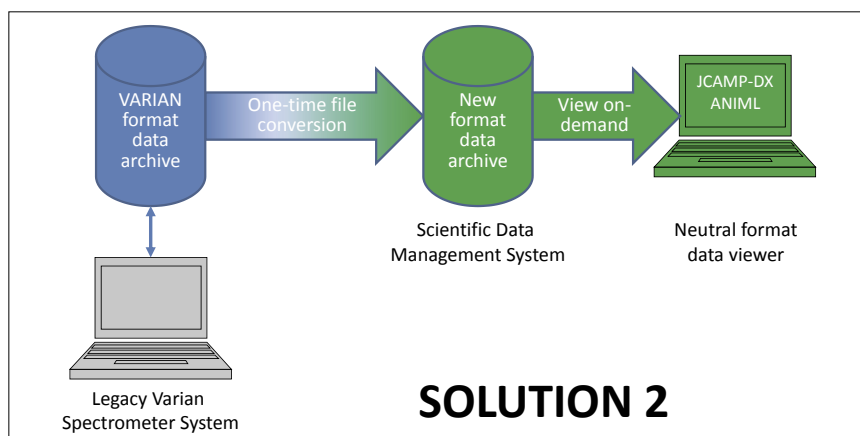

Figure 2. Use of vendor-neutral formats and scientific data management systems.

Strengths	Weaknesess
■ Removes legacy systems from environment mitigating risk ■ Builds on similar work already carried out and validated in the community by those with such e-record retention policies ■ Domain experts in Varian formats/systems still available ■ Agilent still supporting instrumentation	■ No publically available documented experiences of the full range of Varian data available ■ Substantial investment / testing required ■ Possible software development required/ no "off the shelf" complete single vendor solution ■ Capex required for secure data storage servers etc.

Opportunities	Threats
■ Possible broad community support as very many laboratories may want to go down this route at the same time ■ Other vendors may see this as a good commercial opportunity/business to move into ■ Clear scientific community need for standardisation bodies to respond to ■ Will yield a more robust general scientific data archiving strategy for an organisation	■ Cost ■ Conversions may be incomplete or difficult to automatically validate electronically ■ NMR communities often tend to store FID raw data rather than processed spectra makes this route more complex than for other spectroscopy types ■ Insufficient experience in this strategy in the NMR community globally

store un-processed time-domain FID raw data rather than the fully processed result files, so that the vendor-neutral format must allow for subsequent rather complex re-processing.

There are a number of vendors with various levels of offerings in this area. Waters' Dan Chapman (Product Manager, Waters NuGenesis LMS, SDMS) pointed out that the Scientific Data Management System (SDMS) in Waters NuGenesis® Lab Management System (LMS) automatically captures, secures, accesses and disseminates information from analytical technologies that includes Varian data. So for those labs that have a vast quantity of legacy Varian data, NuGenesis LMS is an ideal long-term data archive solution that will preserve the data with full search

capability for the required length of time. Agilent themselves, of course, have OpenLab ECM with support for technology-neutral formats and associated data viewers. For people looking for an organisation with an offering in this area who might be interested in developing a solution, Mukunth Venkatesan (CEO and Director of Agaram Technologies) has suggested developing a bulk convertor to JCAMP or ASCII formats and upload through their SDMS with provision of a viewer.

Solution Three: Third-party NMR specialist software processing solutions

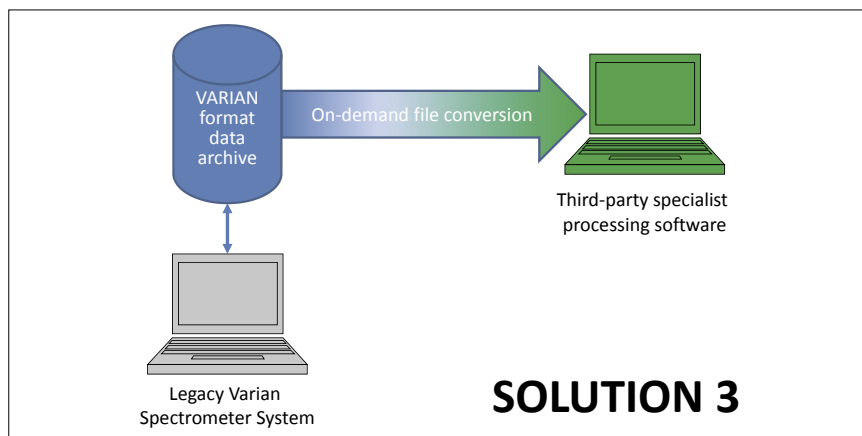One serious advantage that the NMR community has always benefited from

SOLUTION 3

Figure 3. Use of third-party, non-instrument vendor software solutions.

Strengths	Weaknesess
■ Probably the lowest cost solution in the short-term ■ Number of suppliers already in the market place ■ Processing from FID always available using the latest/fastest hardware/software platforms ■ May actually improve processing due to better algorithm implementations than currently available	■ Needs extensive testing against all Varian formats/experiments/file versions in archive ■ Relies still on longer-term support of computer systems supplying the data ■ Probably needs additional archive for converted and processed data to avoid repetition

Opportunities	Threats
■ Avoidance of potential short-term investment requirement ■ Potential broader deployment of instrument vendor-neutral NMR data processing ■ Provides a reasonable breathing space for other scientific data processing companies to come up with better commercial solutions ■ Data may reach end-of-life before even needing to be converted	■ Third-party independent solution providers (although "large" has not been much of a recommendation in this scenario!) ■ With only a few small specialist suppliers there is an increased risk of them going out of business ■ Small suppliers require disproprionate effort to stay up-to-date with rapidly changing device/operating system environments

over several other spectroscopy types is a strong provision of third-party data analysis and reporting software from scientific data processing companies outside the pool of instrument manufacturers. Considering the complexity of the required data processing for NMR raw data, this is quite surprising—but also maybe one of the root causes. Solution Three assesses the reliance of non-instrument manufacturer NMR data processing solutions to keep the Varian data archives viable.

Mike Partington (Senior Sales Director Europe and Japan) was again very helpful when we went in search of data on ACD/Labs' capabilities to mitigate

our Varian problem. He made an interesting observation that *"All analytical techniques have faced cycles of growth and contraction. VG, Nicolet, Bear, GE, and Finnigan are all companies that made positive contributions to various analytical instrumentation modes, but have disappeared. The most recent case of interest for NMR is Varian/Agilent. Data from VnmrS and VnmrJ has been used to solve a vast array of analytical problems for more than a quarter of a century. This data needs to be preserved and available for analysis for at least as long as the format has existed."* ACD/Labs has the Spectrus platform as an off-the-shelf

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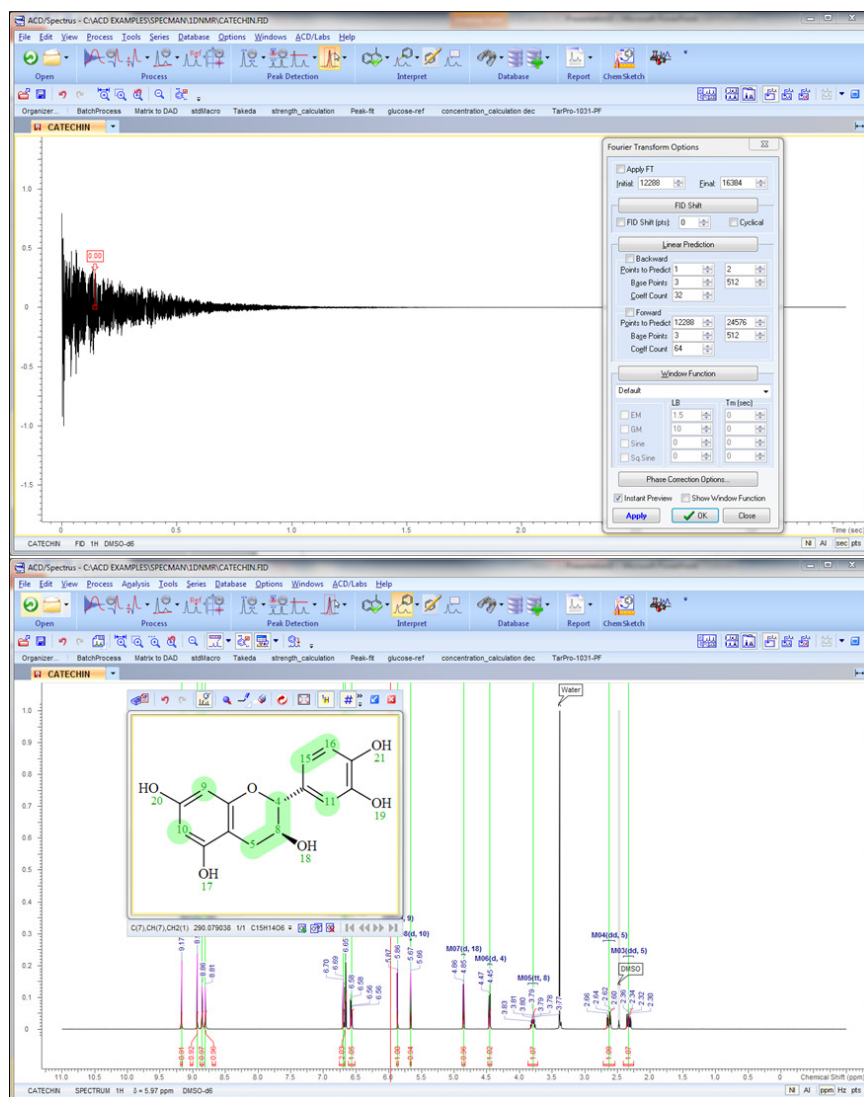**Figure 4.** 1D data imported from VnmrJ into the ACD/NMR Suite, before and after automated processing and interpretation.

Following the various SWOT analyses we think that the best solution is probably a combination of the three proposed solutions depending on your particular laboratory circumstances. First, it is probably a great idea to secure all your native NMR data into a safe, flexible, validateable and maintainable electronic content management system such as an SDMS. Second, retrieval from the SDMS system into a specialist NMR data handling software either from another instrument vendor as in Solution One or a dedicated NMR third-party software vendor as in Solution Three. So… no panics… even with Agilent/Varian leaving the NMR arena in the foreseeable future, we are still blessed with good commercial solution providers with high-quality products and vast experience to allow us to take this issue in our stride and continue to focus (after a short hiccup) on continuing to provide top quality spectroscopic analyses!

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commercial solution within which the ACD/NMR Workbook Suite supports a number of Varian file formats including *.fdf, fid0001.fdf, *.txt and *.fid. The data stored in the Spectrus environment is live, allowing reviewing, re-interpretation and re-processing to address new questions that may arise during the lifetime of a given molecular entity. Figure 4 shows an example of 1D data imported from VnmrJ, before and after automated processing and interpretation.

Juan Carlos Cobas Gómez (co-founder and President of Mestrelab Research) was good enough to tell us about the LinkedIn discussion we cited at the beginning of the column. He pointed out that, from the Mnova point of view, it is

preferable to have the data in the actual native NMR instrument vendor format rather than as JCAMP-DX files as they can import these directly. Even with the extensive implementation of JCAMP-DX in Mnova, especially for NMR data, there is always the possibility that during the Varian-to-JCAMP conversion some piece of information can be dropped. He also pointed out that there are many 3D and higher dimensionality NMR spectra in VNMR format which are not contemplated in the current JCAMP-DX NMR format.[5–8]

Conclusion

We have some work to do if we are going to avoid the fate of the Dodo.