

# Central spectroscopic data systems: why are chromatographers so much better equipped?

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I do not like being jealous, but looking at the systems our chromatographers have at their fingertips to control, program, monitor and analyse their experiments from a central Chromatography Data System makes me wish the spectroscopy community would catch up! The chromatographers are very fortunate in that their main vendors have a good offering of Chromatography Data Systems (CDS) which can run instruments from pretty much all of the various main chromatography instruments on the market. Why are we spectroscopists so poorly served?

## Typical CDS

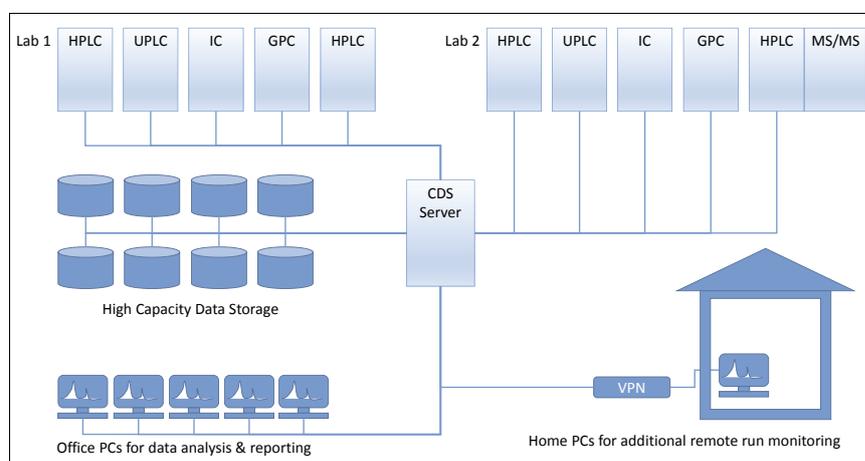
Depending on the size of your organisation, a central CDS can serve multiple laboratories in multiple locations, spread across different buildings, sites and even countries. In fact, it is possible to deploy these systems in a secure robust disaster recovery configuration which allows a fallback position of running the CDS from another continent. Essentially the only limiting factor is the availability of the network backbone infrastructure.

The enormous flexibility has been made possible by the exchange of instrument control specifications and tools between what would otherwise be competing vendors in the same instrument functionality space. This means that analysts are free to select the analyt-

ical system which they feel delivers the best performance for their particular area of work whilst selecting the control software which they feel best fits into their overall data analysis and reporting world. They have no need to compromise by being forced to buy a CDS from the same manufacturer as their instrument hardware.

The vendors must be applauded for having the strength to continue these collaborations, as you can well understand the pressure from the commercial side to try and gain a business advantage by not continuing this information exchange. In such deployments there must be serious discussion with the

users, management, compliance and IT support community if the addition of a Scientific Data Management System (SDMS) is actually to bring benefits. For laboratories working within a regulatory compliance framework, modern centralised CDS systems will normally be compliance-ready on installation and can operate alone (Figure 1). There may well be benefits arising in the area of long-term compliant archiving depending on the stability and granularity of the organisation. Where corporate policy may be able to dictate a centralised document archiving system across an organisation, this is significantly more



**Figure 1.** Potential modern CDS Deployment—now available with integrated mass spectrometry instrument control, data acquisition and analysis.

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difficult in the area of scientific data handling.

These systems have also made it possible for easy remote monitoring of the ongoing work which I have seen enhance the work–life balance amongst colleagues.

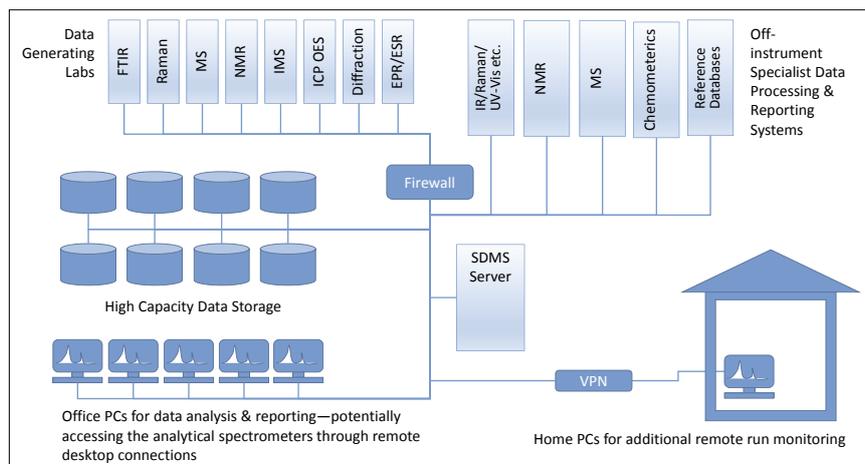
## Adding spectroscopy

Recently, there have been updates to CDS systems which have started to include support for hyphenated instrumentation. Currently the instrumentation support has been limited to a selection of the instruments within the particular CDS vendor's own range of spectrometers. This integration has included complex mass spectrometry instrumentation control and data analysis with reference spectroscopic database integration. As a first step this is greatly to be welcomed—and we can only hope that the collaboration between vendors in exchanging instrument control information will extend in future to the spectroscopic detectors as well.

Unfortunately, we may well run into the old ideological battle which is always fun to watch between those who identify themselves as chromatographers—who see hyphenated systems such as an UPLC-MS/MS as just a top of the range chromatography system with an overly expensive detector; and spectroscopists who would just see the front end as a programmable sample preparation robot enhancement to the inlet of the spectrometer. I always try to promote the thought that they are all actually just analysts and they should be optimising all areas of their instrumentation to achieve the best results.

As we have seen in recent articles there is the potential for remote spectroscopic instrument control between different vendors,<sup>1</sup> but in this particular case I would think it necessary to add that I would guess the specific collaboration was eased by the long-standing good relationship between the parties involved and the lack of competition in the instrumentation market between them.

There have been many initiatives involving direct competitors, especially in the USA, to develop the “unified instrument control protocol” to allow central-



**Figure 2.** Potential for a Spectroscopic Data System—still a bit of a mess!

ised instrumental management systems to handle a multitude of different instruments. Some of the systems prototyped have been used by individual vendors, but I am unaware of any great impact in our deployed instrumentation park.

## Can we rival the chromatographers' functionality?

Well the answer is not very inspiring and worryingly has not really changed much in the last ten years or so. Figure 2 shows one version of how an organisation may combine their available spectroscopic systems, data processing tools and an SDMS to get close to what the chromatographers' can boast is available out-of-the-box from several vendors in their space.

In a corporate environment one of the problems may well be incompatibilities between the laboratory PC infrastructure, due to the reliance on increasingly ageing spectrometer control systems and the demand to continually update to the latest operating systems. This is mainly driven by security reasons for all computers on the main corporate network. One workaround shown in Figure 2 is the introduction of segregation of the laboratory network from the corporate office network by a firewall. This adds another, although not insurmountable, level of complication to an integrated solution.

Although many spectrometer control packages now come with varying levels of complexity in the in-built data processing, many analysts have their own

personal preferences when it comes to advanced spectroscopic data processing, chemometric analysis or the use of particular reference database solutions. Maintenance update releases and security patches of these systems usually have no problems in remaining compliant with corporate IT policy so are usually found deployed on the normal corporate network.

If your organisation operates in a regulatory compliant space, there is probably little choice but to deploy an SDMS of some nature to meet the demands of the regulators around data integrity.

## Conclusions

In conclusion it is possible for a spectroscopic environment to mimic the functionality available to our brother and sister chromatographers, but we are still required to deploy a highly fragmented—and therefore vulnerable solution if we are to get close to what they have at their fingertips. I suppose hope is on the horizon with the introduction of hyphenated instrument support to recent CDS releases... but do we really want to be told by chromatographers how we need to work?

## References

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