A Closer Look at Chemical and Solvent Demands for LC-MS Applications

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Analytical laboratories are increasingly under pressure to perform – the precision of equipment used by the sector is improving, raising customer expectations for lower levels of detection and accuracy, while shorter turnaround times are being demanded. This combination of factors is intensifying the demands on analytical laboratories, which in turn is placing a corresponding burden on laboratory suppliers.

For example, the demand for high quality chemicals, such as solvents, has never been greater as sub-standard products can contain contaminants that can impair findings and block systems. Also, as laboratory equipment gets more sensitive, the requirement for increased levels of chemical purity to permit lower detection levels, rises in tandem, intensifying the issue. The need to eliminate potential contaminants, compromised results and false readings in analytical laboratories is vital, so only the best quality chemicals should be used. Fortunately, a reputable supplier will be prepared to provide samples and detailed data sheets in order to prove the effectiveness of its products.

Also, some laboratory requirements such as accuracy, reliability and timeliness lead to additional testing, such as a dedicated application test for the specified use of the chemicals that they purchase on incoming goods, including commodity products. It is often the case that the supplier has to provide customised test data and certification for them so when the product arrives the customer can proceed with analytical testing and not spend time evaluating products in the raw materials stage. Laboratories want a product that is ready to use straight from the container *(Figure 1)*.

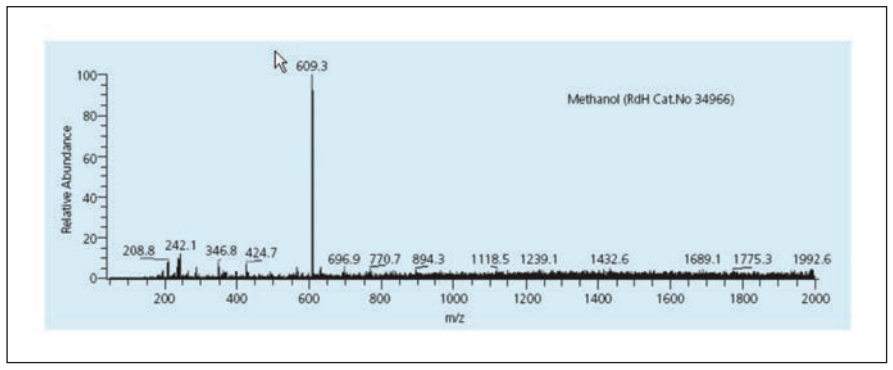

Figure 1. The Reserpine test shows a reserpine spectrum measured in Methanol; no signals should be greater than [M+H]+ = 609 (100ppb reserpine; ESI, positive mode).

Importantly, having access to high-purity, custom formulations produced to exact specifications can help minimise the need for manual blending in the laboratory and therefore provide health and safety benefits to people directly associated with the work. Finding a supplier that will process a chemical to a level not ordinarily seen in the marketplace not only saves time and therefore money, it also helps to maximise staff welfare by reducing potentially hazardous blending.

Moreover, by eliminating the need for manual blending a laboratory can redeploy resources to more value-added activities that help it reach its scientific and technical goals. Laboratories also benefit from eliminating the waste that can result from formulation errors while at the same time reducing chemical handling, which helps make for a safer working environment.

While some supply trends are general, analytical laboratories have some very specific requirements such as for chemicals used in liquid chromatography–mass spectrometry (LC-MS). Because of the need for legally defensible results produced in the process and because of its extremely high levels of sensitivity it is essential to only use chemicals with the highest obtainable levels of purity. Any contaminants can provide erroneous results through contaminant peaks, high backgrounds and matrix effects. Poor quality chemicals/ solvents may also block LC-MS filters, which can generate undesirable back pressure.

LC-MS is fast becoming a routine apparatus in a modern analytical laboratory. Along with the increased use of LC-MS technology, new ion sources, high-resolution LC systems and rapid mass spectrometers with enhanced ion optics and detectors have lowered the limits of detection. Meanwhile the use of dedicated and application tested high purity mobile phase became more and more popular. Beside strict specifications that are promised by all commercial available mobile phases, there are still differences that will effect a measurement. *Figure 2* shows the comparison between a water/acetonitrile gradient of an HPLC grade and LC-MS Chromasolv grade from Honeywell.

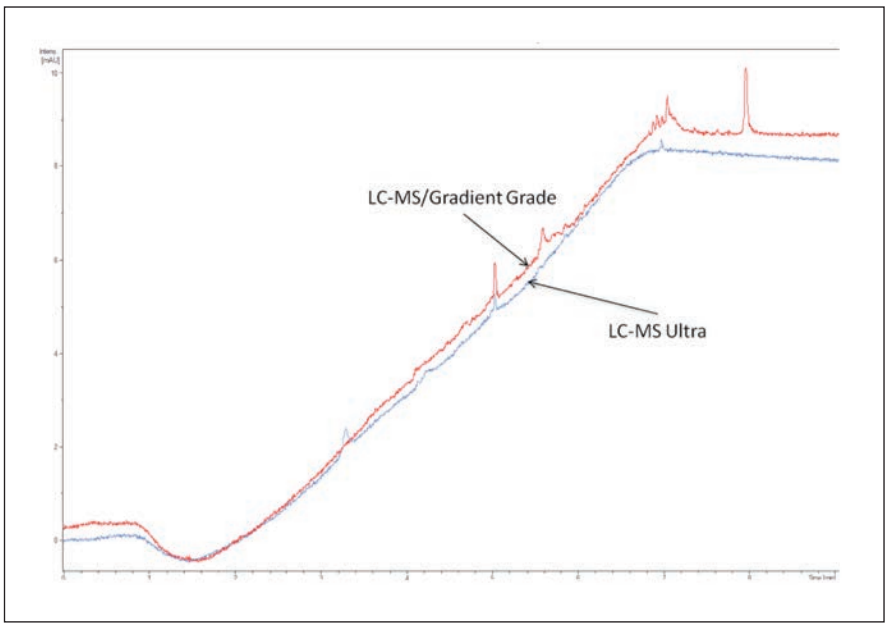

Figure 2. Comparison LC-MS/Gradient Grade under UHPLC Conditions

In order to be suitable for LC-MS chemicals will generally have been through an additional purification step as well as rigorous testing. Different manufacturers use different techniques to achieve this and while all might claim to be the same standard, very often they are not. Poor quality solvents and chemicals can contain particulate matter that can block inlet and inline filters, columns and contaminate detector cells but most importantly they can make low level detection difficult *Figure 2* exhibits the difference in sensitivity between two grades *Figures 3 and 4* show a chromatogram with a 5 ppm injection of reserpine utilising the same gradient. Analytical laboratories should therefore only procure solvents for use in LC-MS that have been micro-filtered; not all suppliers offer this level of treatment.

The rapid growth of ultrahigh-performance liquid chromatography has provided greatly reduced analysis times and its coupling with mass spectrometry for detection, is driving the need for even greater levels of purity, albeit at reduced chemical volumes. The background mass spectrum noise seen in *Figure 3* (red line) originates only from the HPLC grade water, this is highlighted in *Figures 5* and *6*. Therefore, the solvent quality should be directly linked to the analysis method.

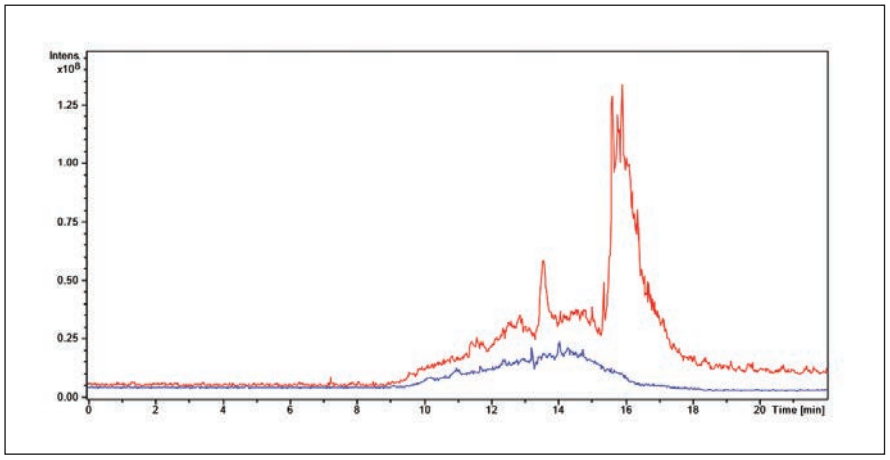

Figure 3. HPLC baseline produced by a gradient from 100% Water (Riedel-de Haën LC-MS CHROMASOLV 39253) to 100% acetonitrile (Riedel-de Haën LC-MS CHROMASOLV 34967) blue chromatogram. The red chromatogram is the same gradient using basic HPLC grade water and acetonitrile. The contamination originates only from the HPLC grade water.

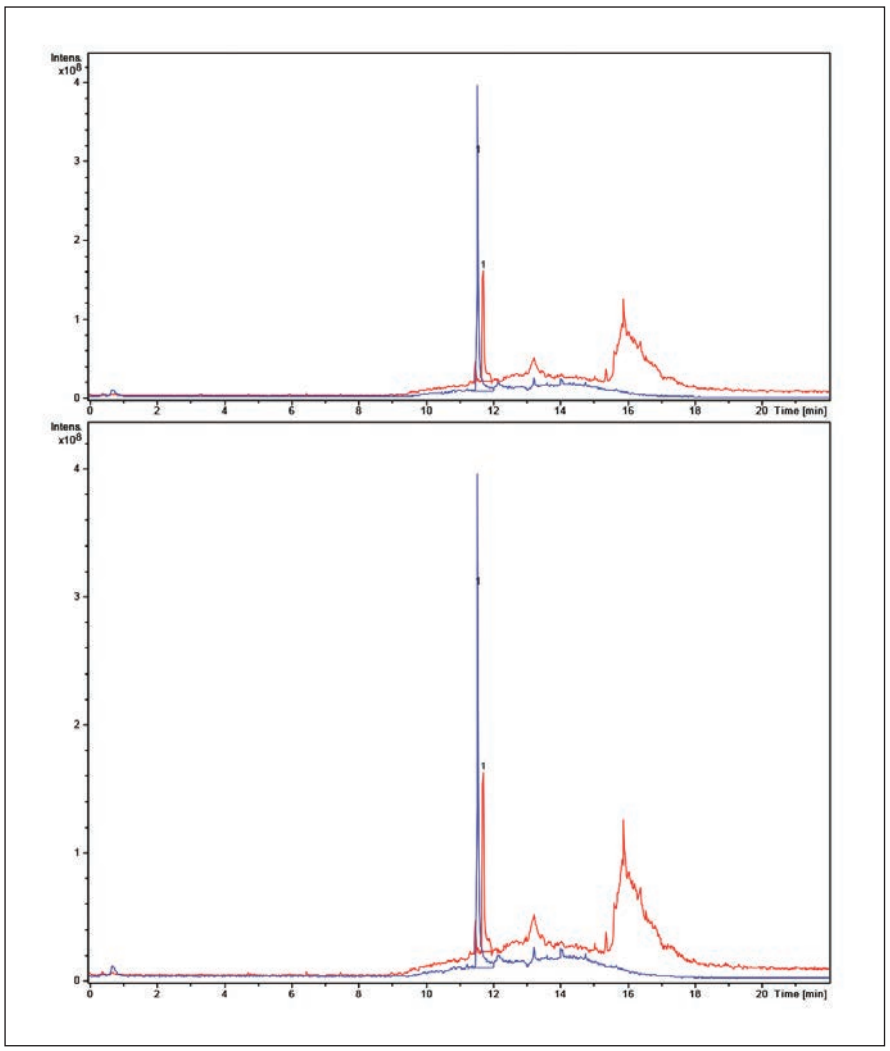

Figure 4. In this example the chromatogram shows a 5 ppm injection of reserpine using the same gradient conditions. The red line shows HPLC grade water / acetonitrile and the blue line shows LC-MS water / acetonitrile (Riedel-de Haën 39253 and Riedel-de Haën 34967).

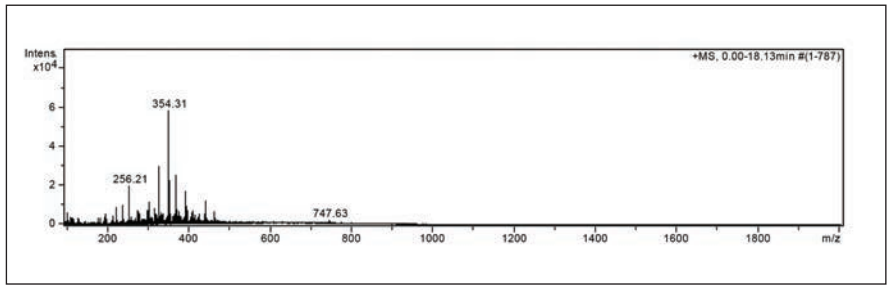

Figure 5. The average mass spectrum of LC-MS grade Water and LC-MS grade Acetonitrile (Riedel-de Haën 39253 versus 34967) is shown. Figure 6 is the direct comparison with an HPLC grade water.

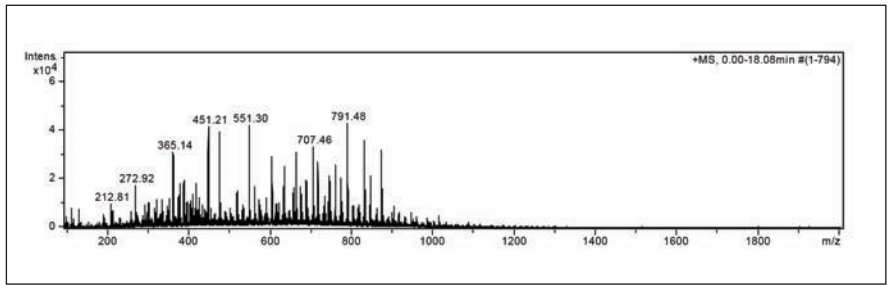

Figure 6. The average mass spectrum of HPLC grade water versus LC-MS grade acetonitrile (Riedel-de Haën 34967) is shown. In conclusion to the measurement above the contamination originates only from the HPLC grade water.

Timely deliveries of variable amounts on specific deadlines are not optional requirements for today's analytical laboratory – they are essential for efficient analytical laboratory operation. Custom formulations are increasingly being seen as a 'must have' option, too. Analytical laboratories therefore need to work with chemicals suppliers that offer the highest possible levels of purity as well as in bespoke formulations. These products also need to be delivered in the required quantities on the requested date in order to ensure throughput levels are maintained. Not all suppliers offer this class of service, a shortcoming that can compromise a laboratories ability to meet their testing demand.

Honeywell's LC-MS Chromasolv solvents and blends do offer the same and comparable outstanding quality. They ensure the specification requirements regardless of differences in the nature of the chemicals and their behaviour. All products are developed for routine analysis, e.g. proteins and peptides (Water/acetonitrile with 0.1% Formic acid, 0.01% TFA or water/acetonitrile with 0.1% TFA), small molecules (Water/acetonitrile with 0.1% Formic Acid). Pure solvents and blends can also be adapted to special chromatographic needs with our high purity additives.