White Paper

Agilent
Trusted Answers

What Solvents Are You Putting Into Your LC/MS Instrument?

Introduction

Today, luxury car manufacturers typically require the buyer to put the highest grade of fuel into the car when refilling the tank. The higher-powered engines in these luxury cars have multiple sensors that monitor the status and performance of the engine. Premium fuels allow the car to maintain its performance, reduce the amount of contaminant buildup, and meet the manufacturer's rigorous specifications.

Similarly, as an LC/MS instrument manufacturer, Agilent understands that LC/MS performance is optimized using high-quality solvents. We designed our Agilent InfinityLab Ultrapure LC/MS solvents with instrument performance in mind. Our solvents are developed and manufactured to reduce their levels of metal and organic contaminants. To decrease the potential for contamination from the container itself, and to extend solvent shelf life, we take extreme care in choosing solvent bottles and caps. The following examples showcase the improvements we have made, and the performance of these solvents in comparison with existing manufacturers.

Improved solvent performance

LC/MS contaminants results

With ever-increasing sensitivity made possible by improving LC/MS technologies, it is important to have solvents with low background contamination to distinguish your analyte from the baseline noise. To illustrate minimized background contaminants, InfinityLab Ultrapure solvents were directly infused into an Agilent 6550 iFunnel quadrupole time-of-flight LC/MS source. The reduction of contaminating species facilitates increased sensitivity and decreased ion suppression.

Figures 1, 2, and 3 show Agilent InfinityLab Ultrapure LC/MS methanol, water, and acetonitrile with fewer background contaminants or equivalent background than the other vendors tested, respectively.

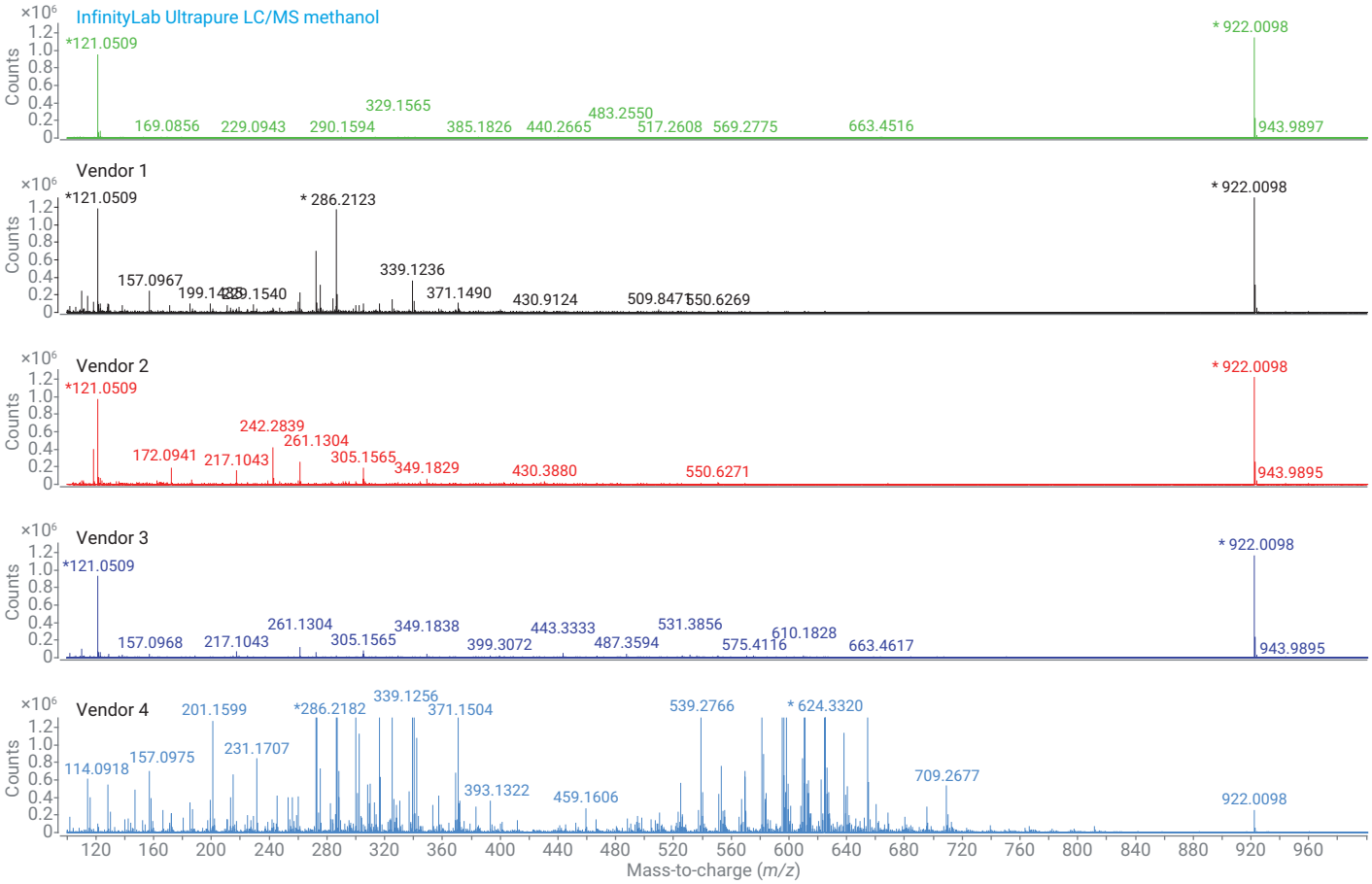


Figure 1. Full scan direct infusion comparison of four vendors and InfinityLab Ultrapure LC/MS methanol in positive polarity mode using a 6550 iFunnel quadrupole TOF LC/MS. *m/z* 121 and 922 are reference solution ions.

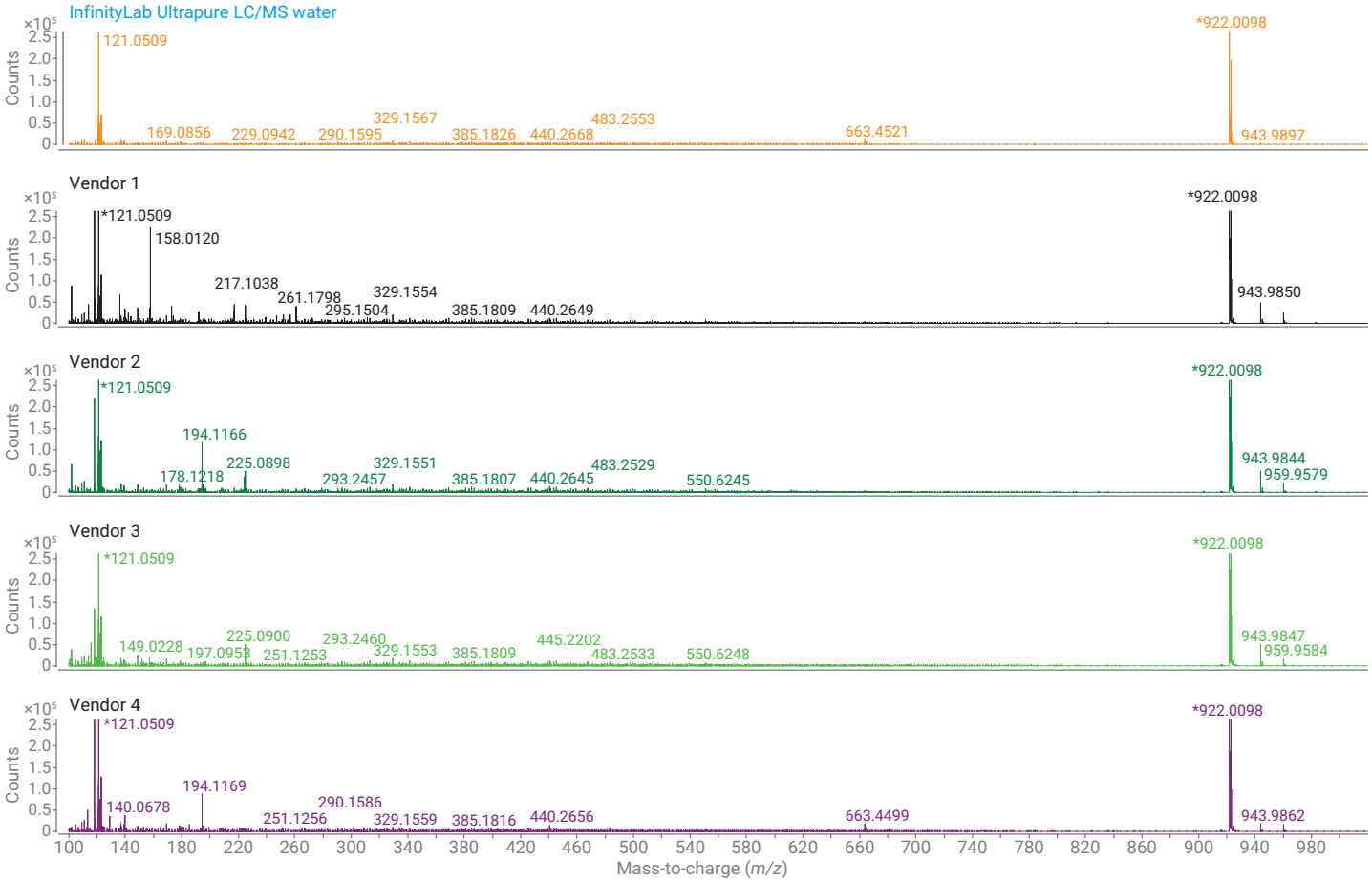


Figure 2. Full scan direct infusion comparison of four vendors and InfinityLab Ultrapure LC/MS water in positive polarity mode using a 6550 iFunnel quadrupole time-of-flight LC/MS. *m/z* 121 and 922 are reference solution ions.

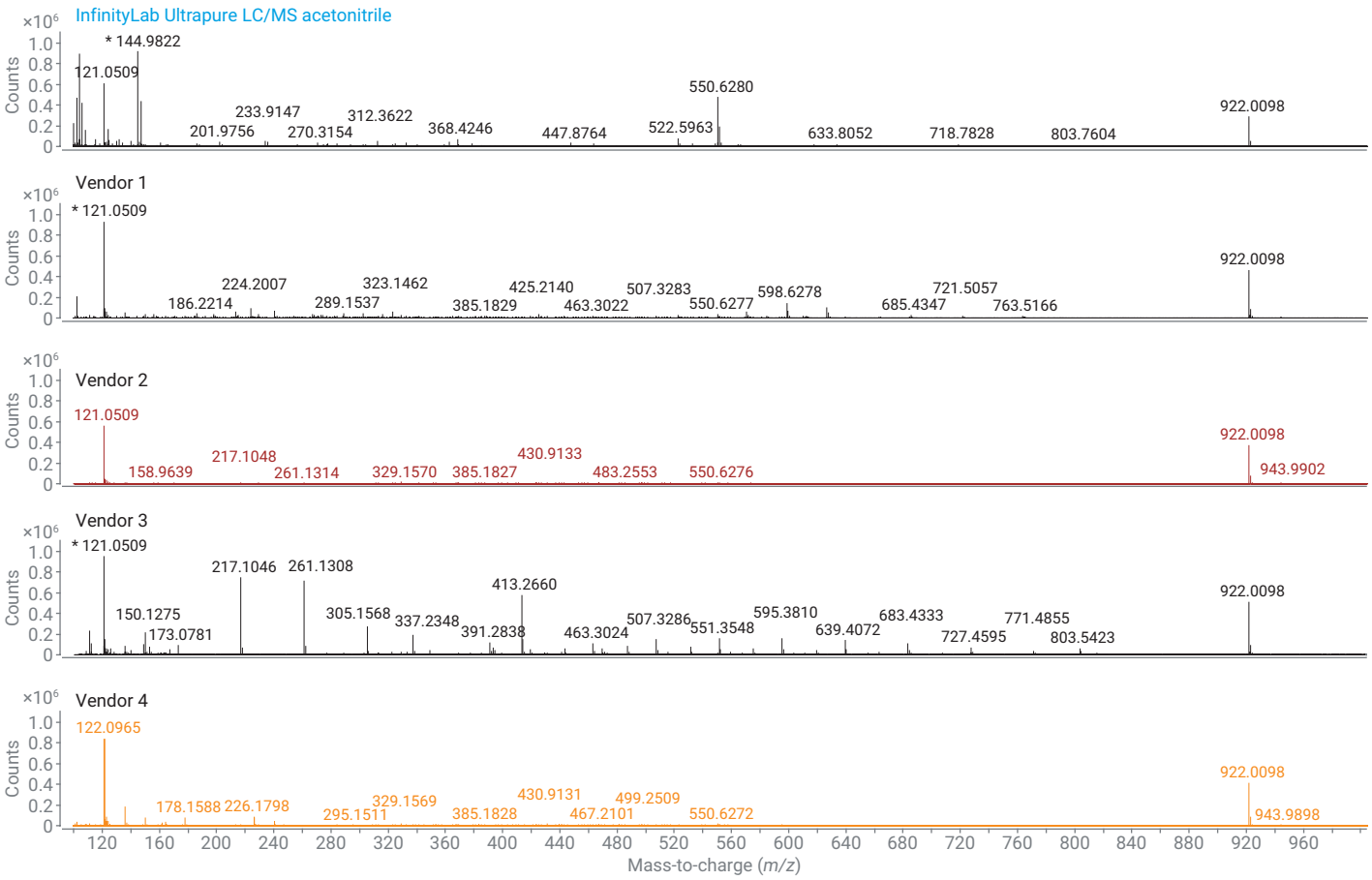


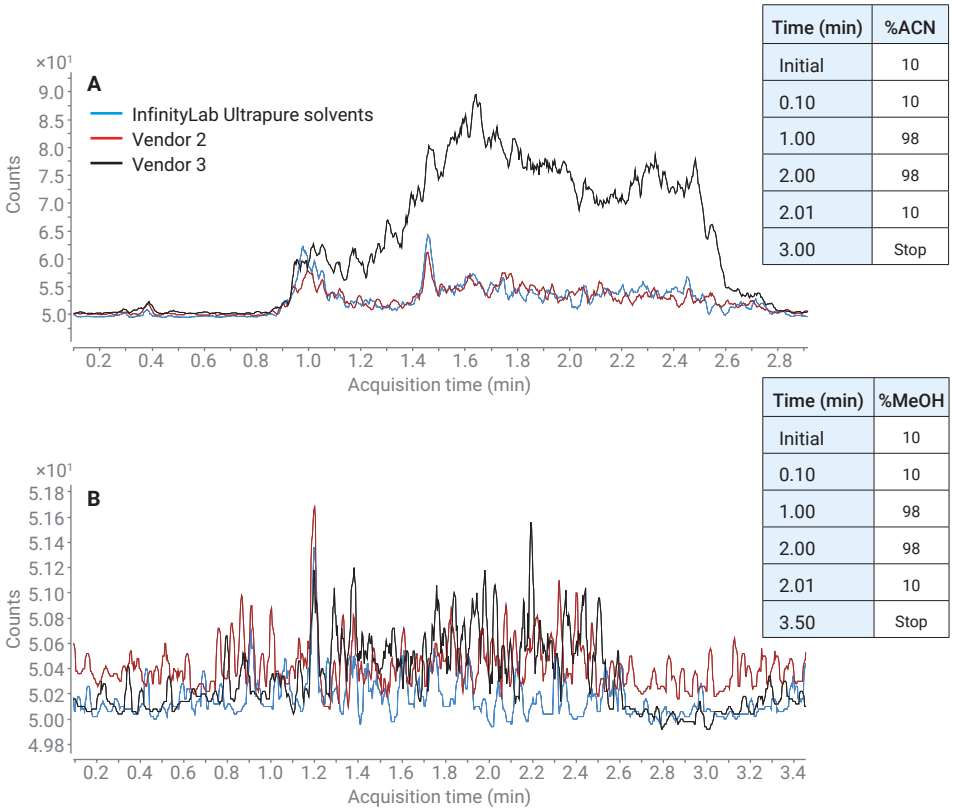
Figure 3. Full scan direct infusion comparison of four vendors and InfinityLab Ultrapure LC/MS acetonitrile in positive polarity mode using a 6550 iFunnel quadrupole time-of-flight LC/MS. *m/z* 121 and 922 are reference solution ions.

LC/MS gradient data

To ensure low background even when the solvent ratio changed, InfinityLab Ultrapure solvents were run in parallel with two other vendors on a gradient. Low background means consistently low noise throughout a gradient run (Figure 4), giving increased sensitivity for even the most challenging analytes. Our solvents outperform or directly compete with other high-quality solvents on the market. Gradient data were collected with a 6495B triple quadrupole LC/MS using instrument checkout methods.

Low metal ion adducts

In quantitative LC/MS analysis, it is important to have low concentrations of metal ions. One of the greatest contributors to this prevalent issue is solvent quality. We tested our InfinityLab Ultrapure solvents using sulfadimethoxine, a commonly used analyte known for easily forming sodium adducts. The higher the intensity of the sulfadimethoxine $[M+H]^+$ ion, the lower the sodium in the solvent. InfinityLab Ultrapure methanol, water, and acetonitrile all surpass competitor solvents, producing the highest intensity $[M+H]^+$ ions, revealing less metal adduct formation and more accurate quantitation (Tables 1 and 2).



Time (min)	%ACN
Initial	10
0.10	10
1.00	98
2.00	98
2.01	10
3.00	Stop

Time (min)	%MeOH
Initial	10
0.10	10
1.00	98
2.00	98
2.01	10
3.50	Stop

Figure 4. A)Acetonitrile/water with 0.1 % formic acid, positive mode. B) Methanol/water, negative mode. Column: Agilent ZORBAX RRHD Eclipse Plus, 3 × 50 mm (p/n 959757-302).

Table 1. Sulfadimethoxine sodium adduct formation results using acetonitrile/water with 0.1 % formic acid. InfinityLab Ultrapure acetonitrile use produces the highest intensity $[M+H]^+$ ion, indicating fewer sodium and potassium adducts. A 6550 iFunnel quadrupole TOF LC/MS was used to generate the results, which were averaged between lots tested for each vendor.

	Vendor 1 (2 lots)		Vendor 2 (3 lots)		InfinityLab (3 lots)	
Species	% of Analyte	%RSD	% of Analyte	%RSD	% of Analyte	%RSD
$[M+H]^+$	69.5	1.0	73.1	1.2	82.7	2.4
$[M+Na]^+$	26.8	2.0	22.9	3.8	14.4	16.7
$[M+K]^+$	3.7	5.6	4.0	18.5	2.9	19.4

Table 2. Sulfadimethoxine sodium adduct formation results using methanol/water with 0.1 % formic acid. InfinityLab Ultrapure methanol use produces the highest intensity $[M+H]^+$ ion, indicating fewer sodium and potassium adducts. A 6550 iFunnel quadrupole TOF LC/MS was used to generate the results, which were averaged between lots tested for each vendor.

	Vendor 1 (2 lots)		Vendor 2 (3 lots)		InfinityLab (3 lots)	
Species	% of Analyte	%RSD	% of Analyte	%RSD	% of Analyte	%RSD
$[M+H]^+$	78.6	0.6	72.7	5.8	83.2	2.3
$[M+Na]^+$	19.1	2.1	23.6	18.9	15.1	8.9
$[M+K]^+$	2.3	4.1	3.8	6.1	1.9	20.8

LC/MS packaging results

Use of the right packaging is essential for ensuring the long-term stability of solvents. By choosing the optimum bottles and caps, we can ensure the performance of our solvents, even after storing them for long periods. For example, an instrument detection limit (IDL) checkout using reserpine on an Agilent Ultivo triple quadrupole LC/MS was achieved without issues after storing the solvents for nine months at room temperature. IDLs between 1.7 and 3.8 fg of reserpine were found, which is well below the specification limit of ≤10.0 fg. Solvents from three different lots were used (Figure 5).

Conclusions

The importance of solvent quality cannot be underestimated when running LC/MS instrumentation. Using InfinityLab Ultrapure LC/MS solvents will significantly enhance the sensitivity of your LC/MS instruments. InfinityLab Ultrapure LC/MS solvents perform as well or better than our competitors by ensuring less contamination. You can be certain of experiencing lower baseline noise, fewer sodium adducts, and less ion suppression relative to solvents from other vendors. The innovative packaging also increases solvent shelf life, and reduces metal contamination.

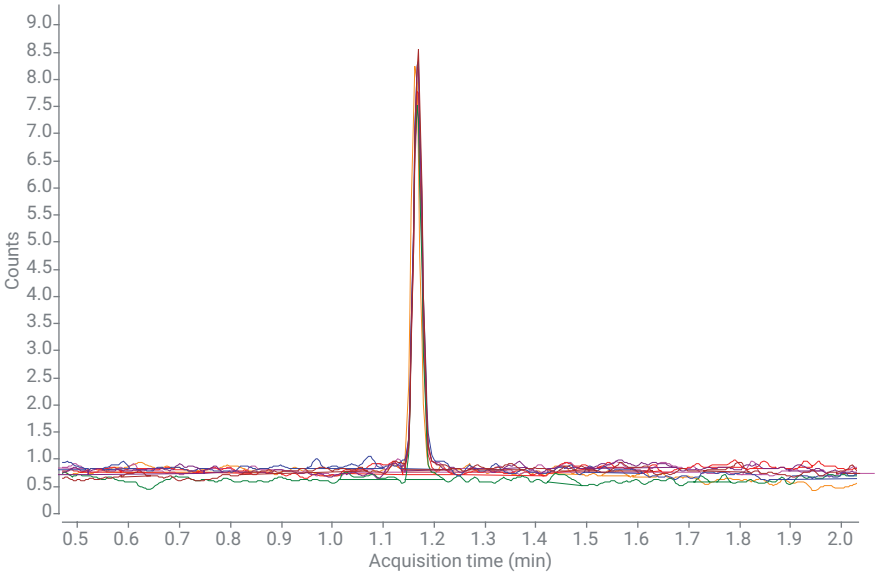


Figure 5. Instrument detection limit determination, with eight consecutive injections of 20 fg of reserpine using solvents after nine months of storage. An Ultivo triple quadrupole LC/MS was used to generate the results.

Agilent InfinityLab Ultrapure LC/MS solvents

Product name	Part number
InfinityLab Ultrapure LC/MS acetonitrile	5191-4496
InfinityLab Ultrapure LC/MS methanol	5191-4497
InfinityLab Ultrapure LC/MS water	5191-4498

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