

LC-MS CHROMASOLV®

High Purity Solvents As an analytical tool LC-MS is often chosen for its sensitivity and specificity. However, impurities in the mobile phase can seriously diminish the ability to detect and identify compounds that exist at very low levels. LC-MS CHROMASOLV® solvents from Riedel-de Haën undergo 34 distinct tests to ensure they meet the stringent criteria required for sensitive LC-MS and LC-UV analyses. Some of the most important features are:

- Application-tested for LC-MS using the reserpine test
- Very low level of inorganic and metal ions for high sensitivity and spectral interpretation
- Free of particles and non-volatile compounds
- High UV-transmittance for UV-Diode Array application
- Low gradient baseline

LC-MS Solvents

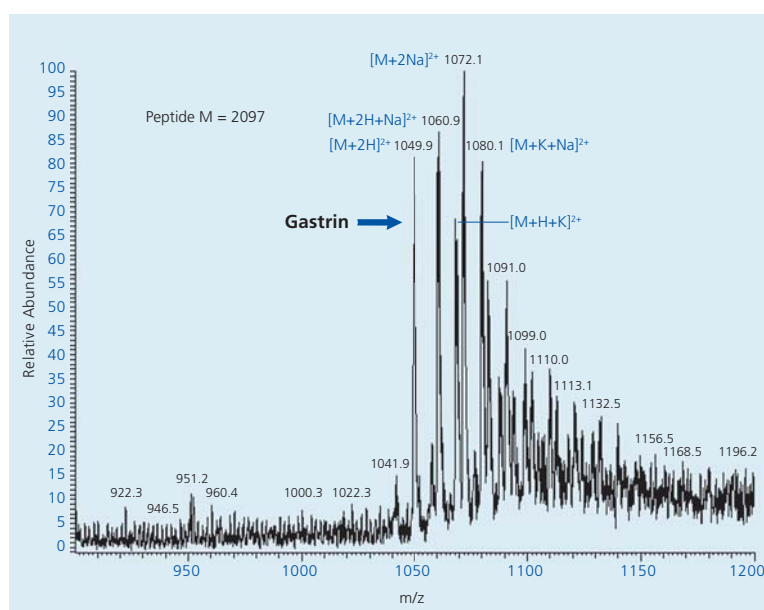
As an analytical tool LC-MS is often chosen for its sensitivity and specificity. However, impurities in the mobile phase can seriously diminish the ability to detect and identify compounds that exist at very low levels. Furthermore, particulate and non-volatile impurities can clog susceptible and delicate hardware components and cause expensive system down-time.

LC-MS CHROMASOLV[®] solvents from Riedel-de Haën undergo 34 distinct tests to ensure they meet the stringent criteria required for sensitive LC-MS and LC-UV analyses. Some of the most important features are:

- Application-tested for LC-MS using the reserpine test
- Very low level of inorganic and metal ions for high sensitivity and spectral interpretation
- Free of particles and non-volatile compounds to maintain system integrity
- High UV-transmittance for UV-Diode Array applications
- Low gradient baseline even with your own optimized protocols

MS detection relies on two factors that are not necessary in UV detection: the analytes must be ionized and they must be volatile. HPLC mobile phase solvents and buffers that are suitable for UV detection are often unsuitable when MS detection is employed. For example, sodium and potassium phosphate, two of the most common buffers in HPLC with UV detection, cannot be used in LC-MS because they are not volatile and suppress ionization. Additionally, they can complicate spectral interpretation, as we describe in the following discussion.

Figure 1 ESI mass spectrum of human gastrin dissolved in water having a sodium and potassium content higher than 10 ppm (gastrin molecular ion = 1049.8 m/z). A fence originated by the metal ion cluster can be clearly noted (peaks between 1051 and 1150 m/z).



Investigation of Cluster Formation in Presence of Alkali Ions

When using mobile phases that are contaminated with alkali metals, particularly sodium and potassium, interpretation of the mass spectra is complicated and sensitivity is decreased. Ideally, the analyte should give molecular ions by forming adducts with protons, [M+H]⁺. However, when other cations are present as contaminants in the mobile phase, undesirable adducts are formed, e.g. [M+Na]⁺, making spectral interpretation difficult.

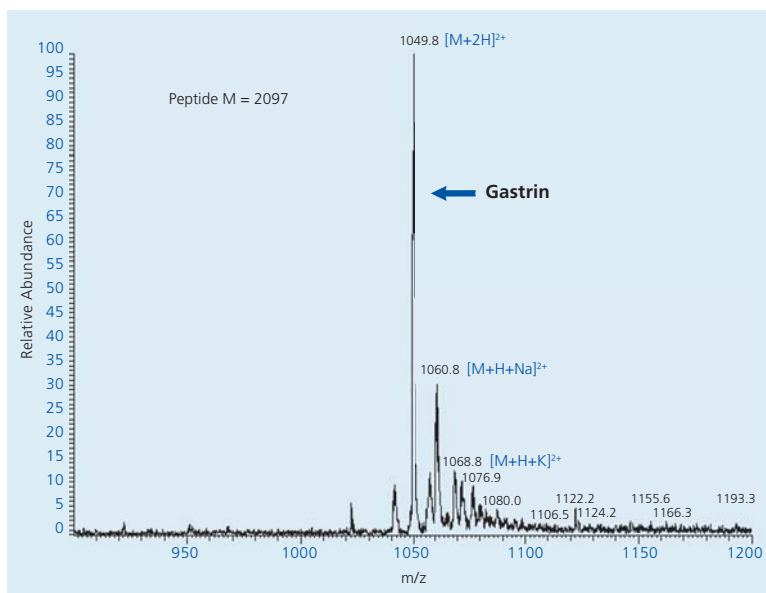
We investigated the influence of metal ions on the quality of LC-MS spectra using human gastrin (M = 2097) as a model peptide. The sample was infused with a microspray representing the conditions of a capillary nanospray. When operating ESI in positive ion mode, the preferred ionization reaction is the formation of [M+H]⁺ ions. In the case of peptides, a protonated, double-charged [M+2H]²⁺ ion is generated. For gastrin, a molecular ion with m/z = 1049.8 [M+2H]²⁺ is expected.

First, human gastrin was dissolved in commercially available HPLC water containing 0.2% formic acid. Typically, for the standard HPLC-grade, the potassium and sodium content is higher than 10ppm. The high metal content causes formation of metal ion clusters with the peptide. As a result the mass spectrum is difficult to interpret; the dominating clusters appear as a fence of double and multicharged ions (**Figure 1**). Such artifacts make it difficult to determine the **true peak** which is the protonated double charged molecular ion of gastrin ([M+2H]²⁺). Additionally, major problems will occur with the automatic MS-MS mode, where the most abundant peaks are selected for further collisions to give the amino acid sequence.

Next, we replaced the HPLC-grade water with LC-MS CHROMASOLV[®]-water, which has very low concentration of sodium and potassium ions (< 0.1 ppm). Note in **Figure 2** the mass spectrum reveals very few metal ion clusters; only [M+H+Na]²⁺ and [M+H+K]²⁺ were found in a relatively low abundance. The protonated double charged molecular ion peak of gastrin ([M+2H]²⁺) can be easily discerned, isolated and further fragmented to yield the amino acid sequence. Not only is the mass spectrum using the LC-MS CHROMASOLV[®]-water easier to interpret, an added benefit to the fewer artifacts is the nearly 10-fold increase in sensitivity compared to the standard HPLC-grade water.

Conclusions

Because alkali metal ion concentration has such a profound effect on the quality of the LC-MS results, we increased the quality by reducing the specifications for the alkali elements sodium and potassium for all of our LC-MS CHROMASOLV[®]-solvents (see **Table**). The only exception was ethyl acetate because it is used primarily for sample preparation rather than as a mobile phase. The purity and quality of LC-MS CHROMASOLV[®] solvents from Riedel-de Haën allow the LC-MS to realize its maximum sensitivity and specificity.



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Figure 2 ESI mass spectrum of human gastrin in LC-MS CHROMASOLV® Water. The gastrin molecular ion can be found at 1049.8 m/z. Only a few clusters are observed (between 1051 and 1100 m/z). Sensitivity was enhanced 10-fold.

Table Specifications for LC-MS CHROMASOLV®-Solvents from Riedel-de Haën

	Water	Acetonitrile	Methanol	2-Propanol	Ethylacetate
Cat. No.	39253	34967	34966	34965	34972
Pack Sizes	1 L	1 L / 2.5 L	1 L / 2.5 L	1 L / 2.5 L	1 L / 2.5 L
Assay (GC) (min)	-	99.9%	99.9%	99.9%	99.7%
Fluorescence at 254 nm (max)	1 ppb	0.5 ppb	1 ppb	1 ppb	-
Fluorescence at 365 nm (max)	1 ppb	0.5 ppb	1 ppb	1 ppb	-
Chloride (Cl) (max)	0.000001%	-	-	-	-
Fluoride (F) (max)	0.000001%	-	-	-	-
Nitrate (NO₃) (max)	0.00001%	-	-	-	-
Sulfate (SO₄) (max)	0.00001%	-	-	-	-
Free acid (max)	-	0.001%	0.001%	0.001%	-
Free alkali (as NH₃) (max)	-	0.0002%	0.0005%	0.0005%	0.0005%
Non-volatile matter (max)	0.001%	0.0002%	0.0005%	0.0005%	0.0005%
Water (Karl Fischer) (max)	-	0.01%	0.02%	0.05%	0.03%
Transmittance at 200 nm (min)	95%	95%	-	-	-
Transmittance at 230 nm (min)	99%	99%	75%	75%	-
Transmittance at 260 nm (min)	-	-	98%	98%	50%
HPLC gradient (254nm) (max)	1 mAU	0.2 mAU	2 mAU	2 mAU	-
Silver (Ag) (min) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	-
Aluminum (Al) (max)	0.5 ppm	0.5 ppm	0.5 ppm	0.5 ppm	-
Barium (Ba) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	-
Calcium (Ca) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm
Cadmium (Cd) (max)	0.05 ppm	0.05 ppm	0.05 ppm	0.05 ppm	-
Cobalt (Co) (max)	0.02 ppm	0.02 ppm	0.02 ppm	0.02 ppm	-
Chromium (Cr) (max)	0.02 ppm	0.02 ppm	0.02 ppm	0.02 ppm	-
Copper (Cu) (max)	0.02 ppm	0.02 ppm	0.01 ppm	0.02 ppm	-
Iron (Fe) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	-
Potassium (K) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm
Magnesium (Mg) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm
Manganese (Mn) (max)	0.02 ppm	0.02 ppm	0.01 ppm	0.02 ppm	-
Sodium (Na) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm
Nickel (Ni) (max)	0.02 ppm	0.02 ppm	0.02 ppm	0.02 ppm	-
Lead (Pb) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	-
Tin (Sn) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	-
Zinc (Zn) (max)	0.1 ppm	0.1 ppm	0.1 ppm	0.1 ppm	-
Particle test	+	+	+	-	-
LC-MS suitability test (reserpine test)	+	+	+	+	+

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