

# Scharlau



*Beyond HPLC...*  
...LC-MS solvents & mixtures

*Beyond HPLC, the LC-MS technique combines the advantages of chromatographic separation with those of mass spectrometry. The structural information given by mass spectrometry about the separated compounds allows its identification and quantification, even if they are in complex matrixes. Those characteristics makes the LC-MS very useful for the analysis of organic compounds in biological samples, the analysis of contaminants in environmental samples, as well as in proteomics and genomics.*



Doing the transition from HPLC to LC-MS is not trivial. It is necessary to adapt methods to the new analytical conditions in order to obtain the maximum benefits associated to the LC-MS. In this context, the user might ask about the necessity of using solvents of guaranteed quality for LC-MS.

The sensitivity of the LC-MS equipment is increased with the use of cleaner eluents. A solvent of HPLC quality is not always appropriate for its use in LC-MS, since some impurities that are not detected by ultraviolet spectroscopy could interfere in mass spectrometry.

Our solvents and mixtures for LC-MS respond to these new necessities and guarantee the best results thanks to their special characteristics:

- **Low content of metallic impurities (alkalines and alkaline earth cations)**
- **Microfiltered through 0,22µm**
- **Minimum level of free acidity and free alkalinity**
- **Low water content**
- **Low level of non-volatile impurities**
- **Controlled by LC-MS**
- **Packed under special conditions**
- **Certificate of batch analysis**

### *What will you gain by using our solvents and mixtures for LC-MS?*

- **Greater sensitivity**
- **Spectra identification becomes simpler**
- **More efficiency in the formation of molecular ions**
- **Longer HPLC column life**
- **Savings in equipment maintenance costs**
- **Guarantee of a product controlled by LC-MS**

Metallic impurities at the ppm level, that don't affect in HPLC, distort the mass spectra, modifying the abundance of the molecular ions of interest and making the interpretation of the spectra more complicated.

Next are shown two spectra of the same peptide where the positive effect of using acetonitrile and water of LC-MS quality is observed.

The analyzed peptide is human gastrin and the major ion  $[M+2H]^{2+}$  should respond to  $m/z$  1050.

In fig. 1 it is observed how the peak of the major ion  $[M+2H]^{2+}$  is masked by other peaks corresponding to adducts formed with alkaline metals  $[M+Na+H]^{2+}$  or  $[M+K+H]^{2+}$ .

In fig. 2 we can observe that  $[M+2H]^{2+}$  is the major ion when using Scharlau acetonitrile and water LC-MS.

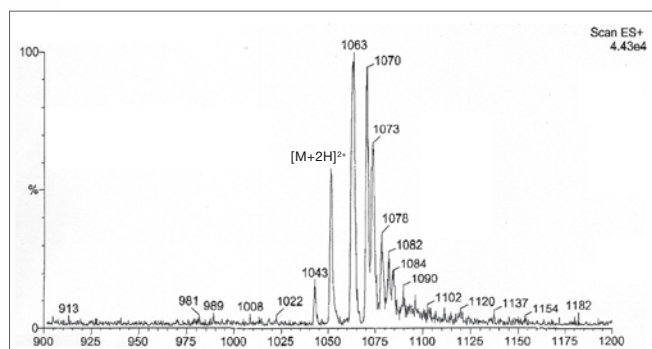


Figure 1. HG spectrum obtained with acetonitrile and water of HPLC quality.

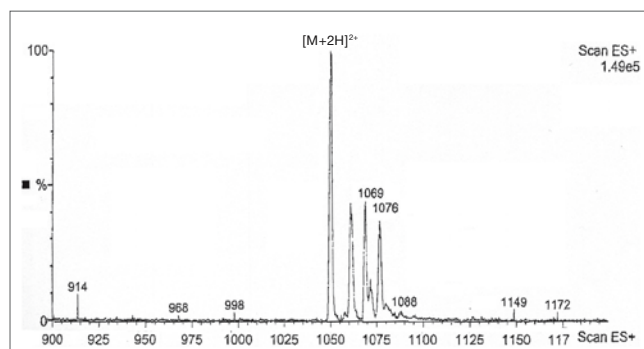


Figure 2. HG spectrum obtained with acetonitrile and water of LC-MS quality from Scharlau.

LC-MS analytical conditions:

Eluent: ACN/H<sub>2</sub>O mixture, 50/50, v/v, with 0,2% formic acid  
 Flux: 250 µl/min. Split  
 Injection volume: 50µl of a 10µg/ml human gastrin solution  
 Detection: ESI + Frag. 3500V Source T: 150°C

Parameter	Acetonitrile LC-MS AC0371	Methanol LC-MS ME0326	Water LC-MS AG0006	2-Propanol LC-MS AL0326	Ethyl acetate LC-MS AC0158
Assay (G.C.)	min. 99,9 %	min. 99,9 %		min. 99,9 %	min. 99,8 %
Conductivity (25°C)			max. 1 µS/cm		
Density (20°/4°)	0,779 - 0,783	0,791 - 0,792		0,784 - 0,785	0,899 - 0,902
Acidity	max. 0,0002 meq/g	max. 0,0002 meq/g		max. 0,0001 meq/g	
Alkalinity		max. 0,0002 meq/g			max. 0,0002 meq/g
Aluminium (Al)	max. 0,00005 %	max. 0,00005 %	max. 0,00005 %	max. 0,00005 %	
Barium (Ba)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	
Cadmium (Cd)	max. 0,000005 %	max. 0,000005 %	max. 0,000005 %	max. 0,000005 %	
Calcium (Ca)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %
Chlorides (Cl)			max. 0,000001 %		
Chromium (Cr)	max. 0,000002 %	max. 0,000002 %	max. 0,000002 %	max. 0,000002 %	
Cobalt (Co)	max. 0,000002 %	max. 0,000002 %	max. 0,000002 %	max. 0,000002 %	
Copper (Cu)	max. 0,000002 %	max. 0,000001 %	max. 0,000002 %	max. 0,000002 %	
Fluorides (F)			max. 0,000001 %		
Identity (IR-spectrum)	passes test	passes test		passes test	passes test
Iron (Fe)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	
Lead (Pb)	max. 0,00001 %	max. 0,000002 %	max. 0,00001 %	max. 0,00001 %	
Magnesium (Mg)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %
Manganese (Mn)	max. 0,000002 %	max. 0,000001 %	max. 0,000002 %	max. 0,000002 %	
Nickel (Ni)	max. 0,000002 %	max. 0,000002 %	max. 0,000002 %	max. 0,000002 %	
Nitrates (NO <sub>3</sub> )			max. 0,00001 %		
Non-volatile matter	max. 0,0001 %	max. 0,0005 %	max. 0,0001 %	max. 0,0005 %	max. 0,0005 %
Potassium (K)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %
Silver (Ag)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	
Sodium (Na)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %
Sulfates (SO <sub>4</sub> )			max. 0,00001 %		
Tin (Sn)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	
Water (K.F.)	max. 0,01 %	max. 0,02 %		max. 0,05 %	max. 0,03 %
Zinc (Zn)	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	max. 0,00001 %	
Min. transmission/max. absorbance in a 1,0 cm cell at wavelength:	T(%) A (AU)				
195 nm	80 % 0,097 AU				
200 nm	95 % 0,022 AU		95 % 0,022 AU		
205 nm		20 % 0,699 AU			
210 nm	97 % 0,013 AU			20 % 0,699 AU	
215 nm		50 % 0,301 AU		50 % 0,301 AU	
220 nm	98 % 0,009 AU				
230 nm			99 % 0,004 AU		
240 nm		90 % 0,046 AU		90 % 0,046 AU	
255 nm					20 % 0,699 AU
258 nm					50 % 0,301 AU
265 nm					90 % 0,046 AU
Gradient grade (210 nm)	0,012 AU		max. 0,005 AU		
Maximum background absorbance					
Maximum peak absorbance	0,001 AU				
Gradient grade (254 nm)	0,0002 AU	0,0002 AU	max. 0,001 AU	max. 0,005 AU	
Maximum peak absorbance					
Microfiltered through membranes of pore diameter 0,22 µm	✓	✓	✓	✓	✓
Suitability for use in LC-MS	passes test	passes test	passes test	passes test	passes test

## LC-MS mixtures

In the preparation of eluents for LC-MS it is common to add modifiers in order to promote the formation of molecular ions, thus improving spectral peak shape. Ultra pure acetic acid, formic acid, ammonium acetate or trifluoroacetic acid are frequently used for that purpose.

Scharlau offers ready to use solvent/modifier mixtures. Using these mixtures greatly simplifies eluent preparation and guarantees its suitability for LC-MS analysis.

Description	Ref.
Acetonitrile with 0,1% acetic acid, LC-MS	AC0374
Acetonitrile with 0,1% formic acid, LC-MS	AC0373
Acetonitrile with 0,1% trifluoroacetic acid, LC-MS	AC0372
Water with 0,1% acetic acid, LC-MS	AG0009
Water with 0,1% formic acid, LC-MS	AG0008
Water with 0,1% trifluoroacetic acid, LC-MS	AG0007
Water with 0,1% ammonium acetate, LC-MS	AG0010
Methanol with 0,1% acetic acid, LC-MS	ME0329
Methanol with 0,1% trifluoroacetic acid, LC-MS	ME0327
Methanol with 0,1% ammonium acetate, LC-MS	ME0330

## Auxiliary products

Once the daily work with LC-MS equipment has been concluded, it is convenient to eliminate the remains of salts of its interior by rinsing with water during a certain time. Once the salts have been eliminated, it is recommended to keep a water/2-propanol mixture in the equipment, to inhibit the growth of microorganisms.

Description	Ref.
Formic acid solution, 10% in water, for cleaning, LC-MS	AC1075
2-propanol/water mixture, 50/50, for cleaning, LC-MS	ME0797
Ammonium acetate solution 10 mmol/l in water, buffered to pH = 7, LC-MS	AM0262



## Certificate of Analysis

All our chemicals are shipped together with its certificate of analysis. Real analysis data from the batch and expiry date of the product are printed in every certificate.

## Quality



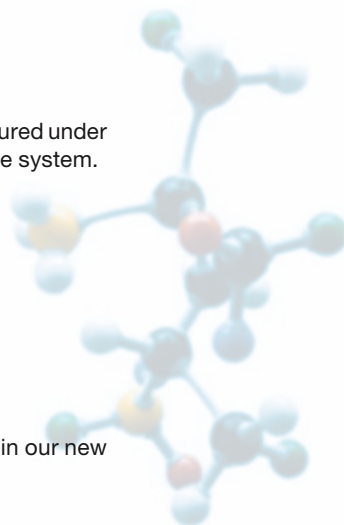
Scharlau chemicals are manufactured under ISO 9001: 2000 quality assurance system.

## Availability

More than 5.000 references are ready to be shipped in our new warehouse near Barcelona.

## www.scharlau.com

You can access to our catalogue on line, and get copies of COA and MSDS whenever you need.



CAT-LCMSE6



Scharlau Chemie S.A.  
www.scharlau.com

Scharlab S.L.  
www.scharlab.com  
export@scharlau.com  
Tel. +34 93 745 64 26  
Fax +34 93 715 27 65