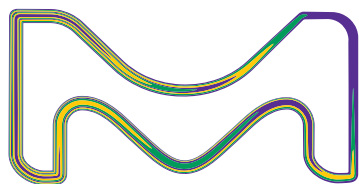


cleaner

LC-MS sample prep

LC-MS grade solvents and reagents with
the Whatman® Mini-UniPrep® system



The life science business of
Merck KGaA, Darmstadt,
Germany operates as
MilliporeSigma in the
U.S. and Canada.

Analytical Products

Whatman® Mini-UniPrep® Syringeless Filters

Whatman Mini-UniPrep Syringeless Filters provide a faster, easier way to remove particulates from samples being prepared for HPLC/UHPLC analysis. Syringeless filters simplify your workflow and reduce waste generated in the lab by replacing four different components with one Mini-UniPrep



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2 versions are available:



1. The Mini-UniPrep G2 Syringeless Filter with an inner glass storage vial

- Inner storage vials made of borosilicate glass
- Glass construction minimizes the risk of leachables contaminating the sample
- Use with hand-held manual compressor or multicompressor shown below

2. The Original Mini-UniPrep Syringeless Filter with polypropylene housing

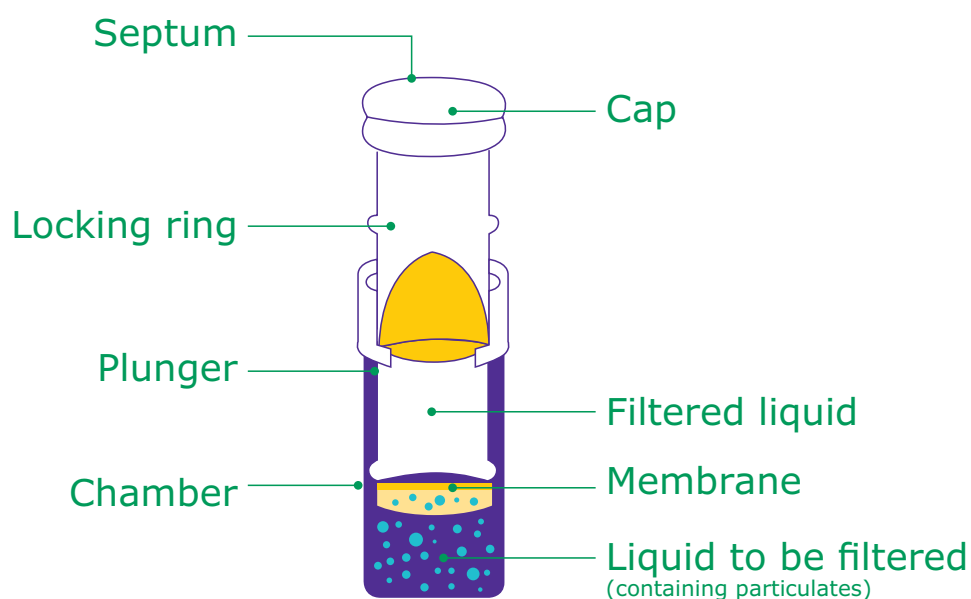
- Polypropylene housing
- Use with 6-position multicompressor



The Mini-UniPrep syringeless filters are compatible with most autosamplers

- Easy-to-use design supports sample preparation outside of the lab if needed
- Process samples in one-third the time of traditional syringe filtration
- Replaces syringe, syringe filter, vial, and cap in one consumable
- Polypropylene or glass chamber options to prevent interference from chemical leaching
- Amber vials available for light sensitive samples
- Multi-compressors available for ease of use
- 12 × 32 mm vial can be used to filter up to 400 µL

Parts of a Mini-UniPrep filter



	Mini-UniPrep	Mini-UniPrep G2
Dimensions:	Equivalent in size to 12 mm × 32 mm vials	Equivalent in size to 12 × 32 mm vials
Materials of construction:		
Chamber:	Polypropylene	Borosilicate glass
Plunger housing:	Polypropylene	Polypropylene
Plunger inner storage vial:	N/A	Borosilicate glass
Filter medium:	As specified	As specified
Septum:	Silicone with PTFE liner	Silicone with PTFE liner
Cap:	Polypropylene	Polypropylene
Maximum operating temp:	50°C (122°F)	50°C (122°F)
Max. unfiltered sample capacity:	400 µL	500 µL
Max. filtered sample capacity:	350 µL	330 µL
Dead volume:	50 µL	170 µL
Recommended minimum filtering volume:	100 µL	220 µL placed in the chamber to obtain 50 µL in inner storage vial
Nominal force needed to compress:	Approx. 8.2 kg (18 lbs)	Approx. 11.3 kg (25 lbs)
Autosampler needle height adjustment:	3 mm from the bottom of Mini-UniPrep	5 mm from the bottom of Mini-UniPrep G2
Autosampler compatibility:	Any autosampler that accommodates standard 12 × 32 mm profile vials	Any autosampler that accommodates standard 12 × 32 mm profile vials

Mini-UniPrep G2 syringeless filters with inner glass storage vial

Note: Adjust autosampler needle height to a minimum of 5 mm from the bottom of the Mini-UniPrep G2 unit.

Membrane	Pore size (µm)	Housing	Cap	Product No. (Pack size 1000/pack)	Product No. (Pack size 1000/pack)
RC	0.2	Translucent	Normal	GN203NPERC	GN503NPERC
RC	0.45	Translucent	Normal	GN203NPURC	GN503NPURC
PTFE	0.2	Translucent	Normal	WHAGN203NPEORG	GN503NPEORG
PTFE	0.2	Translucent	Slit septum	GS203NPEORG	GS503NPEORG
PTFE	0.2	Amber	Normal	GN203APEORG	NA
PTFE	0.45	Translucent	Normal	WHAGN203NPUORG	GN503NPUORG
PTFE	0.45	Translucent	Slit septum	GS203NPUORG	GS503NPUORG
PVDF	0.2	Translucent	Normal	WHAGN203NPEAQU	GN503NPEAQU
PVDF	0.2	Translucent	Slit septum	GS203NPEAQU	GS503NPEAQU
PVDF	0.2	Amber	Normal	GN203APEAQU	NA
PVDF	0.45	Translucent	Normal	WHAGN203NPUAQU	GN503NPUAQU
PVDF	0.45	Translucent	Slit septum	GS203NPUAQU	GS503NPUAQU
Nylon	0.2	Translucent	Normal	GN203NPENYL	GN503NPENYL
Nylon	0.2	Translucent	Slit septum	GS203NPENYL	GS503NPENYL
Polypropylene	0.2	Translucent	Normal	WHAGN203NPEPP	GN503NPEPP
Polypropylene	0.2	Translucent	Slit septum	GS203NPEPP	NA
Glass fiber	0.45	Translucent	Normal	GN203NPUGMF	GN503NPUGMF
Glass fiber	0.45	Translucent	Slit septum	GS203NPUGMF	NA

Description	Pack size	Product No.
Mini-UniPrep G2 Hand Compressor	1	WAMUPG2HCPWC1
Mini-UniPrep G2 Multi-Compressor	1	WAMUPG2MCPWC8
Mini-UniPrep G2 Multi-Compressor Tray	1	WHAMUPG2MCWT8
Multi Compressor - 6 positions	1	WHACR000006

For more information
Mini-UniPrep syringeless filters visit:
SigmaAldrich.com/GE

Mini-UniPrep filter vial with polypropylene housing

Note: Adjust autosampler needle height to a minimum of 3 mm from the bottom of the Mini-UniPrep unit.

Membrane	Pore size (µm)	Housing	Cap	Product No. (Pack size 100/Pack)	Product No. (Pack size 1000/pack)
PTFE	0.2	Translucent	Standard	WHAUN203NPEORG	WHAUN503NPEORG
PTFE	0.2	Translucent	Slit septum	WHAUS203NPEORG	WHAUS503NPEORG
PTFE	0.2	Amber	Standard	WHAUN203APEORG	NA
PTFE	0.45	Translucent	Standard	WHAUN203NPUORG	WHAUN503NPUORG
PTFE	0.45	Translucent	Slit septum	WHAUS203NPUORG	WHAUS503NPUORG
PTFE	0.45	Amber	Standard	WHAUN203APUORG	NA
PVDF	0.2	Translucent	Standard	WHAUN203NPEAQU	WHAUN503NPEAQU
PVDF	0.2	Translucent	Slit septum	WHAUS203NPEAQU	WHAUS503NPEAQU
PVDF	0.2	Amber	Standard	WHAUN203APEAQU	NA
PVDF	0.45	Translucent	Standard	WHAUN203NPUAQU	WHAUN503NPUAQU
PVDF	0.45	Translucent	Slit septum	WHAUS203NPUAQU	WHAUS503NPUAQU
PVDF	0.45	Amber	Standard	WHAUN203APUAQU	NA
PES	0.2	Translucent	Standard	WHAUN203NPEPES	WHAUN503NPEPES
PES	0.2	Translucent	Slit septum	WHAUS203NPEPES	WHAUS503NPEPES
PES	0.2	Amber	Standard	WHAUN203APEPES	NA
PES	0.45	Translucent	Standard	WHAUN203NPUPES	WHAUN503NPUPES
PES	0.45	Amber	Standard	WHAUN203APUPES	NA
PES	0.45	Translucent	Slit septum	WHAUS203NPUPES	WHAUS503NPUPES
RC	0.2	Translucent	Standard	WHAUN203NPERC	WHAUN503NPERC
RC	0.45	Translucent	Standard	WHAUN203NPURC	WHAUN503NPURC
Nylon	0.2	Translucent	Standard	WHAUN203NPENYL	WHAUN503NPENYL
Nylon	0.2	Translucent	Slit septum	WHAUS203NPENYL	WHAUS503NPENYL
Nylon	0.2	Amber	Standard	WHAUN203APENYL	NA
Nylon	0.45	Translucent	Standard	WHAUN203NPUNYL	WHAUN503NPUNYL
Nylon	0.45	Translucent	Slit septum	WHAUS203NPUNYL	WHAUS503NPUNYL
Nylon	0.45	Amber	Standard	WHAUN203APUNYL	NA
PP	0.2	Translucent	Standard	WHAUN203NPEPP	WHAUN503NPEPP
PP	0.2	Translucent	Slit septum	WHAUS203NPEPP	WHAUS503NPEPP
PP	0.2	Amber	Standard	WHAUN203APEPP	NA
PP	0.45	Translucent	Standard	WHAUN203NPUPP	WHAUN503NPUPP
PP	0.45	Translucent	Slit septum	WHAUS203NPUPP	WHAUS503NPUPP
PP	0.45	Amber	Standard	WHAUN203APUPP	NA
DpPP	0.45	Translucent	Standard	WHAUN203NPUDPP	WHAUN503NPUDPP
DpPP	0.45	Translucent	Slit septum	WHAUS203NPUDPP	WHAUS503NPUDPP
DpPP	0.45	Amber	Standard	WHAUN203APUDPP	NA
Glass fiber	0.45	Translucent	Standard	WHAUN203NPUGMF	WHAUN503NPUGMF
Glass fiber	0.45	Translucent	Slit septum	WHAUS203NPUGMF	WHAUS503NPUGMF
Glass fiber	0.45	Amber	Standard	WHAUN203APUGMF	NA

Solvents and Blends for LC-MS

Superior resolution and sensitivity

Why use LC-MS grade solvents?

- No ghost peaks
- Full reproducibility
- Extends the lifetime of your columns
- Optimized and tested for LC-MS applications
- Minimal background ion suppression
- Global availability

Why Pre-Blended?

- Reduces the risk of contamination
- Saves time
- No cleaning of glassware or filtration
- Less exposure to hazardous chemicals

As LC-MS is a highly sensitive analytical technique, impurities in your solvents can have an impact on the accuracy and reproducibility of your analytical results. Have confidence in your analysis by using our high purity solvents and blends designed to meet the demanding requirements of LC-MS applications, ensuring baseline stability, lowest impurity levels, and in addition, high UV transmittance.

Developed specifically for LC-MS, we have introduced a range of high purity solvents pre-blended with acetic acid, formic acid or trifluoroacetic acid, to provide convenient ready-to-use mobile phases for accurate LC-MS. We have also extended our product range to add four new LC-MS grade solvents including ethyl acetate, hexane, heptane and isopropanol.

This complete product portfolio sets the standard for accurate, reproducible and high-resolution analytical separations for superior performance and sensitivity.



For more information visit:
[SigmaAldrich.com/lcms-solvents](https://www.sigmaaldrich.com/lcms-solvents)

Product No.	Name	Description	Package Size
159004.2500 159004.4000	Acetonitrile + 0.1% Acetic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L GL 4 L GL*
159002.1000 159002.2500 159002.4000	Acetonitrile + 0.1% Formic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL 4 L GL
159014.2500 159014.4000	Acetonitrile + 0.1% Trifluoroacetic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L GL 4 L GL*
159007.2500 159007.4000	Water + 0.1% Acetic acid (v/v)	Water for Chromatography (LC-MS grade) LiChrosolv®	2.5 L GL 4 L GL*
159013.2500 159013.4000	Water + 0.1% Formic acid (v/v)	Water for Chromatography (LC-MS grade) LiChrosolv®	2.5 L GL 4 L GL*
480112.2500 480112.4000	Water + 0.1% Trifluoroacetic acid (v/v)	Water for Chromatography (LC-MS grade) LiChrosolv®	2.5 L GL 4 L GL*
100029.1000 100029.2500 100029.9010 100029.9030	Acetonitrile	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL 10 L ST** 30 L ST**
106035.1000 106035.2500	Methanol	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL
115333.1000 115333.2500 115333.4000 115333.9010 115333.9030	Water	Water for Chromatography (LC-MS grade) LiChrosolv®	1 L GL 2.5 L GL 4 L GL* 10 L ST** 30 L ST**
103649.1000 103649.2500	Ethyl acetate	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL
103701.1000 103701.2500	Hexane	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL
103654.1000 103654.2500	Heptane	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL
102781.1000 102781.2500 102781.4000	2-Propanol	Hypergrade for LC-MS LiChrosolv®	1 L GL 2.5 L GL 4 L GL*

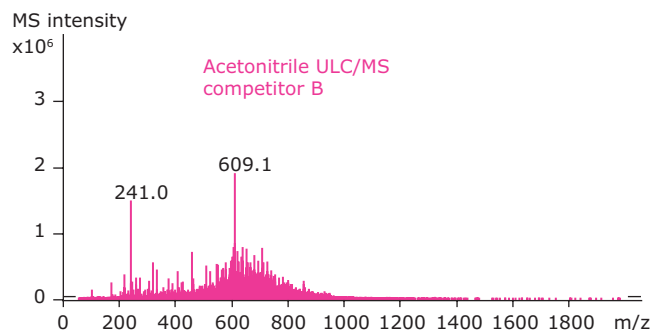
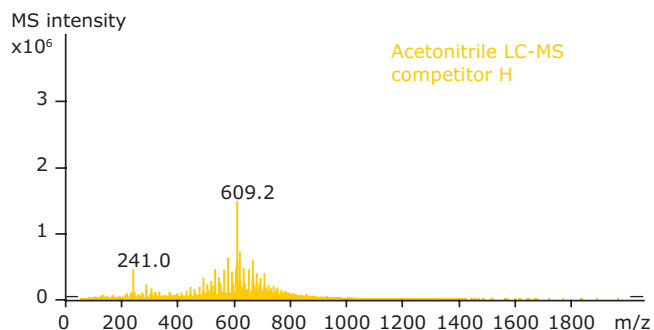
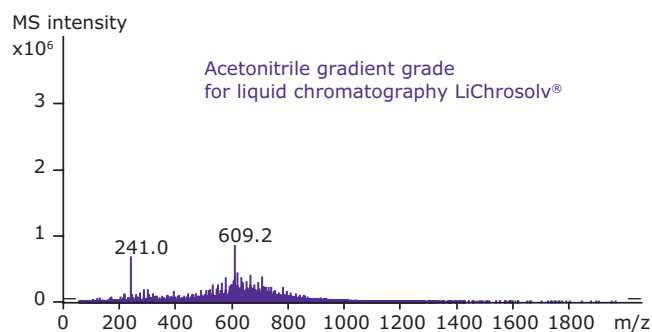
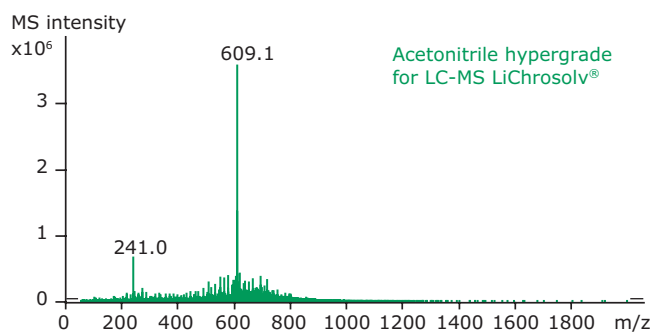
* special treated amber glass bottle

** returnable

All solvents are filtered through 0.2 µm. | GL = glass bottle | ST = stainless steel returnable barrel only in EU

For Dispensing tools and couplings of solvents to LC-MS, visit
[SigmaAldrich.com/safety-accessories](https://www.sigmaaldrich.com/safety-accessories)

Why your choice of solvent matters



MS conditions

System	Bruker Esquire 3000+ ion trap MS
Detection	Pos. ESI-MS, m/z range 50 – 2000
Flow rate	0.2 mL/min via syringe pump
Temperature	25°C
Sample	Reserpine (m/z 609.1), internal standard (m/z 241.0)

Mass spectra displaying the results of reserpine comparing different acetonitrile qualities from MilliporeSigma and two alternative competitors.

The mass spectra of these four different acetonitrile grades clearly shows the variation in the intensity of the reserpine signal ($[M+H]^+ = 609$), as well as the extent of the background signals. The differences in the intensity of the reserpine signal are caused by ion suppression. This effect occurs due to interfering trace contaminants that can be present in acetonitrile, which can be avoided using the correct high grade solvent for this purpose.

LC-MS Reagents and Additives

Features:

- LC-MS application tested for consistent quality according to the reserpine test
- Optimized to improve ionization and resolution
- Extremely low levels of inorganic and organic impurities
- Manufactured specifically for accurate and fast LC-MS
- Highest quality acids, bases & salts - specified in the certificate of analysis

Introduction

It is common practice in LC-MS to add certain reagents to the mobile phase, or to introduce them post-column prior to the interface to influence analyte ionization. Most often the goal is for an improvement in the analyte signal. In addition, some additives may be used to suppress unwanted signals, or selectively enhance the signal of particular compounds in a mixture. For example, glycosidic species in a mixture of peptides.

To help you obtain the highest quality analysis, we offer a wide range of high purity mobile phase additives for LC-MS applications. The LC-MS portfolio includes the most commonly used acids, bases and volatile salts of high purity tested for LC-MS applications.

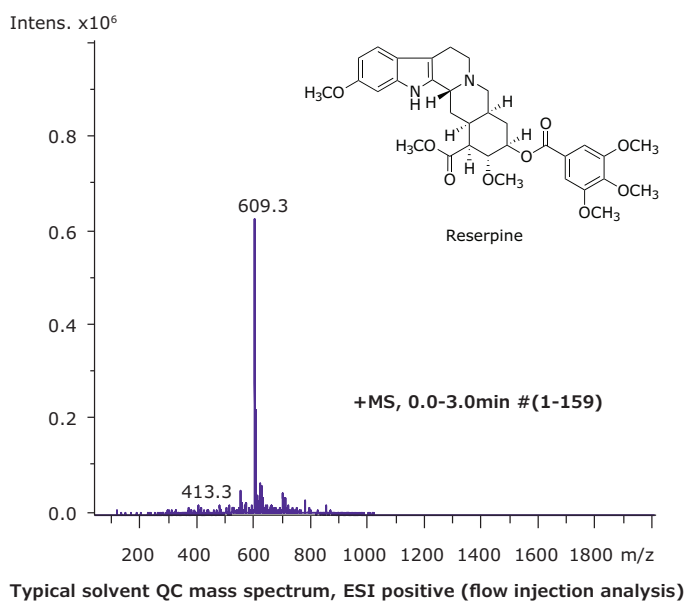
Impurities, such as alkali ions, plasticizers or surfactants, that can be commonly found in lower-grade solvents are particularly problematic as they interfere strongly with LC-MS, resulting in

higher background noise and formation of adducts. Only ultrapure reagents enable high signal-to-noise ratios, which results in the highest and most reliable performance for small and large molecule applications.

Reserpine test

All of our LC-MS solvents and reagents are specified using the standard reserpine test. Reserpine (608.68) is used as the reference substance to quantify possible impurities in the LiChropur® LC-MS reagents. It is performed by diluting 2.5% (v/v) acid, base or 2.5% (w/v) salt in 50/50 (v/v) acetonitrile/water. Every lot produced is analyzed via flow injection analysis mass spectrometry (FIA-MS). The dissolved reagent and the appropriate reserpine reference solutions are introduced into the MS ion source syringe pumps. The total ion chromatogram (TIC) is accumulated during three minutes. The relative intensities of the detected masses are compared with the reserpine signal.

For electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) in the positive mode, the specified amount of reserpine is 2 ppb for acids and bases, and 20 ppb for salts. In the negative mode, the specified amount of reserpine is 20 ppb for both.



Acid additives

Volatile, low molecular weight organic acids such as formic and acetic acid improve ionization and resolution of a wide range of molecules. Addition of organic acids to the mobile phase can help to overcome the ionization-suppressing effect of trifluoroacetic acid (TFA) present in the mobile phases used for the analysis of proteins and peptides.

Neutral salts

Neutral volatile salts, such as ammonium acetate or ammonium formate are typically used as buffer compounds to control the analytes (and phases) ionization state, which has a strong influence on the LC-MS separation and performance.

Sodium adduct formation

Alkali adducts diminish instrument sensitivity. When adduct formation tendency is strong, often the addition of defined amounts of sodium ions (mostly pre-column) can help to obtain uniform and stable molecular ions for detection in LC-MS.

Product No.	Substance	Description	Package Size
5.33001.0050	Acetic acid	100% for LC-MS LiChropur®	50 mL
5.33002.0050	Formic acid	98-100% for LC-MS LiChropur®	50 mL
5.33003.0050	Ammonia solution	25% for LC-MS LiChropur®	50 mL
5.33004.0050	Ammonium acetate	for LC-MS LiChropur®	50 g
5.33005.0050	Ammonium hydrogen carbonate	for LC-MS LiChropur®	50 g

Extensive QC testing ensuring highest specification

Residue on ignition (evaporation residue) tests show the low content of insoluble matter in the reagent. This provides confidence that your eluents have the low particle content needed for accurate LC-MS measurement.

Sodium and potassium ions are particularly likely to form adducts with the analyte molecules. This leads to complex mass spectra leading to time-consuming data evaluation. The content of trace metals is in the low ppb range for LiChropur® LC-MS reagents to minimizing the risk of adduct formation in the ion source for cleaner results.

Our LiChropur® LC-MS reagents are stored in borosilicate bottles to prevent leaching of alkali ions out of the glass. The content of the potentially complex forming ions aluminum, copper and iron is also specified.

Full specification can be found in the certificate of analysis for each of our LC-MS grade products.

Specification (Acids/Bases)

Assay (acidimetric)	≥ 98,0%
Colour	≤ 10 Hazen
Residue on ignition	≤ 2 ppm
Al	≤ 5.0 ppb
Ca	≤ 10.0 ppb
Cu	≤ 1.0 ppb
Fe	≤ 5.0 ppb
K	≤ 5.0 ppb
Mg	≤ 2.0 ppb
Na	≤ 5.0 ppb
NH ₄ ⁺	≤ 10 ppm
LC-MS Suitability ESI Positive (Reserpine Test)	≤ 2 ppb (tested with ion trap MS). Intensity of background mass peak based on reserpine
LC-MS Suitability ESI Negative (Reserpine Test)	≤ 20 ppb (tested with ion trap MS). Intensity of background mass peak based on reserpine

For more information HPLC buffers, visit
[SigmaAldrich.com/lcms-reagents](https://www.sigmaaldrich.com/lcms-reagents)

Chemical Derivatization Reagents for LC-MS

Modern mass spectrometry techniques such as APCI or ESI are highly successful in providing valuable structural information, and allow the detection of very low analyte concentrations in various sample matrices. For certain samples e.g. non-polar compounds, and in research areas, such as clinical metabolomics and forensics analytics, there are many cases where such methods can be insufficiently sensitive.

Derivatization reactions in mass spectrometry are used to improve ionization efficiency¹⁻⁴. The derivatization reagents have functional groups possessing high proton (cation) affinity that stabilize a positive charge. Of similar importance when derivatizing is the improvement of qualitative analysis by modifying fragmentation behavior to form unique product ions and the shifting. Finally, derivatization can enhance precise quantitative analysis for profiling of relatively small analyte molecules, particularly in metabolomics.

References

1. Zaikin V, Halket J, 2009. A handbook of derivatives for mass spectrometry. Chichester: IM Publications LLP,
2. Santa T. 2013. Derivatization in liquid chromatography for mass spectrometric detection *Drug Discov. Ther.* 7:9-17
3. Santa T. 2011. Derivatization reagents in liquid chromatography/electrospray ionization tandem mass spectrometry. *Biomed. Chromatogr.* 25:1-10
4. Santa T, Al-Dirbashi OY, Fukushima T. 2007. Derivatization reagents in liquid chromatography/electrospray ionization tandem mass spectrometry for biomedical analysis. *Drug Discov. Ther.* 1:108-118.

For more information, visit
SigmaAldrich.com/derivatization

Product No.	Derivatization Reagent	Analyte Functional Group	Typical Application
69706	6-Bromo-3-pyridinylboronic acid	1,2-Dihydroxy	Brassinosteroids
05689	Diethyl ethoxymethylenemalonate	Amine	Amino acids
29208	(N-Succinimidylloxycarbonylmethyl) tris(2,4,6-trimethoxyphenyl)phosphonium bromide	Amine	Protein sequence analysis
61224	N-Succinimidyl 4-(dimethylamino)benzoate	Amine	Glycerophosphoethanolamine lipids
73177	1-Fluoro-2,4-dinitrobenzene	Amine	Prim./sec. aliphatic amines
94076	{1-[2-(Diethylamino)ethoxy]-2-isothiocyanatoethyl}benzene	Amine	—
59934	2,5-Dioxopyrrolidin-1-yl N-tri(pyrrolidino) phosphoranylideneaminocarbamate	Amine	Amino acids
73103	Dibenzyl ethoxymethylenemalonate	Amine	Amino acids
03334	Dansylhydrazine	Carbonyl	—
06963	4-(Diethylamino)benzhydrazide	Carbonyl	—
08843	2-Hydrazinopyridine	Carbonyl	Steroids
4465962	Amplifex Keto Reagent Kit	Carbonyl	—
5037804	Amplifex Diene Reagent Kit	Diene	—
59799	4-(Diethylaminomethyl)benzhydrazide	Carbonyl	—
65562	2-Picolylamine	Carbonyl	Steroids
89397	Girard's reagent T	Carbonyl	Nucleosides
92989	4-(Dimethylamino)benzohydrazide	Carbonyl	—
93742	Pentafluorophenylhydrazine	Carbonyl	Oligosaccharides
75821	1,2-Benzo-3,4-dihydrocarbazole-9-ethyl-p-toluenesulfonate	Carboxylic acid	Fatty/bile acids
79291	4-[2-(N,N-Dimethylamino)ethylaminosulfonyl]-7-(2-aminoethylamino)-2,1,3-benzoxadiazole	Carboxylic acid	Fatty acids
42579	4-Phenyl-1,2,4-triazoline-3,5-dione	Diene	Vitamin D
97622	2-Mercaptoethanol	Double bond	Microcystins
00721	4-(Dimethyl-d ₆ -amino)benzoyl chloride	Hydroxy	Deuterium mass shift
03641	Dansyl chloride	Hydroxy	—
05022	N,N-Dimethylglycine	Hydroxy	Cholesterol
06696	3-Amino-9-ethylcarbazole	Hydroxy	Sugars
67954	4-(Dimethylamino)benzoyl chloride	Hydroxy	17β-Estradiol
72702	3,5-Dinitrobenzoyl chloride	Hydroxy	Tetrahydrocorticosterones
41368	p-Toluenesulfonyl isocyanate Product No.	Hydroxy	Steroids

Our combined LC-MS columns offer

LC-MS results can be improved by choosing a column that meets the needs of your desired separation. We offer leading column technologies that were specifically developed for the trending research in life science.

ultra LC-MS

Think . . . Ascentis® Express
LC-MS Columns

Ascentis® Express is the leading Fused-Core® column providing high speed at low back pressure results.



chiral LC-MS

Think . . . Chirobiotic®
LC-MS Columns

Chirobiotic® Columns offer 6 products for Reversed-Phase LC-MS that are proprietary and provide high resolution of Chiral compounds. Frequently referenced in academic journals. Columns are ideal for Analytical Chiral Chromatography.



walk-up/open Access

Think . . . Chromolith®
LC-MS Columns

Chromolith® family of monolithic columns are proprietary technology for the most demanding applications in terms of ruggedness for dirty samples.



Metabolomics

Think . . . SeQuant®
LC-MS Columns

SeQuant® Columns offer 3 products for HILIC LC-MS that are proprietary and provide high resolution of polar compounds. Frequently referenced in academic journals. Columns are Zwitterionic, ideal for Metabolomics Chromatography.

High pH Method

Think . . . Eternity™
LC-MS Columns

Kromasil® Eternity™ Columns offer products that are designed for high pH separation of basic compounds. Kromasil® columns are exclusively sold through MilliporeSigma.

MABs, proteins, ADCs, glycans

Think . . . BIOshell™
LC-MS Columns

BIOshell™ columns are designed for the needs of modern biochromatography. With a wide range of pore sizes for the important molecules in life science.

Analytical Products

MilliporeSigma
400 Summit Drive
Burlington, MA 01803

SigmaAldrich.com

To place an order or receive technical assistance:
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