Increase Analytical Accuracy LC/MS: Solvents, Blends, Standards, Surfactants



Reliability. Purity. Certainty.



Chemicals from Thermo Fisher Scientific brands offer a wide range of reagents, blends and standards designed to deliver more accurate results for liquid chromatography and mass spectrometry (LC/MS) analysis. The products in this brochure are specifically formulated, tested and validated on the latest instruments from leading brands to offer superior performance for LC/MS, and they're conveniently provided in ready-to-use sizes with innovative packaging.

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Surfactants

Alfa Aesar™ surfactants are compatible with mass spectrometry used in proteomics analysis.

The compounds listed here showed minimal matrix interference in proteomics target analysis by mass spectrometry.

Description	Pack Size	Cat. No.
Anionic Acid Labile Surfactant I (AALS I)	5mg	AAJ67647LB0
Anionic Acid Labile Surfactant II (AALS II)	5mg	AAJ67832LB0
Cationic Acid Labile Surfactant I (CALS I)	5mg	AAJ67743LB0
Cationic Acid Labile Surfactant II (CALS II)	5mg	AAJ67525LB0
Non-Ionic Acid Labile Surfactant I (NALS I)	5mg	AAJ67592LB0
Non-Ionic Acid Labile Surfactant II (NALS II)	5mg	AAJ67682LB0
Zwitterionic Acid Labile Surfactant I (ZALS I)	5mg	AAJ67729LB0
Zwitterionic Acid Labile Surfactant II (ZALS II)	5mg	AAJ67721LB0

Preserving Product Integrity

Standards

Standardization verifies instrument function and its suitability for the next analysis. By regularly calibrating your instruments using reliable chromatography standards, you'll always have confidence in the accuracy of your data.

Type of Mass Spec Standards	Size	Cat. No.
2,4,6-Tris(heptafluoropropyl)-1,3,5-triazine	1g, 5g	AAL16883
2,4,6-Tris(perfluoroheptyl)-1,3,5-triazine	100mg, 500mg	AAL16678
2,4,6-Tris(trifluoromethyl)-1,3,5-triazine, 98%	1g, 5g	AAB22001
Bis(pentafluorophenyl)phenylphosphine, 97%	0.25g, 1g	AAA11014
Perfluorokerosene-941	1g	AAL16595
Perfluorokerosene-L	1g, 5g	AAL16597
Perfluorotributylamine	1g, 5g, 25g	AA19126
Tris(pentafluorophenyl)phosphine, 97%	1g, 5g	AAL02748
Ultramark™ 1621	250mg, 1g	AAL16698
Ultramark 1960F	1g	AAL16695
Ultramark 2500F	1g	AAL16696
Ultramark 3200F	1g	AAL16697
Protein Mass Spec Certified Standards Assortment: Albumin, Carbonic Anhydrase, Cytochrome C, Lysozyme, Myoglobin	1 Kit	AAJ67734QA
Protein LC-MS Standard, Certified Ribonuclease A, Cytochrome C, Lysozyme, Myoglobin, Carbonic Anhydrase, 5mg Protein per Vial	1 Vial	AAJ67628LPL
Reversed Phase LC-MS Peptide Retention Standard, Certified: Angiotensin I, Angiotensin II, Albumin fragment LVAASQAALGL, Albumin fragment TCVADESAENCDK, and Reference Peptide IAIANIIDEIIEK, 500pmol Each Peptide per Vial	1 Vial	AAJ67668LPL

Specialty Flush Solutions and Probe Washes

Thermo Scientific[™] flush solutions are designed to remove difficult-to-clean contaminants from your instruments, and probe wash solutions remove carryover between sample runs. Isopropanol acetonitrile acetone (9/9/2) flush solution (Cat. No. MB124) is formulated for difficult-to-remove blood and urine sample residue.

Thermo Scientific probe washes are ultra-filtered and designed to flush common reverse phase contaminants from LC/MS instrumentation. Select the mixture most appropriate for the nature of the suspected containment.

Flush Solutions

Description	Size	Packaging	Cat. No.
Flush Solution, Isopropanol Acetonitrile Acetone (9/9/2), LC/MS Grade	1L	Borosilicate Glass Bottle	MB124-1
Flush Solution, isoproparior Acetoritine Acetorie (9/9/2), EC/MS Grade	2.5L	Amber Glass Bottle	MB124-212

Probe Wash Solutions

Description	Size	Packaging	Cat. No.
Probe Wash, Water with 2% Acetonitrile	2.5L	Amber Glass Bottle	T001252500
Probe Wash, Water with 40% Acetonitrile and 0.1% Formic Acid	2.5L	Amber Glass Bottle	T001262500

Preserving Product Integrity

Mobile Phase Blends, Optima LC/MS Grade

Fisher Chemical[™] Optima[™] LC/MS solvents and blends have set the standard of excellence for consistent, reproducible performance in the mobile phase of LC/MS. These Optima LC/MS solvent blends provide a consistent concentration of FA (Formic Acid) or TFA (Trifluoroacetic Acid), a very low mass baseline (noise level), exceptionally low metal ion content, and UV background. Moreover, the proteasefree specification of the aqueous blends supports proteomics research, as peptides or proteins could be degraded if the mobile phase solution is contaminated with protease.

Key Features

- Extensive functional testing to ensure:
 - Low mass spectrometry background noise (LC/MS)
 - Minimal metal impurities
 - Lowest impurity background using diode array detection (LC/UV)
- Lot-to-lot consistency
- Low impurity levels and low residue values help to extend LC/MS column life
- Very effective in solubilizing hydrophobic polypeptides
- Only product line with verified absence of proteases in aqueous blends

Advantages

- Ready to use
- Avoids the contamination or safety risk and cost with inhouse blended solvents
- Eliminates the need to clean glassware or measure corrosive acids
- Eliminates batch-to-batch variation
- Avoids human error during blend preparation

Applications

- Proteomics
- Pharmaceutical research
- Drug discovery
- Biomedical research



Aqueous Blends

Description	Size	Case Quantity	Cat. No.
Water with 0.05% TFA, Optima LC/MS	4L	4/Case	LS115-4
	500mL	6/Case	LS118-500
Materiality 0,10/ FA Optime L C/MC	1L	6/Case	LS118-1
Water with 0.1% FA, Optima LC/MS	2.5L	4/Case	LS118-212
	4L	4/Case	LS118-4
	500mL	6/Case	LS119-500
Materiality 0,10/ TEA Optime LC/MC	1L	6/Case	LS119-1
Water with 0.1% TFA, Optima LC/MS	2.5L	4/Case	LS119-212
	4L	4/Case	LS119-4
Water with 0.05% FA in 10mM Ammonium Formate, LC/MS	1L	6/Case	MB123-1

Organic Blends

Description	Size	Case Quantity	Cat. No.
Acetonitrile with 0.05% TFA, Optima LC/MS	4L	4/Case	LS117-4
	500mL	6/Case	LS120-500
Acetonitrile with 0.1% FA, Optima LC/	1L	6/Case	LS120-1
MS	2.5L	4/Case	LS120-212
	4L	4/Case	LS120-4
	500mL	6/Case	LS121-500
Acetonitrile with 0.1% TFA, Optima	1L	6/Case	LS121-1
LC/MS	2.5L	4/Case	LS121-212
	4L	4/Case	LS121-4
Acetonitrile with 0.1% FA in 80% Water, Optima LC/MS	500mL	6/Case	LS122-500
Methanol with 0.05% FA in 10mM Ammonium Formate, LC/MS	1L	6/Case	MB122-1

Visit **fishersci.com/LCMS** or **fishersci.ca/LCMS** for more information, including a white paper titled Optimizing Mobile Phase Solvent Purity for LC/MS.

Preserving Product Integrity

Product Specifications

	LS118	LS119	LS120	LS121
Description	Water with 0.1% (v/v) Formic Acid, Optima LC/MS	Water with 0.1% (v/v) Trifluoroacetic Acid, Optima LC/MS	Acetonitrile with 0.1% (v/v) Formic Acid, Optima LC/MS	Acetonitrile with 0.1% (v/v) Trifluo- roacetic Acid, Optima LC/MS
Sizes	500mL, 1, 2.5 and 4L	500mL, 1, 2.5 and 4L	500mL, 1, 2.5 and 4L	500mL, 1, 2.5 and 4L
Assay % (V/V)	0.095 to 0.105%	0.095 to 0.105%	0.095 to 0.105%	0.095 to 0.105%
Color (APHA), Max	10	10	10	10
Optical Absorbance				
254nm	0.01	0.003	0.03	0.03
230nm	0.55	0.06	0.75	0.4
220nm	0.85	0.18	1.25	0.55
210nm	1.25	0.55	1.3	0.6
LC/MS Gradient Suitability	Pass Test	Pass Test	Pass Test	Pass Test
Residue After Evaporation (max)	1 ppm	1 ppm	1 ppm	1 ppm
Protease	Not Detected	Not Detected	N/A	N/A
Ionic Impurities (Maximum)				·
Aluminum (Al)	20 ppb	20 ppb	25 ppb	25 ppb
Calcium (Ca)	50 ppb	50 ppb	50 ppb	50 ppb
Copper (Cu)	10 ppb	10 ppb	10 ppb	10 ppb
Iron (Fe)	10 ppb	10 ppb	10 ppb	10 ppb
Lead (Pb)	10 ppb	10 ppb	10 ppb	10 ppb
Magnesium (Mg)	10 ppb	10 ppb	10 ppb	10 ppb
Manganese (Mn)	10 ppb	10 ppb	10 ppb	10 ppb
Nickel (Ni)	10 ppb	10 ppb	10 ppb	10 ppb
Potassium (K)	20 ppb	20 ppb	20 ppb	20 ppb
Silver (Ag)	10 ppb	10 ppb	10 ppb	10 ppb
Sodium (Na)	50 ppb	50 ppb	50 ppb	50 ppb
Zinc (Zn)	20 ppb	20 ppb	20 ppb	20 ppb

Need tailored solvents or solvent blends?

With our experience in manufacturing, processing and testing high-purity solvents, we can customize solvents and blends to your specifications. Visit **fishersci.com/SCS** or **fishersci.ca/SCS** to learn more or request a quote today.



Preserving Product Integrity

Solvents, Optima LC/MS Grade

The partnering of liquid chromatography (LC) with mass spectrometry (MS) has created an indispensable tool for many fields of research. As instrumentation advances lead to ever-lower analyte detection limits, it is crucial for the chromatographer to consider the level of purity when selecting appropriate solvents for use in the LC/MS mobile phase. The Fisher Chemical[™] product line offers superior high-purity solvents designed to meet the required purity level of advanced LC/MS systems.

Improved Performance

Fisher Chemical[™] Optima[™] LC/MS solvents lead the industry with an unprecedented LC/UV gradient suitability specification, developed by coupling advanced UHPLC technology with PDA detection optics. As a result, each lot of Optima LC/ MS solvent is screened for UV-absorbing contaminants at every wavelength in the 200-400nm range to afford smooth baselines, reduced interferences, and increased confidence in your analyses.

Key Features

- Optimized for UHPLC/UV for extremely low levels of UV-absorbing impurities
- Sub-micron filtration to prolong the life and effectiveness of UHPLC components (inlet filters, check valves and seals, injectors and columns) and reduce instrument downtime and maintenance costs
- Filtration provides very low particle content for maximum purity
- Protease tested perfect for proteomics workflows



•			1	
	Acetonitrile A955	Methanol A456	Water W6	2-Propanol A461
Color (APHA), Max				5
Optical Absorbance	AU , Max			
280nm	0.005	0.005	0.005	
260nm		0.005	0.005	
254nm	0.005	0.01	0.005	0.005
240nm			0.01	
230nm	0.01	0.1	0.01	0.05
225nm	0.015			
220nm	0.015	0.2	0.01	0.1
215nm	0.025			
214nm		0.4		
210nm	0.03	0.5	0.01	0.4
205nm	0.04			
200nm	0.05			
195nm	0.15			
190nm	1.00			
LC/UV Gradient	Single, Max			
254	0.0005	0.001	0.0005	
220		0.005		
210	0.002		0.005	
LC/UV Gradient	Single, Max			
Protease			Not Detected	
LC/MS at Positive Mode Max	50 ppb Reserpine	50 ppb Reserpine	50 ppb Reserpine	
LC/MS at Negative Mode Max	50 ppb Aldicarb	50 ppb Aldicarb	50 ppb Aldicarb	
Water (KF)	0.01%	0.02%		0.05%

Acetonitrile A955 2-Propanol A461 Methanol A456 Water W6 **Residue after** Evaporation. 0.8 1 1 1 ppm, Max LC/MS Pass Test Suitability Titratable 0.008 0.0003 Acid,mEQ/g Titratable Base. 0.0006 0.0002 mEQ/a **Titratable Acid** 0.0001 or Base meq/g **Trace Ionic** ppb, Max Impurities Aluminum (Al) 25 10 10 10 Barium (Ba) 5 10 10 Cadmium (Cd) 5 10 10 Calcium (Ca) 25 20 20 10 5 10 10 Chromium (Cr) Cobalt (Co) 5 10 10 Copper (Cu) 5 10 10 5 Iron (Fe) 5 10 10 5 Lead (Pb) 5 10 10 5 5 Magnesium (Mg) 10 10 10 5 Manganese (Mn) 5 10 10 Nickel (Ni) 5 10 10 5 Potassium (K) 10 10 10 10 Silver (Ag) 5 10 10 5 50 Sodium (Na) 50 50 20 Tin (Sn) 5 10 10 Zinc (Zn) 10 10 10 10 Total Halogens (as Not Detected chloride)

Product Specifications

Preserving Product Integrity

Reagents, Optima LC/MS Grade

The Fisher Chemical[™] Optima[™] LC/MS product line now includes reagents such as formic acid (FA) and trifluoroacetic acid (TFA), coupled with their ready-to-use aqueous and organic blends. These mobile phase additives are use-tested, and data show that their mass baselines are very low for positive mode in TIC with single quadrupole and ion trap mass detector; very low LC/UV response using a diode array detector; and exceptionally low metal ion content with ICP/ MS (which makes MS interpretation easier due to reduced metal adduct formation). For proteomics research, aqueous additives and blends are protease-free so that target peptides or proteins are not destroyed by these pervasive hydrolyzing enzymes.

Key Features:

- Low mass spectrometry background noise
- Lowest impurity background using diode array detection (LC/UV)
- Minimal metal impurities
- Aqueous mobile phase blends free of proteases
- Lot-to-lot consistency
- Extended column life due to low impurity levels using Optima LC/MS solvents and additives

For smaller volumes and easy dilutions, FA and TFA are also available in convenient 0.5mL, 1mL and 2mL ampules.

Formic Acid

Fisher Chemical[™] Optima[™] LC/MS grade formic acid (FA) is an ultrapure reagent used as a mobile phase additive for its ability to reduce MS signal suppression and volatility and thus enhance the signal detection limit.

When preparing mobile phase blends, FA can be used with Optima LC/MS solvents such as acetonitrile, water, and methanol.

- Packaged in HDPE bottles to avoid possible glass bottle breakage from carbon monoxide pressure buildup (a natural decomposition product of formic acid)
- A proprietary surface treatment is used on our HDPE bottles to create a barrier between the bottle and its contents, preventing plasticizer contamination
- For smaller volumes, FA is also available in 0.5, 1 and 2mL ampules.

Description	Pack Size	Cat. No.
	50mL	A117-50
	10 x 1mL	A117-10X1AMP
Formic Acid	1mL	A117-1AMP
	0.5mL	A117-05AMP
	2mL	A117-2AMP

Preserving Product Integrity

Trifluoroacetic Acid

Fisher Chemical[™] Optima[™] LC/MS Grade trifluoroacetic acid is an ultrapure reagent used as an additive for the formulation of solvent blends for the mobile phase in LC/MS applications due to its volatility.

Trifluoroacetic acid is often added to the mobile phase to enhance chromatographic separations.

When reversed-phase chromatography is applied to protein and peptide analysis, TFA is frequently used as an ion-pairing reagent in mobile phases. Although TFA is known to suppress MS ionization, use of a low concentration of TFA can enhance retention and improve peak shape of a product during the analytical separations. For preparing mobile phase blends, trifluoracetic acid can be used with Optima LC/MS solvents such as acetonitrile, water, and methanol.

Description	Size	Cat. No.
Trifluoroacetic Acid, Optima LC/MS	50mL	A116-50
Trifluoroacetic Acid, Optima LC/MS	10 x 1mL	A116-10X1AMP
Trifluoroacetic Acid, Optima LC/MS	1mL	A116-1AMP
Trifluoroacetic Acid, Optima LC/MS	0.5mL	A116-05AMP
Trifluoroacetic Acid, Optima LC/MS	2mL	A116-2AMP



Product Specifications

	A117 Formic Acid	A116 Trifluoroacetic Acid
Appearance	Clear, colorless, fuming liquid	Clear, colorless, fuming liquid
Assay	99.5% min	99.5% min
Color (APHA), Max	10	10
Optical Absorbance	0.1% Aqueous, au, Max	As Is, au, Max
300nm		0.03
275nm		0.06
254nm	0.01	0.003
230nm	0.55	0.06
220nm	0.85	0.18
210 nm	1.25	0.55
Residue after Evapo	pration (at 0.1% aqueous), 1 ppm Max
Chloride	5 ppm	
Sulfate (SO4)	50 ppm	
Sulfite (SO3)	20 ppm	
Water (KF)		0.05%
Trace Ionic Impuriti	es (at 0.1% aqueous), pp	b, Max
Aluminum (Al)	20	20
Calcium (Ca)	50	50
Copper (Cu)	10	10
Iron (Fe)	10	10
Lead (Pb)	10	10
Magnesium (Mg)	10	10
Manganese (Mn)	10	10
Nickel (Ni)	10	10
Potassium (K)	10	20
Silver (Ag)	20	10
Sodium (Na)	10	50
Zinc (Zn)	50	20

Preserving Product Integrity

Acetic Acid, Ammonium Acetate, and Ammonium Formate

Achieving the full analytical potential of LC/MS instruments requires the use of highly purified solvents and ionic additives. Fisher Chemical[™] Optima[™] LC/MS ammonium formate, ammonium acetate, and acetic acid are ultrapure reagents used to modify the LC/MS mobile phase in order to improve chromatographic peak shape and provide stable analyte signals in the MS detector.

Ammonium acetate and ammonium formate are volatile salts. often used for improving ionization under neutral conditions in either the positive or negative ESI-MS mode. Acetic acid is commonly used for enhancing chromatography separation under acidic conditions.

For preparing mobile phase blends, acetic acid, ammonium acetate, and ammonium formate can be added to Fisher Chemical Optima LC/MS solvents such as acetonitrile, water, and methanol.

Description	Size	Packaging	Cat. No.
Acetic Acid, Optima LC/MS	50mL	Nalgene [™] Poly Bottle,	A113-50
Ammonium Acetate, Optima LC/MS	50g	Amber Glass Bottle	A114-50
Ammonium Formate, Optima LC/MS	50g	Amber Glass Bottle	A115-50
Ammonium Hydroxide, Optima	250mL	HDPE Bottle	A470-250

*The proprietary surface treatment creates a contamination barrier between the bottle and the acetic acid.

Acetic Acid Is Now Available in Glass Ampules

Fisher Chemical Optima LC/MS acetic acid is now custom-packaged in amber borosilicate ampules under inert atmospheric conditions to provide the freshest additive for preparing aqueous and organic mobile phase blends.

Description	Pack Size	Cat. No.
Acetic Acid, Optima LC/MS	1mL ampule	A113-1AMP
	10 x 1mL ampule	A113-10X1AMP

Advantages

- Convenient ready-to-use, 1mL ampule
- Safe eliminates the need to measure corrosive acids
- Reproducible ampules are filled to +/-0.05% to reduce batch-to-batch variation
- Expedient 1mL ampule is used to prepare 1L of fresh 0.1% v/v acetic acid mobile phase blend in a matter of seconds

Key Features

- Minimal metal impurities
- Low mass spectrometry background noise
- Lowest impurity background using diode array detection (LC/UV)
- Lot-to-lot consistency
- Extended column life due to low impurity levels using OPTIMA LC/MS mobile phase solvents and additives









Preserving Product Integrity

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Product Specifications	Acetic Acid	Ammonium Acetate	Ammonium Formate		
	A113	A114	A115		
Appearance	Clear, colorless fuming liquid	Fine white crystals with lumps	Fine white crystals with lumps		
Assay, % min	99.7% min	99% min	99% min		
Color (APHA), max	10 max				
Optical Absorbance	au, Max				
350nm	0.02				
280nm	0.05				
255nm	1.0	1.0			
LC/MS Gradient Suitability (at 0.1% aqueous)	Pass Test	Pass Test	Pass Test		
Trace Ionic Impurities (at 0.1% aqueous),	ppb, Max				
Aluminum (Al)	20 ppb	20 ppb	20 ppb		
Calcium (Ca)	50 ppb	50 ppb	50 ppb		
Copper (Cu)	10 ppb	10 ppb	10 ppb		
Iron (Fe)	10 ppb	10 ppb	10 ppb		
Lead (Pb)	10 ppb	10 ppb	10 ppb		
Magnesium (Mg)	10 ppb	10 ppb	10 ppb		
Trace Ionic Impurities (at 0.1% aqueous),	ppb, Max				
Manganese (Mn)	10 ppb	10 ppb	10 ppb		
Nickel (Ni)	10 ppb	10 ppb	10 ppb		
Potassium (K)	20 ppb	20 ppb	20 ppb		
Silver (Ag)	10 ppb	10 ppb	10 ppb		
Sodium (Na)	50 ppb	50 ppb	50 ppb		
Zinc (Zn)	20 ppb	20 ppb	20 ppb		
Residue after Evaporation, ppm, Max	5 ppm				
Residue on Ignition, % Max		0.01%	0.005%		
Chloride, % Max	0.00004%	0.0005%	0.001%		
Nitrate (NO3), % Max	0.00004%	0.001%			
Sulfate (SO4), % Max	Not Detected		0.005%		
Protease (at 0.1% aqueous)	0.1% max	Not Detected	Not Detected		
Water (KF), % Max		1%	2%		
Shelf Life	1 Year	2 Years	3 Years		

Preserving Product Integrity

Innovative Packaging

Our high-purity solvents are designed with researchers in mind, and we focus on preserving the integrity of the product while being conscious of the environmental impact of our packaging. Our solvents are available in a variety of innovative packages that offer you reliability, purity and convenience.

QR Codes Retrieve SDS and CofA

Just scan the label to get instant access to SDS and lot-specific CofA. Visit fishersci.com/QR to learn more.



Safe-Cote Solvents - Safely Serving Science

Safe-Cote[™] bottles feature a plastic coating that traps liquids and glass fragments if the bottle breaks, preserving the product, protecting you, and avoiding a potentially dangerous spill and cleanup.

Visit fishersci.com/safecote to learn more.

Lock in Safety and Quality with Fisher Chemical FisherLOCK Caps

Secure, tamper-evident Fisher Chemical[™] FisherLOCK[™] caps hold the lips of our amber glass bottles and preserve the integrity of your chemicals. The color-coded bands at the bottom of the cap are based on industry-standard color coding for proper storage and handling, so you can easily identify hazards.

Next-Generation Products

As instrumentation evolves, new lines of solvents are being developed so researchers can amplify productivity with improved detection of impurities and interference-free baselines. Higher-purity solvents are packaged in borosilicate glass bottles:

- Minimizes Na+ and K+ metal adduct formation in high-purity solvents
- Use directly on the instrument
- Graduated for ready reference

EcoSafPak Shipping Containers

EcoSafPak[™] packaging is Styrofoam free, environmentally friendly and sturdy. It surpasses the most demanding ISTA (International Safe Transport Association) 3A tests, including 17 drops that simulate real-world shipping as well as vibration and stability testing to ensure that the frame protects the product. This packaging is produced by manufacturers that are SFI (Sustainable Forest Initiative)-certified, indicating compliance to certain principles, objectives and performance measures developed by professional foresters, conservationists and scientists to promote the perpetual growth and harvest of trees for the long-term protection of wildlife, plants, soil and water.

Visit fishersci.com/ecosafpak or fishersci.ca/ecosafpak to learn more.





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