

# Analytical Technique: Chromatography

## Guide to Key Solvents, Blends, Acids, and Instruments



Reliability.  
Purity.  
Certainty.



Discover. Synthesize. Analyze. Customize.

## The Best Performance for Your Chromatography

Whatever your field of activity — research, routine analysis or quality control — we can supply the solvents, blends, and reagents you need in grades, sizes, and packaging that meet your requirements. Our solvents are specifically formulated and tested on Thermo Scientific™ instruments and instruments from other leading manufacturers, so you can be sure they'll stand up to the challenges of HPLC, UHPLC/MS and GC applications, including:

- Pharmaceutical and biopharmaceutical research
- Environmental analysis
- Proteomics and metabolomics
- Forensic toxicology
- Personal care
- Clinical diagnostics

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## Manufacturing Capabilities

Our long-standing expertise in distillation, blending, processing, testing and packaging has led to a broad range of products for everything from drug discovery to production.

Our chemical manufacturing facilities are ISO 9001-certified with quality processes designed to meet rigorous testing measures that ensure lot-to-lot and bottle-to-bottle consistency. They are central to the development and production of high-purity solvents, additives and wash solutions for chromatography and mass spectrometry instrument systems, molecular biology reagents for life sciences applications, and reagents for automated clinical analyzers.

Additionally, we specialize in semi-bulk and bulk delivery, special testing, custom synthesis, and packaging and labeling of solvents or blends (including proprietary mixes) tailored to your needs.

Visit [fishersci.com/SCS](http://fishersci.com/SCS) or [fishersci.ca/SCS](http://fishersci.ca/SCS) for more information.



## Have technical questions or need information about our chemicals?

Our team of manufacturing chemists, chemical specialists, account representatives and customer service personnel are committed to bringing you the highest level of customer service, technical assistance and fast, accurate delivery.



Customer Service: **1-800-766-7000**

Chemical Technical Support: **1-800-227-6701**  
(Available in the United States, Puerto Rico and Canada.)

Service and support personnel are available Monday through Friday from 8:00 a.m. to 6:30 p.m. ET.



# Find Your Chromatography Chemicals

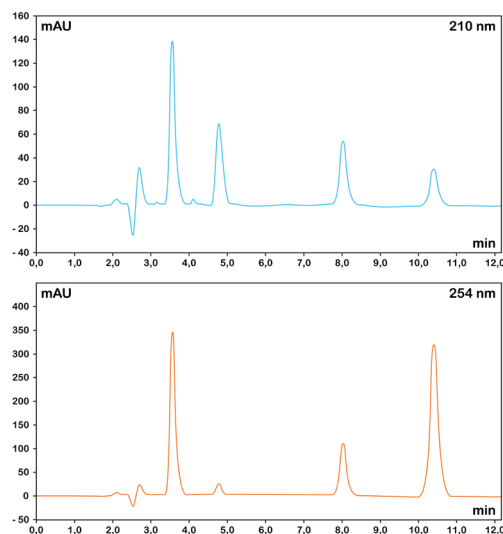
Use this table to find the best Fisher Chemical™ solvent grade for your applications:

Application	Instrument or Detector Type	Fisher Chemical Solvent Grade
Calibrating	MS	(Alfa Aesar) Standards
HPLC	LC Coupled with UV Detector	HPLC, Optima
High-Throughput Gradient HPLC	LC Gradient Grade Coupled with UV Detector	Optima
Clinical or Proteomics Chromatography Workflows	LC Coupled with Mass Detector	Optima LC/MS Mobile Phase Blends
UHPLC	LC Coupled with UV Detector UHPLC/UV	Optima LC/MS
UHPLC/MS	LC Coupled with Mass Detector	UHPLC/MS
High-Throughput UHPLC/MS	LC and UHPLC Coupled with Mass Detector	UHPLC/MS
GC	GC, GC/MS	Optima, GC Resolv
GC	GC with Electron Capture Detector	Pesticide
GC	GC with Headspace Analyzer	GC Headspace
MS for Proteomics	MS	(Alfa Aesar) Surfactants

## Standards

Calibration using reliable, verifiable chromatography standards must be performed regularly to ensure confidence in the accuracy of the data.

Alfa Aesar™ Mass Spectroscopy Standards	Sizes	Cat. No.
2,4,6-Tris(heptafluoropropyl)-1,3,5-triazine	5g, 1g	AAL16883
2,4,6-Tris(perfluoroheptyl)-1,3,5-triazine	500mg, 100mg	AAL16678
2,4,6-Tris(trifluoromethyl)-1,3,5-triazine, 98%	5g, 1g	AAB22001
Bis(pentafluorophenyl)phenylphosphine, 97%	0.25g, 1g	AAA11014
Perfluorokerosene-941	1g	AAL16595
Perfluorokerosene-L	5g, 1g	AAL16597
Perfluorotributylamine	25g, 5g, 1g	AA19126
Tris(pentafluorophenyl)phosphine, 97%	5g, 1g	AAL02748
Ultramark™ 1621	1g, 250mg	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, Carbonic Anhydrase, Cytochrome C, Lysozyme, Myoglobin	1 Vial	AAJ67628LPL
Reversed Phase LC/MS Peptide Retention Standard, 500pmol Each Peptide per Vial, Certified: Angiotensin I, Angiotensin II, Albumin Fragment LVAASQAALGL, Albumin Fragment TCVADESAENCDK, and Reference Peptide IAANIIDEIIEK	1 Vial	AAJ67668LPL





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## UHPLC/MS

Reach the highest level of UHPLC/MS performance with Fisher Chemical™ Optima™ UHPLC/MS grade solvents. These ultra-high-purity solvents are specifically for mass spectrometry instrumentation.

### Key Features

- Solvent specifications based on S/N ratio of the propazine product ion from MS/MS fragmentation
- LC/UV gradient suitability specifications are tested in the full 200–400nm range
- Borosilicate glass significantly reduces metal cation leaching (Na<sup>+</sup> and K<sup>+</sup>)
- Submicron filtration for maximum purity

### Advantages

- Designed to ensure low metal ion adduct formation and improve peak profiles
- Submicron filtration reduces clogging of instrument, column and check valve
- Provides a smooth baseline with minimal interference



## Application Example

Designed with innovative technology and fine detail, the Thermo Scientific™ Vanquish™ UHPLC System delivers a new standard in high-end UHPLC — more results with better separations and easier interaction simultaneously, without compromise. Conceived for the uniquely efficient 1.5µm solid core particle Thermo Scientific™ Accucore™ Vanquish™ C18 UHPLC columns, this fully integrated and biocompatible system features high sample capacity for high-throughput workflows, industry-leading pumping performance, amazingly low S/N and linearity, two-mode thermostating, active preheating and more, all in a system that's driven by the gold-standard CDS software.



UHPLC-MS Solvents	Packaging	Sizes	Cat. No.
Acetonitrile	Clear Borosilicate Glass Bottles	1L, Case of 6	A9561
Methanol	Clear Borosilicate Glass Bottles	1L, Case of 6	A4581
Water	Clear Borosilicate Glass Bottles	1L, Case of 6	W81

Visit [thermoscientific.com/vanquish](https://thermoscientific.com/vanquish) to learn more.



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## LC/MS

Fisher Chemical™ Optima™ LC/MS grade solvents lead the industry with LC/UV suitability specifications developed using advanced UHPLC technology coupled with PDA and MS detectors.

For reproducible performance of your LC/MS mobile phase, choose Optima LC/MS grade products:

- Solvents
- Mobile phase blends
- Reagents and additives

### Key Features

- Higher signal intensity and lower metal ion content (tested for up to 17 metals)
- Innovative LC/UV gradient test with photo diode array detector
- Submicron filtration for maximum purity
- Water is tested for absence of protease

### Advantages

- Designed to ensure low metal ion adduct formation and improve peak profiles
- Submicron filtration reduces clogging of instrument, column and check valve
- Provides a smooth baseline with minimal interference
- Water ideal for proteomic workflows



## Application Example

From forensic toxicology to environmental analysis and pharmaceutical research, a constant in almost every field is the need for greater productivity — to quantify more samples in less time with greater reliability and confidence, and to do it all on ever-tighter budgets. The Thermo Scientific™ Endura™ Triple Quadrupole Mass Spectrometer meets these needs with unsurpassed value. It delivers best-in-class sensitivity, run after run and day after day, regardless of sample type or matrix, and does so with an ease of use that takes the worry out of method development and operation.





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LC/MS Solvents	Packaging	Sizes	Cat. No.
Acetonitrile	Amber Glass Bottles	500mL, 1, 2.5 and 4L	A955
Methanol	Amber Glass Bottles	500mL, 1, 2.5 and 4L	A456
Water	Amber Glass Bottles	500mL, 1, 2.5 and 4L	W6
2-Propanol	Amber Glass Bottles	500mL, 1, 2.5 and 4L	A461

These solvents are formulated for UHPLC/UV and HPLC/MS.

Visit [thermoscientific.com/en/product/tsq-endura-triplequadropole-mass-spectrometer.html](https://thermoscientific.com/en/product/tsq-endura-triplequadropole-mass-spectrometer.html) to learn more.

## LC/MS Blends

Fisher Chemical™ Optima™ LC/MS solvents have set the standard of excellence for consistent, reproducible performance in the mobile phase of LC/MS. These same high-purity solvents are offered as blends with Optima LC/MS modifiers — like formic (FA) or trifluoroacetic (TFA) acids — to provide ready-to-use products for LC/MS applications.

### Key Features

- Low background noise (LC/MS)
- Minimal metal impurities
- Optimized for UHPLC/UV over the full UV range (200-400nm) to ensure extremely low levels of UV-absorbing impurities

### Advantages

- Suitable for MS detection
- Lower costs and fewer errors associated with preparing blends, along with consistent results.
- Extends LC/MS column life (low impurity levels and low residue values)



Optima LC/MS Blends	Packaging	Sizes	Cat. No.
Acetonitrile with 0.1% FA	Amber Glass Bottles	500mL, 1, 2.5 and 4L	LS120
Acetonitrile with 0.1% TFA	Amber Glass Bottles	500mL, 1, 2.5 and 4L	LS121
Water with 0.05% TFA	Amber Glass Bottles	4L	LS115
Acetonitrile with 0.05% TFA	Amber Glass Bottles	4L	LS117
Water with 0.1% FA	Amber Glass Bottles	500mL, 1, 2.5 and 4L	LS118
Water with 0.1% TFA	Amber Glass Bottles	500mL, 1, 2.5 and 4L	LS119
80% Acetonitrile with 0.1% FA	Amber Glass Bottles	500mL	LS122



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## LC/MS Specialty Mobile Phase Blends

The Thermo Scientific™ brand offers two premium mobile phase blends of ammonium formate and formic acid. The blends were developed for analyzing vitamin D, hormones and immunosuppressive drugs, and the volatility of the additives makes these blends suitable for LC/MS. They are ideal for use in nano LC/MS and other LC/MS applications.

### Key Features

- Highest purity demanded by LC/MS applications
- Low metal ion content to ensure minimal metal contamination
- Ultra-filtered to ensure low levels of particulates
- Premixed, ready-to-use LC/MS blend

Fisher Chemical™ LC/MS FA blend LS122 is recommended for use with the Thermo Scientific™ EASY-nLC™ 1200 and Thermo Scientific™ UltiMate™ 3000 RSLCnano Systems. This blend's reduced acetonitrile concentration improves performance, especially of early eluting, hydrophilic peptides.



EASY-nLC™ 1200 System

UltiMate™ 3000 RSLCnano Systems

## Application Example

These specialized solvent blends have been developed for use with the Thermo Scientific™ Prelude SPLC™ System and are ideal for cutting-edge research applications in areas such as proteomics, metabolomics, clinical chemistry and drug discovery.

LC/MS Specialty Mobile Phase Blends	Packaging	Sizes	Cat. No.
Methanol with 10mM Ammonium Formate with 0.05% Formic Acid	Borosilicate Glass Bottles	1L	MB122
Water with 10mM Ammonium Formate with 0.05% Formic Acid	Borosilicate Glass Bottles	1L	MB123





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## LC/MS Flush Solutions and Probe Washes

Thermo Scientific™ flush solutions are designed to remove difficult-to-clean contaminants from the instruments and remove carryover between sample runs. Isopropanol/acetonitrile/acetone (9/9/2) flush solution (Cat. No. MB124) is formulated for difficult-to-remove serum (blood) and urine samples.

LC/MS Flush and Wash Solutions	Packaging	Size	Cat. No.
Acetonitrile/IPA/Acetone (9/9/2)	Amber Glass Bottles	2.5L	MB124212
Probe Wash, Water with 2% Acetonitrile	Amber Glass Bottles	2.5L	T001252500
Probe Wash, Water with 40% Acetonitrile and 0.1% Formic Acid	Amber Glass Bottles	2.5L	T001262500

## LC/MS Additives

Fisher Scientific™ Optima™ LC/MS grade additives are available for use in the mobile phase, and they use-tested to ensure suitability.

### Key Features

- Low spectrometry background noise
- Minimal metal impurities
- Lowest impurity background using diode array detection

### Advantages

- Available in ampules (for small volumes) and HDPE bottles (for larger amounts)
- Ampules are pre-scored and sized for convenience

LC/MS Additives	Packaging	Size	Cat. No.
Acetic Acid	HDPE Bottles	1mL Ampules, 50mL Bottles	A113
Ammonium Acetate	Amber Glass Bottles	50g	A114
Ammonium Formate	Amber Glass Bottles	50g	A115
Formic Acid	HDPE Bottles	0.5, 1 and 2mL Ampules, 50mL Bottles	A117
Trifluoroacetic Acid	HDPE Bottles	0.5, 1 and 2mL Ampules, 50mL Bottles	A116

## Chromatography Columns and Consumables

Thermo Scientific columns and consumables offer solutions for pharmaceutical, food and beverage, forensic and toxicology, proteomics, clinical, and environmental customers.

- Sample preparation — a broad range of manual and semi-automated SPE consumable solutions, as well as systems for automated solvent extraction, solid phase extraction and evaporation
- Columns — get reliable, reproducible results with a comprehensive selection of LC and BioLC columns
- Vials and closures — choose from a large selection of vials and closures to meet your requirements

Visit [separatedbyexperience.com](http://separatedbyexperience.com) to learn more.



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## HPLC

Fisher Chemical™ Optima™ grade solvents meet purity requirements in the ppm range and are the best choice for basic chromatography work. They are manufactured for applications where contaminant-free performance is essential: HPLC/UV or HPLC/PDA, GC/TCD, spectrophotometry, environmental testing and other analytical applications.

### Key Features

- Contaminant-free to ppb and ppm levels
- Supplied in specially cleaned bottles

Description	Packaging	Sizes	Cat. No.
<b>Premium HPLC Optima Solvents</b>			
Acetone	Amber Glass Bottles and Safe-Cote™ Bottles (4L only)	1 and 4L	A929
Acetonitrile	Amber Glass Bottles and Safe-Cote Bottles (4L only)	1 and 4L	A996
Chloroform (with ~50ppm Amylene as a Preservative)	Amber Glass Bottles	4L	C297
Ethyl Acetate	Amber Glass and Safe-Cote Bottles	4L	E196
NEW Ethyl Acetate/Ethanol 3:1 Solution	Amber Glass Bottles	1 and 4L	E151
Hexanes	Amber Glass Bottles and Safe-Cote Bottles (4L only)	1 and 4L	H303
n-Hexane,95%	Amber Glass Bottles and Safe-Cote Bottles (4L only)	1 and 4L	H306
Methanol	Amber Glass Bottles and Safe-Cote Bottles (4L only)	1 and 4L	A454
Methylene Chloride	Amber Glass Bottles and Safe-Cote Bottles (4L only)	2.5 and 4L	D151
Petroleum Ether	Amber Glass Bottles and Safe-Cote Bottles	4L	E120
2-Propanol	Amber Glass Bottles and Safe-Cote Bottles	4L	A464
Tetrahydrofuran	Amber Glass Bottles and Safe-Cote Bottles (4L only)	1 and 4L	T427
Toluene	Amber Glass Bottles and Safe-Cote Bottles	4L	T291
Water	Amber Glass Bottles and Safe-Cote Bottles	4L	W7
<b>HPLC Grade Solvent Blends</b>			
Acetonitrile with 0.05% TFA	Amber Glass Bottles	4L	HB98124
Acetonitrile with 0.1% FA	Amber Glass Bottles	4L	HB98234
Acetonitrile with 0.1% TFA	Amber Glass Bottles	4L	HB98134
Water with 0.05% TFA	Amber Glass Bottles	4L	HB5124
Water with 0.1% TFA	Amber Glass Bottles	4L	HB5134
Water with 0.1% FA	Amber Glass Bottles	4L	HB5234



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## HPLC Grade Solvents

HPLC grade solvents are specifically for use in preparatory chromatography with HPLC instruments.

### Key Features

- Meet ACS specifications
- Submicron filtered
- Actual lot analysis on label
- Supplied in specially cleaned bottles or aluminum cans
- Blanketed with inert gas to maintain purity
- Certificate of Analysis available online or scan CofA QR code on label

HPLC Grade Solvents	Packaging	Sizes	Cat. No.
Acetone	Amber Glass Bottles, Safe-Cote™ Bottles, NOWPak I and FisherPak	1, 4, 19 and 115L	A949
Acetonitrile	Amber Glass Bottles, Safe-Cote Bottles (1 and 4L only), NOWPak I	1, 2.5, 4 and 19L	A998
Alcohol	Amber Glass Bottles, FisherPak	4 and 200L	A995
1-Butanol	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	A383
n-Butyl Chloride	Amber Glass Bottles, Safe-Cote Bottles	4L	B4294
Chloroform (~50ppm Pentene as a Preservative)	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	C607
Chloroform (~0.75% Ethanol as a Preservative)	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	C606
Cyclohexane	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	C620
Dimethyl Sulfoxide	Amber Glass Bottles	4L	D1594
Ethyl Acetate	Amber Glass Bottles, Safe-Cote Bottles, NOWPak I	1, 4 and 19L	E195
Ethyl Ether, Anhydrous (Stabilized)	Aluminium Can, FisherPak	4 and 19L	E198
Heptane	Amber Glass Bottles, Safe-Cote Bottles, FisherPak	1, 4, 19 and 200L	H350
Hexanes	Amber Glass Bottles, Safe-Cote Bottles, FisherPak	1, 4, 50, 115 and 200L	H302
Isooctane	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	O296
Methanol	Amber Glass Bottles, Safe-Cote Bottles, NOWPak I	1, 4 and 19L	A452
Methyl tert-Butyl Ether	Amber Glass Bottles, FisherPak	4 and 200L	E127
Methylene Chloride (Not Stabilized)	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	D150
Methylene Chloride (Stabilized)	Amber Glass Bottles, Safe-Cote Bottles, FisherPak	1, 4 and 50L	D143
Methylene Chloride (with Cyclohexene Preservative)	Amber Glass Bottles, Safe-Cote Bottles (4L only)	1 and 4L	D138
Pentane	Amber Glass Bottles, Safe-Cote Bottles, Steel Drums	1, 4 and 19L	P399
2-Propanol	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	A451
Tetrahydrofuran	Amber Glass Bottles, Safe-Cote Bottles, FisherPak	1, 4 and 50L	T425
Toluene	Amber Glass Bottles, Safe-Cote Bottles	1 and 4L	T290
1,2,4-Trichlorobenzene	Amber Glass Bottles	4L	O48464
Triethylamine	Amber Glass Bottles	100mL	O4884100
Vinyl Acetate	BasicPak	115L	O5057FB 115
Water	Amber Glass Bottles, Safe-Cote Bottles, NOWPak I	1, 4 and 19L	W5

Other sizes may be available.



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## Surfactants

Surfactants are compatible with mass spectrometry used in proteomics analysis. The compounds listed here show minimal matrix interference in proteomics target analysis by mass spectrometry.

Certified Mass Spec Surfactants	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 II (NALS II)	5mg	AAJ67682LB0
Non-Ionic Acid Labile Surfactant I (NALS I)	5mg	AAJ67592LB0
Zwitterionic Acid Labile Surfactant II (ZALS II)	5mg	AAJ67721LB0
Zwitterionic Acid Labile Surfactant I (ZALS I)	5mg	AAJ67729LB0

## GC Headspace Solvents

To achieve optimum laboratory testing conditions, solvents must be free of interference that could contaminate headspace and potentially mask your results. If you use a solvent not routinely tested for the absence of low-boiling organics, you'll risk the accuracy of your research.

The solution is simple: Use a better solvent, get more reliable results. But how can you be sure which solvent is actually better? Fisher Chemical™ Headspace grade solvents produce a clean solvent baseline with no extraneous peaks.



Residual Solvent Class	GC Headspace Solvent Suitability Specification	ICH Residual Solvent Concentration Limit
1	1ppm max.	2ppm (Benzene)
2	10ppm max.	50ppm (Methylbutyl-ketone)
3	50ppm max.	NA

<sup>1</sup>International Conference of Harmonization

### Key Features

- Processed to high purity for accurate and repeatable determination of trace levels of Class 1, Class 2, and Class 3 residual solvents in samples
- Tested by UV absorbance to ensure low organic contamination
- Processed for low water content to facilitate organic volatile impurity extraction
- Packaged with an inert atmosphere to maximize (unopened) shelf life



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GC Headspace Grade Solvents	Size	Cat. No.
Water	1L	W101
DMSO, Dimethyl Sulfoxide	1L	D1391
DMF, N,N-Dimethylformamide	1L	D1331
DMAC, N,N-Dimethylacetamide	1L	D1601
NMP, N-Methyl-2-Pyrrolidone	1L	N1401

## Pesticide Grade Solvents

Fisher Chemical™ Pesticide Grade Solvents are the economical choice for analyzing pesticide residue using GC with electron capture detector (ECD). When higher purity to the parts-per-billion level is required, select GC Resolv™ Grade Solvents.

Pesticide Grade Solvents	Grade	Size	Packaging	Cat. No.
Acetone	GC Resolv	4L	Amber Glass Bottles	A9284
n-Hexane	GC Resolv	4L	Amber Glass Bottles	H3074
Methanol	GC Resolv	4L	Amber Glass Bottles	A4574
Methylene Chloride	GC Resolv	4L	Amber Glass Bottles	D1544
Acetone	Pesticide	4L	Amber Glass Bottles	A404
Chloroform (with Amylene preservative)	Pesticide	4L	Amber Glass Bottles	C6034
Cyclohexane	Pesticide	4L	Amber Glass Bottles	C5534
Ethyl Acetate	Pesticide	4L	Amber Glass Bottles	E1914
Ethyl Ether	Pesticide	4L	Amber Glass Bottles	E1994
Hexanes	Pesticide	4L	Amber Glass Bottles	H3004
Isooctane	Pesticide	4L	Amber Glass Bottles	O2974
Methanol	Pesticide	4L	Amber Glass Bottles	A4504
Methylene Chloride	Pesticide	4L	Amber Glass Bottles	D1424
Pentane	Pesticide	4L	Amber Glass Bottles	P4004
Petroleum Ether	Pesticide	4L	Amber Glass Bottles	P4804
2-Propanol	Pesticide	4L	Amber Glass Bottles	A5194

### TRACE GC Ultra Chromatographs

With the most complete range of proprietary inlets, sensitive detection systems, smart accessories, and ancillary devices, the Ultra platform features unique technologies that raise the standards of speed, sensitivity and separation in gas chromatography.

Visit [thermoscientific.com/chromatography](http://thermoscientific.com/chromatography) to learn more.





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## Acids

The Fisher Chemical™ portfolio of high-purity acids and bases comprises more than 400 products suited to a wide range of laboratory applications, including trace element analysis in sample preparation, HPLC and spectrophotometry. All Fisher Chemical acids are manufactured in ISO 9001-certified facilities and subjected to rigorous quality assurance and testing measures that ensure excellent lot-to-lot and bottle-to-bottle consistency.

Select the grade that is best suited to your application:

Grade	Description	Applications
Optima	<ul style="list-style-type: none"> <li>Extremely high-purity acids</li> <li>Lowest metal content of commercially available acids</li> <li>Analyzed for 65 metals by ICP/MS (impurity levels in ppt)</li> <li>Packaged in specially manufactured and cleaned PFA and FEP fluoropolymer bottles</li> <li>Optima ammonium hydroxide is packaged in specially cleaned HDPE bottles</li> </ul>	<ul style="list-style-type: none"> <li>HPLC</li> <li>GC</li> <li>AA</li> <li>Plasma, ICP, ICP/MS</li> <li>Spectrophotometry</li> <li>Pesticide residue analysis</li> </ul>
TraceMetal	<ul style="list-style-type: none"> <li>Manufactured to achieve metal contamination in ppm to ppb range (proprietary distillation)</li> <li>ICP/MS-analyzed by lot for more than 55 metals</li> <li>Packaged in poly bottles (for safer and easier handling and limited/no breakage during transportation)</li> </ul>	Primarily used to help digest samples for ICP analysis.
HPLC	<ul style="list-style-type: none"> <li>Formulated for liquid chromatography</li> <li>Ensures minimum baseline drift and maximum retention reproducibility</li> <li>Meets all ACS specifications</li> </ul>	<ul style="list-style-type: none"> <li>HPLC</li> <li>Spectrophotometry</li> </ul>
Certified ACS Plus	<ul style="list-style-type: none"> <li>Analyzed for more than 16 metals</li> <li>Meets or exceed ACS specifications</li> </ul>	Analytical applications with tighter metal specifications
Certified ACS	<ul style="list-style-type: none"> <li>Meets or exceed ACS specifications</li> <li>Label includes actual lot analysis</li> </ul>	Analytical applications

### Evolution 600 UV-Vis Spectrophotometer

The Thermo Scientific™ Evolution™ 600 incorporates a high-performance optical design, versatile Thermo Scientific™ VISION™ software packages, and the highest-quality accessories for the most demanding materials science and research applications.

Visit [thermoscientific.com/uv-vis](http://thermoscientific.com/uv-vis) to learn more.





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## High-Purity Acids

Fisher Chemical™ Optima™ grade acids offer the lowest metal content and the highest purity. They are an ideal choice for environmental testing, plasma analysis, electronic research and other exacting procedures requiring the utmost purity, precision and accuracy.

### Applications

- HPLC/MS
- GC
- ICP/MS
- Spectrophotometry
- Pesticide residue analysis

### Key Features

- Analyzed for up to 65 metals (to ppt level) by ICP/MS to provide unequalled purity (Certificate of Analysis supplied with each bottle)
- Packaged in specially manufactured and cleaned PFA and FEP fluoropolymer bottles (Optima Ammonium Hydroxide is packaged in specially cleaned HDPE bottles)
- Produced and packaged in a Class 100 cleanroom environment to ensure maximum purity
- Excellent lot-to-lot consistency for reproducible results

Optima Grade Acids	Packaging	Sizes	Cat. No.
Acetic Acid, Glacial	PFA Bottles	250 and 500mL, 1L	A465
Ammonium Hydroxide	PFA Bottles	250 and 500mL, 1L	A470
Hydrobromic Acid	FEP Bottles	250 and 500mL, 1 and 2L	A471
Hydrochloric Acid	PFA Bottles, FEP Bottles (2L only)	250 and 500mL, 1 and 2L	A466
Hydrofluoric Acid	PFA Bottles	250 and 500mL, 1 and 2L	A463
Hydrogen Peroxide	FEP Bottles	500mL	P170500
Nitric Acid	FEP Bottles	250 and 500mL, 1 and 2L	A467
Perchloric Acid	PFA Bottles	250 and 500mL, 1L	A467
Sulfuric Acid	FEP Bottles	250 and 500mL, 1 and 2L	A468

<sup>†</sup>Products might not be available in all regions. Contact your local sales representative for details



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### XSERIES 2 ICP/MS

The Thermo Scientific™ XSERIES 2™ ICP/MS offers outstanding productivity in a quadrupole ICP/MS for both routine and high-performance analytical work.

Visit [thermoscientific.com/ms](http://thermoscientific.com/ms) to learn more.



### iCAP 6500 ICP Spectrometer

Thermo Scientific™ iCAP™ 6500 ICP Spectrometer is small in size, yet big on performance, offering the best detection capability of any optical ICP, with enhanced productivity and the optimum in application flexibility.

Visit [thermoscientific.com/ms](http://thermoscientific.com/ms) to learn more.



## TraceMetal Acids

Fisher Chemical™ TraceMetal™ grade acids are used primarily in digestion of samples prior to instrument (ICP) analysis. Each lot is analyzed for more than 55 metals by ICP/MS. A proprietary distillation process achieves metal concentrations in the sub-ppb range.

Select TraceMetal grade acids and bases are now available in a plastic bottle consisting of a new high-density polyethylene made with a proprietary resin that provides up to 80% less metallic extractables than glass. This new packaging material for TraceMetal acids and bases provides greater convenience and stability during transportation as well as increased resistance to breakage than conventional glass packaging.

### Packaging Advantages

- Plastic bottles are lighter, safer and easier to handle
- Limited or no breakage during transportation
- Drip lip pour feature for safer pouring in the laboratory
- Fully recyclable package and plastic bottle for reduced waste
- Plastic bottles take up less space than glass bottles, providing better use of space in the laboratory
- Lack of PVC coating reduces waste





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TraceMetal Grade Acids	Packaging	Sizes	Cat. No.
Acetic Acid, Glacial	HDPE Bottles	500mL, 2.5L	A507P
Ammonium Hydroxide	HDPE Bottles	500mL	A512P500
Hydrochloric Acid	HDPE Bottles	500mL, 2.5L	A508P
Hydrofluoric Acid	HDPE Bottles (4L only), LDPE Bottles	500mL, 4L	A513
Nitric Acid	HDPE Bottles	500mL, 2.5L	A509P
Perchloric Acid	HDPE Bottles	500mL, 2.5L	A511P
Sulfuric Acid	HDPE Bottles	500mL, 2.5L	A510P
Water	LDPE Bottles	500mL, 1 and 2L	W9

Ultra Trace Elemental Analysis Grade	Packaging	Sizes	Cat. No.
Water	LDPE Bottles	500mL, 1 and 2L	W9

## Ion Pair and HPLC Acids

Fisher Chemical™, Acros Organics™ and Alfa Aesar™ HPLC grade acids are specifically formulated for use in liquid chromatography. They meet all ACS specifications and ensure minimum baseline drift and maximum retention reproducibility. Ion pair chromatography is used to separate charged substances.

Ion Pair Reagents + HPLC Acids	Size	Cat. No.
1-Butanesulfonic Acid, Sodium Salt, 99+%,	25g	AC343800250
1-Butanesulfonic Acid, Sodium Salt, Anhydrous, +99%	25g	AC396640250
1-Decanesulfonic Acid, Sodium Salt, 99+%, Ion Pair Chromatography, Anhydrous	25 and 100g	AC39671
1-Dodecanesulfonic Acid, Sodium Salt, 99+%, Ion Pair Chromatography, Anhydrous	5 and 25g	AC39672
1-Heptanesulfonic Acid, Sodium Salt, Monohydrate	5, 25, 100 and 500g	AC41127
1-Heptanesulfonic Acid, Sodium Salt, 99+%, Ion Pair Chromatography, Anhydrous	25 and 100g	AC39668
1-Hexanesulfonic Acid, Sodium Salt Hydrate, 98%	5, 25, 100 and 500g	AC41160
1-Hexanesulfonic Acid, Sodium Salt, 99+%, Ion Pair Chromatography, Anhydrous	25 and 100g	AC39667
1-Octanesulfonic Acid, Sodium Salt Anhydrous	5, 25 and 100g	AC41636
1-Octanesulfonic Acid, Sodium Salt	5, 25, 100 and 500g	AC38477
1-Octanesulfonic Acid, Sodium Salt, +99%, Anhydrous	25 and 100g	AC39669
1-Pentanesulfonic Acid, Sodium Salt Monohydrate, 98+%	25 and 100g	AC42320
1-Pentanesulfonic Acid, Sodium Salt, 99+%, Anhydrous	25, 100 and 500g	AC39665
1-Propanesulfonic Acid, Sodium Salt, +99%	25g	AC39666
Acetic Acid, Glacial	500mL	A35-500
Acetic Acid, Ammonium Salt	250g	AC21999
Acetic Acid, Sodium Salt, 99%	50g	AC44688
o-Phosphoric Acid, 85%	500mL	A260500
Trifluoroacetic Acid	100 and 500mL	AC43229
Trifluoroacetic Acid, 99.5+%, Alfa Aesar	100 and 500mL, Packs of 4 Each	AA44630



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## ACS Acids

Fisher Chemical™ ACS grade acids meet or exceed the specifications set by the American Chemical Society and are suitable for analytical applications requiring tight specifications.

This classification includes two grades:

- 1. Certified ACS Grade**
- 2. Certified ACS Plus Grade** (In addition to meeting ACS specifications, these acids are analyzed for more than 16 metals. The actual lot analysis appears on the label.)

Description	Packaging	Sizes	Cat. No.
<b>ACS Grade Acids</b>			
Acetic Acid, Glacial	Glass Bottles, Safe-Cote Bottles	500mL, 2.5L (x6) 2.5L	A38 <sup>†</sup>
Formic Acid	Plastic Bottle	100 and 500mL, 4L	A118P
o-Phosphoric Acid 85%	Glass Bottles, Safe-Cote Bottles	500mL, 1, 2.5 and 4L	A242
Potassium Hydroxide	Plastic Bottles, Plastic Pails	500g, 1, 3 and 10kg	P250
Sodium Hydroxide	Plastic Bottles, Plastic Pails	100 and 500g, 1, 3 and 5kg	S318
Trichloroacetic Acid	Amber Glass Bottles	100 and 500g, 3kg	A322
<b>ACS Plus Grade Acids</b>			
Ammonium Hydroxide	Glass Bottles, Safe-Cote Bottles	500mL, 2.5L (x6) 2.5L	A669 <sup>†</sup>
Hydrochloric Acid	Glass Bottles, Safe-Cote Bottles	500mL, 2.5L (x6) 2.5L	A144 <sup>†</sup>
Nitric Acid	Glass Bottles, Safe-Cote Bottles	500mL, 2.5L (x4) 2.5L	A200 <sup>†</sup>
Sulfuric Acid	Glass Bottles, Safe-Cote Bottles	500mL, 2.5L (x6) 2.5L	A300 <sup>†</sup>

<sup>†</sup>Products might not be available in all regions. Contact your Fisher Scientific Sales Representative for details

## Certified Acids

The Fisher Chemical™ team establishes the purity standard for certified-grade acids and makes sure each lot meets the published maximum limits. These acids are suitable for general analytical procedures.

Certified Acids and Solutions	Packaging	Size	Cat. No.
Hydrochloric Acid Solution, 1N	Plastic Bottles	500mL, 1 and 4L	SA48
Hydrochloric Acid Solution, 2N	Plastic Bottles	500mL	SA431500
Hydrochloric Acid Solution, 6N	Amber Glass Bottles	500mL, 1 and 4L	SA56
Nitric Acid Concentrate	Amber Glass Bottles	100mL	SA95
Nitric Acid Solution, 0.1N (N/10)	Amber Glass Bottles	1L	SA941
Perchloric Acid Solution, 0.1N (N/10)	Amber Glass Bottles	500mL	SP339500
Potassium Hydroxide Solution, 0.1N (in Isopropanol)	Amber Glass Bottles	500mL	ST110500
Propionic Acid	Amber Glass Bottles	500mL	A258500
Sulfuric Acid Solution, 0.02N (N/50)	Plastic Bottles	4L	SA2264
Sulfuric Acid Solution 0.02N (N/50)	Plastic Bottles	1L	SA2261



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## Solvent Selection Guide

Solvent	Available Grades†	MW	Melting Point (°C)	Boiling Point (°C)	Flash Point (°C)	UV Cutoff (nm)	Refractive Index (@ 25°C)	Density (g/mL @ 25°C)	Viscosity (cP @ 20°C)	Polarity Index (P <sup>1</sup> )
Acetone	EFGHOPS	58.08	-94.3	56.1	20	330	1.3568	0.7857	0.36	5.1
Acetonitrile	HOPCU	41.05	-50.0	81.6	2	190	1.3415	0.778	0.36	5.8
1-Butanol	HS	74.12	-88.6	117.7	35	215	1.3972	0.8098	2.98	3.9
Chloroform	HMOPS	119.38	-63.3	61.7	None	245	1.4445	1.484	0.58	4.1
Cyclohexane	HPS	84.16	-6.5	80.7	-20	202	1.4247	0.774	0.90	0.2
N,N-Dimethylacetamide	D	87.12	-60.4	165.1	62.77		1.437	0.937		
N,N-Dimethylformamide	SD	73.09	-61.0	153.0	58	268	1.428	0.944	0.92	6.4
Dimethyl Sulfoxide	HSD	78.13	18.5	189.0	87.8	262	1.4783	1.1014	2.24	7.2
Ethyl Acetate	HOPPhS	88.11	-83.9	77.1	-4	255	1.3695	0.894	0.45	4.4
Ethyl Ether	HPS	74.12	-116.3	34.6	-45	218	1.35	0.7134	0.24	2.8
Glycerol	MPhS	92.09	18.2	290.0	193	205	1.4746	1.2613		
Heptane	HSS	100.2	-90.6	98.4	-4	197	1.3855	0.6838	0.40	0.2
Hexanes	GHOPPhS	86.18	-95.3	69.0	-23	195	1.3759	0.663	0.31	0.1
Isooctane	HOPS	114.23	109.5	99.2	28	205	1.3895	0.6919	0.50	0.1
Methanol	EGHLwOPPtSCU	32.04	-97.8	64.7	12	205	1.3288	0.7915	0.55	5.1
Methylene Chloride	GHOPS	84.93	-96.7	39.5	N/A	233	1.4215	1.318	0.30	3.1
N-Methylpyrrolidinone	M	99.13	-24.4	202.2	95	275	1.469	1.03	1.67	
Pentane	HPS	72.15	-129.7	36.1	-49	190	1.3555	0.6264	0.22	0.0
Petroleum Ether	OP			35-36	-18		1.361	0.64		0.1
2-Propanol	HLwOPPhSCU	60.1	-90.0	82.3	-12	205	1.3772	0.7855	2.40	3.9
Tetrahydrofuran	HOS	72.11	-108.3	66.1	-14	210	1.406	0.8892	0.55	4.0
Toluene	HOScS	92.14	-95.0	110.6	-4	285	1.494	0.866	0.59	2.4
Water	HODCU	18.02	0.0	100.0	N/A		1.333	0.9982	1.00	10.2

†E = Electronic Grade; G = GC Resolv; H = HPLC Grade; Lw = Low water; M = Molecular Biology Grade; O = Optima; P = Pesticide Grade; Ph = Pharmacopeia (USP, NF, FCC, EP, BP, JP); Pt = Purge & Trap; Sc = Scintanalyzed; S = Spectranalyzed C = LCMS, = UHPLC/MS, D = GC Headspace



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## 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](https://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 clean-up. Visit [fishersci.com/safecote](https://fishersci.com/safecote) to learn more.



### Next-Generation Products

As instrumentation evolves, new lines of solvents are being developed to help researchers amplify productivity with improved impurity detection and interference-free baselines. Innovations include:

- Minimized Na<sup>+</sup> and K<sup>+</sup> metal adduct formation in high-purity solvents
- Reagents for direct use on the instrument
- Graduated containers for ready reference



### PTFE Bottles

Our PTFE bottles are durable and inert, and they're designed to preserve the integrity of your high-purity acids.



### Seamless Aluminum Cans

Our lightweight, recyclable seamless aluminum cans are designed to protect against leaks, corrosion and breakage.



### EcoSafPak Shipping Containers

Select solvents are packaged in EcoSafPak™ packaging, which 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](https://fishersci.com/ecosafpak) to learn more.










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## ChemAlert Labels

### Lock in Safety and Quality with FisherLOCK Caps

Secure, tamper-evident Fisher Chemical™ FisherLOCK™ caps hold the lips on most 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.

- |   |  |
|---|--|
| <p> <b>Red — Flammable</b><br/>Store in area segregated for flammable reagents.</p> <p> <b>Blue — Health Hazard</b><br/>Toxic if inhaled, ingested or absorbed through skin.<br/>Store in secure area.</p> <p> <b>Yellow — Reactive and Oxidizing</b><br/>May react violently with air, water or other substances.<br/>Store away from flammable and combustible materials.</p> | <p> <b>White — Corrosive</b><br/>May harm skin, eyes and mucous membranes. Store away from red-, yellow- and blue-coded reagents. Store acids and bases separately.</p> <p> <b>Gray — Moderate Hazard</b><br/>Presents no more than moderate hazard in any of the hazards previously listed.</p> |
|---|--|






### DOT Classifications

The U.S. Department of Transportation (DOT) publishes transportation regulations covering shipments of materials classified as hazardous within the continental United States and its territories. These regulations, covering packaging, marking, labeling and shipping paper descriptions, are published in 49 CFR Parts 100-185. Materials are classified according to the system listed on this page.

DOT Hazard Class/Division	DOT Hazard Description
1	Explosives
2.1	Flammable gas
2.2	Non-flammable gas
2.3	Poison gas
3	Flammable liquid
4.1	Flammable solid
4.2	Spontaneously combustible
4.3	Dangerous when wet
5.1	Oxidizer
5.2	Organic peroxide
6.1	Poison
6.2	Infectious substance
7	Radioactive
8	Corrosive
9	Miscellaneous

### Spill Cleanup Kit Symbols

To simplify ordering the appropriate kit, the following symbols are used to identify chemicals that require special cleanup materials and the type of cleanup kit required. These are one-time-use kits containing everything necessary for spill cleanup.

-  **Acid Spills Emergency Cleanup Kit** for neutralizing and absorbing up to 1L of acid. (Cat. No. 18061A)
-  **Caustic Spill Emergency Cleanup Kit** for neutralizing and absorbing up to 1L of caustic material. (Cat. No. 18061C)
-  **Solvent Spill Emergency Cleanup Kit** for neutralizing and absorbing up to 1L of solvent. (Cat. No. 18061B)

Visit [fishersci.com](http://fishersci.com) to order your spill kit. Search for catalog number 18061E to order the combo pack, which includes all three of these kits.



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# Common Background Contamination Ions in Mass Spectrometry

## Common Adduct Ions in ESI Positive Mode

Solvents	Accurate Mass
(M+H) <sup>+</sup>	M+1.007276
(M+NH <sub>4</sub> ) <sup>+</sup>	M+18.03383
M+Na <sup>+</sup>	M+22.98977
(M+K) <sup>+</sup>	M+38.96371
(M+CH <sub>3</sub> OH+H) <sup>+</sup>	M+33.03349
(M+ACN+H) <sup>+</sup>	M+42.03383
(M+ACN+Na) <sup>+</sup>	M+64.01632
(M+DMSO+H) <sup>+</sup>	M+79.02118
(M+2ACN+H) <sup>+</sup>	M+83.06037

## Common Observed and Predicted Background Ions in ESI Positive Mode

Compounds or Species	Formula	[M+H] <sup>+</sup>	[M+NH <sub>4</sub> ] <sup>+</sup>	[M+Na] <sup>+</sup>	[M+K] <sup>+</sup>
Methanol clusters	CH <sub>3</sub> OH	33.0335	50.0600	55.0154	70.9894
	(CH <sub>3</sub> OH) <sub>2</sub>	65.0597	82.0863	87.0417	103.0156
	(CH <sub>3</sub> OH) <sub>3</sub>	97.0859	114.1125	119.0679	135.0418
Acetonitrile clusters	CH <sub>3</sub> CN	42.0338	59.0604	64.0158	79.9897
	(CH <sub>3</sub> CN) <sub>2</sub>	83.0604	100.0869	105.0423	121.0163
	(CH <sub>3</sub> CN) <sub>3</sub>	124.0869	141.1135	146.0689	162.0428
MeOH + H <sub>2</sub> O clusters	(CH <sub>3</sub> OH)(H <sub>2</sub> O)	51.0446	68.0712	73.0265	89.0005
	(CH <sub>3</sub> OH) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	101.0808	118.1074	123.0628	139.0367
	(CH <sub>3</sub> OH) <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub>	133.1071	150.1336	155.0890	171.0629
Acetonitrile + Methanol clusters	(CH <sub>3</sub> CN)(CH <sub>3</sub> OH)	74.0600	91.0866	96.0420	112.0159
	(CH <sub>3</sub> CN) <sub>2</sub> (CH <sub>3</sub> OH) <sub>2</sub>	147.1128	164.1394	169.0947	185.0687
Dimethylformamide	C <sub>3</sub> H <sub>7</sub> NO	74.0600	91.0866	96.0420	112.0159
DMSO	C <sub>2</sub> H <sub>6</sub> OS	79.0212	96.0478	101.0032	116.9771
	(C <sub>2</sub> H <sub>6</sub> OS) <sub>2</sub>	157.0351	174.0617	179.0171	194.9910
	(C <sub>2</sub> H <sub>6</sub> OS) <sub>3</sub>	235.0491	252.0756	257.0310	273.0050
Acetonitrile/Formic acid	(CH <sub>3</sub> CN)(HCOOH)	88.0393	105.0659	110.0212	125.9952
Acetonitrile/Acetic acid	(CH <sub>3</sub> CN)(CH <sub>3</sub> COOH)	102.0550	119.0815	124.0369	140.0108
Acetonitrile/Dimethylformamide	(CH <sub>3</sub> CN)(C <sub>3</sub> H <sub>7</sub> NO)	115.0866	132.1131		153.0425
DMSO+MeCN clusters	[C <sub>2</sub> H <sub>6</sub> OS+CH <sub>3</sub> CN]	120.0478	137.0743	142.0297	158.0036
Sodium formate	CH <sub>2</sub> O <sub>2</sub> Na			90.9766	
Sodium acetate	C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> Na			104.9923	
(N-Methyl-2-pyrrolidone)	C <sub>5</sub> H <sub>9</sub> NO	100.0757	117.1022	122.0576	138.0316
Triethylamine (TEA)	C <sub>6</sub> H <sub>13</sub> N	102.1277	119.1543	124.1097	140.0836
TRIS	C <sub>4</sub> H <sub>11</sub> NO <sub>3</sub>	122.0812	139.1077	144.0631	160.0371
Dimethylaminopyridine	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	123.0917	140.1182	145.0736	161.0476



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Common Observed and Predicted Background Ions in ESI Positive Mode (Continued)

Compounds or Species	Formula	[M+H] <sup>+</sup>	[M+NH <sub>4</sub> ] <sup>+</sup>	[M+Na] <sup>+</sup>	[M+K] <sup>+</sup>
Diisopropylethylamine	C <sub>9</sub> H <sub>19</sub> N	130.1590	147.1856	152.1410	168.1149
Tripropylamine	C <sub>9</sub> H <sub>21</sub> N	144.1747	161.2012	166.1566	182.1306
Phthalic anhydride	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub>	149.0233	166.0499	171.0053	186.9792
Phenyldiethylamine	C <sub>10</sub> H <sub>15</sub> N	150.1277	167.1543	172.1097	188.0836
1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU)	C <sub>9</sub> H <sub>16</sub> N <sub>2</sub>	153.1386	170.1652	175.1206	191.0945
NaTFA	C <sub>2</sub> F <sub>3</sub> O <sub>2</sub> Na			158.9640	
Diethylene glycol monobutyl ether	C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>	163.1329	180.1594	185.1148	201.0888
	(C <sub>8</sub> H <sub>18</sub> O <sub>3</sub> ) <sub>2</sub>	325.2585	342.2850	347.2404	363.2143
α-Cyano-4-hydroxycinnamic acid (4-HCCA)-H <sub>2</sub> O	C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub>	172.0393	189.0659	194.0212	209.9952
α-Cyano-4-hydroxycinnamic acid (4-HCCA)	C <sub>10</sub> H <sub>7</sub> NO <sub>3</sub>	190.0499	207.0764	212.0318	228.0058
	C <sub>10</sub> H <sub>7</sub> NO <sub>3</sub>	379.0925	396.1190	401.0744	417.0483
	(C <sub>10</sub> H <sub>7</sub> NO <sub>3</sub> ) <sub>3</sub>	568.1351	585.1616	590.1170	606.0909
Butylated hydroxyanisole	C <sub>11</sub> H <sub>16</sub> O <sub>2</sub>	181.1223	198.1489	203.1043	219.0782
Diphenyl ketone	C <sub>13</sub> H <sub>10</sub> O	183.0804	200.1070	205.0624	221.0363
Glycol ether	C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>	185.1148	202.1414	207.0968	223.0707
Tributylamine	C <sub>12</sub> H <sub>27</sub> N	186.2216	203.2482	208.2036	224.1775
n-Butyl benzenesulfonamide	C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub> S	214.0896	231.1162	236.0716	252.0455
Butylated hydroxytoluene	C <sub>15</sub> H <sub>24</sub> O	221.1900	238.2165	243.1719	259.1459
N,N'-Dicyclohexylurea	C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> O	225.1961	242.2227	247.1781	263.1520
	(C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> O) <sub>2</sub>	449.3850	466.4116	471.3669	487.3409
TEA.HCl <sup>95</sup>	C <sub>6</sub> H <sub>15</sub> N.HCl	239.2249	256.2514	261.2068	277.1807
TEA.HCl <sup>97</sup>	C <sub>6</sub> H <sub>15</sub> N.HCl	241.2219	258.2485	263.2038	279.1778
Tetrabutylammonium	C <sub>16</sub> H <sub>36</sub> N	242.2842			
Tributylphosphate	C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P	267.1720	284.1985	289.1539	305.1279
Monomethoxytrityl cation	C <sub>20</sub> H <sub>17</sub> O	273.1274			
Triphenylphosphine oxide	C <sub>18</sub> H <sub>15</sub> OP	279.0933	296.1199	301.0753	317.0492
Oleamide	C <sub>18</sub> H <sub>35</sub> NO	282.2791	299.3057	304.2611	320.2350
Stearamide	C <sub>18</sub> H <sub>37</sub> NO	284.2948	301.3213	306.2767	322.2507
n,n-bis(2-hydroxyethyl) dodecanamide	C <sub>16</sub> H <sub>33</sub> NO <sub>3</sub>	288.2533	305.2799	310.2353	326.2092
Oleamide	C <sub>18</sub> H <sub>35</sub> NO	304.2611	321.2876	326.2430	342.2170
Dibutyl sebacate	C <sub>18</sub> H <sub>34</sub> O <sub>4</sub>	315.2530	332.2795	337.2349	353.2089
Diethylene glycol monobutyl ether	C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>	325.2585	342.2850	347.2404	363.2143
Triphenyl phosphate	C <sub>18</sub> H <sub>15</sub> O <sub>4</sub> P	327.0781	344.1046	349.0600	365.0340
Tributyl tin formate	C <sub>13</sub> H <sub>28</sub> O <sub>2</sub> Sn	337.1184	354.1450	359.1003	375.0743
Erucamide	C <sub>22</sub> H <sub>43</sub> NO	338.3417	355.3683	360.3237	376.2976
Palmitamidopropyl-trimonium chloride	C <sub>22</sub> H <sub>47</sub> N <sub>2</sub> OCl	355.3683	372.3948	377.3502	393.3242
Behentrimonium chloride (BTAC-228)	C <sub>25</sub> H <sub>54</sub> NCl	368.4251			
Bis(2-ethylhexyl) adipate	C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>	371.3156	388.3421	393.2975	409.2715
Diocetyl adipate	C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>	371.3156	388.3421	393.2975	409.2715
Dipalmityldimethylammonium chloride	C <sub>34</sub> H <sub>72</sub> NCl	494.5659			
Didodecyl 3,3'-thiodipropionate	C <sub>30</sub> H <sub>58</sub> O <sub>4</sub> S	515.4129	532.4394	537.3948	553.3687
Stearyl-palmityl dimethylammonium chloride	C <sub>36</sub> H <sub>76</sub> NCl	522.5972			
Didodecyl 3,3'-thiodipropionate oxidized to	C <sub>30</sub> H <sub>58</sub> O <sub>5</sub> S	531.4078	548.4343	553.3897	569.3637
Irganox	C <sub>35</sub> H <sub>62</sub> O <sub>3</sub>	531.4772	548.5037	553.4591	569.4331
Acetic acid-Fe-O- complex	[C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ] <sub>6</sub> -6H+3Fe+O]	537.8790	554.9056	559.8610	575.8349



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Common Observed and Predicted Background Ions in ESI Positive Mode (Continued)

Compounds or Species	Formula	[M+H] <sup>+</sup>	[M+NH <sub>4</sub> ] <sup>+</sup>	[M+Na] <sup>+</sup>	[M+K] <sup>+</sup>
Didodecyl 3,3'-thiodipropionate oxidized to sulfone	C <sub>30</sub> H <sub>56</sub> O <sub>6</sub> S	547.4027	564.4292	569.3846	585.3586
Distearyldimethylammonium chloride	C <sub>38</sub> H <sub>80</sub> NCI	550.6285			
Acetic acid-Fe-O- complex	[(C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ) <sub>6</sub> -6H+H <sub>2</sub> O+3Fe+O]	555.8896			
Acetic acid-Fe-O- complex	[(C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ) <sub>7</sub> -6H+3Fe+O]	597.9001			
3-[(3-Cholamidopropyl)dimethylammonio]-1-propanesulfonate	C <sub>32</sub> H <sub>58</sub> N <sub>2</sub> O <sub>7</sub> S	615.4038	632.4303	637.3857	653.3596
Propionic acid Fe-O complex	[(C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ) <sub>6</sub> -6H+3Fe+O]	621.9729			
Nylon	C <sub>24</sub> H <sub>44</sub> N <sub>4</sub> O <sub>4</sub>	453.3435	470.3701	475.3255	491.2994
	C <sub>36</sub> H <sub>66</sub> N <sub>6</sub> O <sub>6</sub>				
	C <sub>48</sub> H <sub>88</sub> N <sub>8</sub> O <sub>8</sub>	905.6798	922.7063	927.6617	943.6357

Common Background Ions in ESI Negative Mode

Compounds and Species	Ions	Mass of ions
Fragment from acetonitrile	CN <sup>-</sup>	26.0036
Formic acid	HCOO <sup>-</sup>	44.9982
Acetic acid	CH <sub>3</sub> COO <sup>-</sup>	59.0139
Phosphoric acid, and oligonucleotides or phosphopeptides	PO <sub>3</sub> <sup>-</sup>	78.9591
Sulfuric acid and other sulfated materials	SO <sub>3</sub> <sup>-</sup>	79.9574
Methanesulfuric acid	CH <sub>3</sub> SO <sub>3</sub> <sup>-</sup>	94.9808
Sulfuric acid	HSO <sub>4</sub> <sup>-</sup>	96.9601
Phosphoric acid, and oligonucleotides or phosphopeptides	H <sub>2</sub> PO <sub>4</sub> <sup>-</sup>	96.9696
Trifluoroacetic acid, TFA	CF <sub>3</sub> COO <sup>-</sup>	112.9856
Formic acid dimer sodiated anion	[(HCOOH) <sub>2</sub> +Na-2H] <sup>-</sup>	112.9856
Iodine anion (Iodide)	I <sup>-</sup>	126.9050
Pentafluoropropionic acid	CF <sub>3</sub> CF <sub>2</sub> COO <sup>-</sup>	162.9824
n-Butyl benzenesulfonamide	C <sub>10</sub> H <sub>14</sub> NO <sub>2</sub> S <sup>-</sup>	212.0751
Trifluoroacetic acid dimer	CF <sub>3</sub> COOHCF <sub>3</sub> COO <sup>-</sup>	226.9785
Trifluoroacetic acid dimer sodiated anion	[(CF <sub>3</sub> COOH) <sub>2</sub> +Na-2H] <sup>-</sup>	248.9604

Potential Contaminant Ions from Phthalates in ESI Positive Mode, Some Phthalates Form Dimer Ions.

Compounds and Species	Formula	[M+H] <sup>+</sup>	[M+NH <sub>4</sub> ] <sup>+</sup>	[M+Na] <sup>+</sup>	[M+K] <sup>+</sup>
Dimethyl phthalate (DMP)	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	195.0652	212.0917	217.0471	233.0211
Diethyl phthalate (DEP)	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	223.0965	240.1230	245.0784	261.0524
Diallyl phthalate (DAP)	C <sub>14</sub> H <sub>14</sub> O <sub>4</sub>	247.0965	264.1230	269.0784	285.0524
Di-n-propyl phthalate (DPP)	C <sub>14</sub> H <sub>18</sub> O <sub>4</sub>	251.1278	268.1543	273.1097	289.0837
Di-n-butyl phthalate (DBP)	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	279.1591	296.1856	301.1410	317.1150
Diisobutyl phthalate (DIBP)	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	279.1591	296.1856	301.1410	317.1150
Butyl cyclohexyl phthalate (BCP)	C <sub>18</sub> H <sub>24</sub> O <sub>4</sub>	305.1747	322.2012	327.1566	343.1306
Di-n-pentyl phthalate (DNPP)	C <sub>18</sub> H <sub>26</sub> O <sub>4</sub>	307.1904	324.2169	329.1723	345.1463
Dicyclohexyl phthalate (DCP)	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	331.1904	348.2169	353.1723	369.1463
Butyl benzyl phthalate (BBP)	C <sub>19</sub> H <sub>20</sub> O <sub>4</sub>	313.1434	330.1699	335.1253	351.0993
Di-n-hexyl phthalate (DNHP)	C <sub>20</sub> H <sub>30</sub> O <sub>4</sub>	335.2217	352.2482	357.2036	373.1776
Diisohexyl phthalate (DIHP)	C <sub>20</sub> H <sub>30</sub> O <sub>4</sub>	335.2217	352.2482	357.2036	373.1776







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