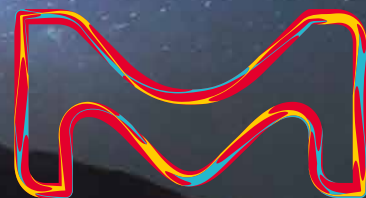


MERCK

Navigate Towards
**Metabolomic
Discovery**



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

Sigma-Aldrich®
Lab & Production Materials

Navigate Towards Metabolomic Discovery

The renaissance of metabolism from molecular physiology to systems medicine requires tools and workflows for obtaining a snapshot of the amount of small molecules present. These low-molecular weight biochemical compounds have been the subject of much classical biochemistry research in the 20th century. The identification of natural substrates and products of enzymatic reactions laid the foundation of metabolic pathway discovery.

Changes in the levels of specific metabolites have been used in routine analysis of healthy and pathological states of humans and animals, but microbial and plant systems benefit as well from the quantification of metabolites. The quantitative and qualitative determination of a larger number of metabolites from a group of related compounds have become possible, primarily through breakthroughs in separation and detection technologies together with the availability of a large number of metabolites. A rapid global analysis can be used as a metabolic fingerprint for phenotype or sample classification. On a more detailed level, workflows for the analysis of specific metabolic pathways and their changes under different experimental conditions are useful for metabolic profiling, with complementary

information to genomic and proteomic studies.

In 1947, Sigma-Aldrich produced the first commercially available form of ATP. Since then, Sigma-Aldrich has consistently expanded its product portfolio to maintain the most comprehensive line of organic metabolites, enzymes, and analytical tools in the world.

Sigma-Aldrich metabolites, enzymes, separation tools and technologies help you navigate the metabolic pathways to biomarker discovery.

The Sigma-Aldrich Metabolomics Resource gives you:

- Nicholson/IUBMB Metabolic Pathways Chart with over 500 links to metabolite, cofactor, and enzyme listings
- High resolution tandem mass spectrometry analysis of select Sigma-Aldrich metabolites from Scripps METLIN Database
- Direct access to 35 Nicholson Metabolic mini-maps
- Animated pathways for teaching and illustration

To get started, visit the Metabolomics Resource at SigmaAldrich.com/metabolomics

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**Sigma-IUBMB Interactive
Metabolic Pathway Tool**



IUBMB-Sigma-Nicholson Interactive Metabolic Pathways Chart

As your partner in discovery, we are here to provide you the products and information that you need to stay on the leading edge of research in metabolomics. This new edition of the iconic IUBMB-Sigma-Nicholson Metabolic Pathways Chart brings increased functionality to a canonical tool. Now, all metabolites, enzymes, and selected pathways are searchable and interactive.

Navigating the Interactive Chart

Colored pins are used to differentiate metabolites from enzymes, red representing metabolites and blue representing enzymes. The pins drop upon searching any of the 1,100 metabolites and enzymes, or their associated pathways. Click the pins to view more information and to see our related products. We hope you enjoy your experience with our new interactive tool.

Key Features and Benefits

- Search any metabolite or enzyme
- Explore the pathways and cycles within the larger picture of metabolism
- Expand pathways and cycles and follow reactions one step at a time

Discover your pathway at SigmaAldrich.com/metpath

TCA Cycle

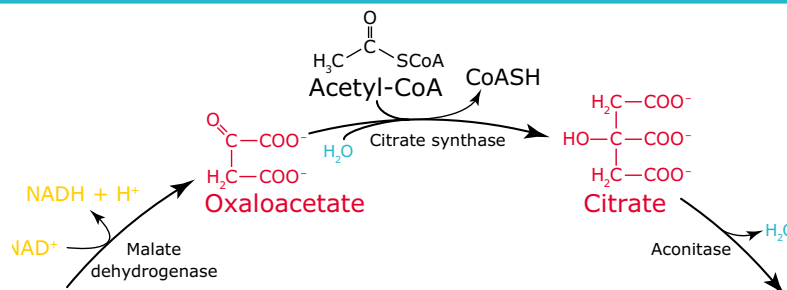
Search

Pathways, metabolites, or enzymes



Explore

Pathways and cycles within the larger picture of metabolism



Expand

Pathways and cycles and follow reactions one step at a time

Search

- Metabolites by CAS number, name, or chemical class
- Enzymes by EC number, name, or enzyme class
- Pathways and cycles including: glycolysis, gluconeogenesis, TCA cycle, pentose phosphate, urea cycle, ketogenesis, and ketolysis

Explore

- New metabolite and enzyme descriptions
- Relevant pathways and related products
- Additional information on the product detail page by clicking on the Sigma-Aldrich Product No.

Acetyl-Coa

Classification: Acyl CoAs

Pathways(s): Glycolysis, TCA Cycle, Lipid metabolism, Glyoxylate Cycle, Ketogenesis, Ketolysis
Synonyms: Acetyl-S-Coa, Acetyl CoA

Acetyl-Coa is an essential cofactor and carrier of acyl groups in enzymatic acetyl transfer reactions. It is formed either by the oxidative decarboxylation of pyruvate in mitochondria, by the oxidation of long-chain fatty acids, or by the oxidative degradation of certain amino acids. Acetyl-Coa is the starting compound for the citric acid cycle (Kreb's cycle). It is also key precursor in lipid biosynthesis, and the source of all fatty acid carbons.

Product Name: Acetyl coenzyme A sodium salt

Product No: A2056

Inborn Errors of Metabolism Chart

Every characteristic of human anatomy and physiology is determined by biochemical reactions catalyzed by enzymes. These in turn are determined by our genetic make-up. If a gene is defective or missing it will result in a defective or missing enzyme, a so-called "inborn error of metabolism." The Inborn Errors of Metabolism Map includes:

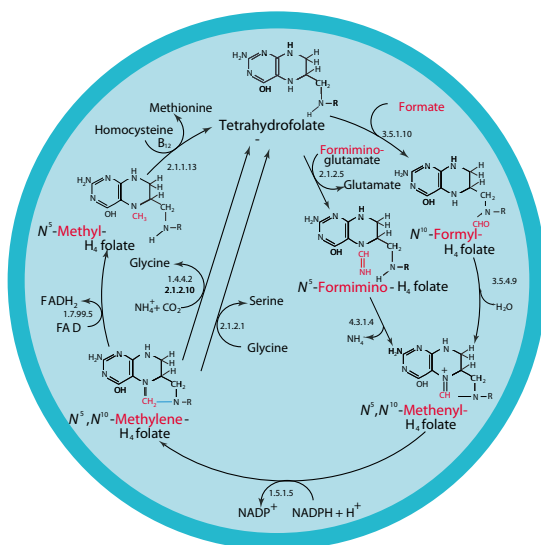
- Over 100 metabolic deficiency diseases which are named on the map

IUBMB-Nicholson Minimaps

Selected individual pathways enlarged to illustrate aspects of metabolism, such as compartmentalization and regulation, expand the information provided by the Metabolic Pathways Chart.

Find the interactive Metabolic Pathways Chart, Minimaps and Animaps at SigmaAldrich.com/metpath

Description	Cat. No.
Inborn Errors of Metabolism, 21st ed. Poster, 22 x 27 in.	I8014
Metabolic Pathways, 22nd Ed. Chart, 12.5 x 19 in.	M3782
Metabolic Pathways, 22nd Ed. Poster, 33 x 50 in.	M3907



ENZYMES

- 1.4.4.2 Glycine dehydrogenase (decarboxylating)
- 1.5.1.3 Dihydrofolate reductase
- 1.5.1.5 Methylene-THF dehydrogenase (NADP⁺)
- 1.7.99.5 5, 10-Methylene-THF reductase (FADH₂)
- 2.1.1.13 5-Methyl-THF-homocysteine S-methyltransferase
- 2.1.1.45 Thymidylate synthase
- 2.1.2.2 Phosphoribosylglycinamide formyltransferase
- 2.1.2.3 Phosphoribosylamidoimidazole-carboxamide formyltransferase
- 2.1.2.5 Glutamate formiminotransferase
- 2.1.2.10 Aminomethyltransferase
- 3.5.1.10 Formyl-THF deformylase
- 3.5.4.9 Methenyl-THF cyclohydrolase
- 4.3.1.4 Formimino-THF cyclodeaminase
- 6.3.3.2 5-Formyl-THF cyclo-ligase
- 6.3.4.3 Formate-tetrahydrofolate ligase

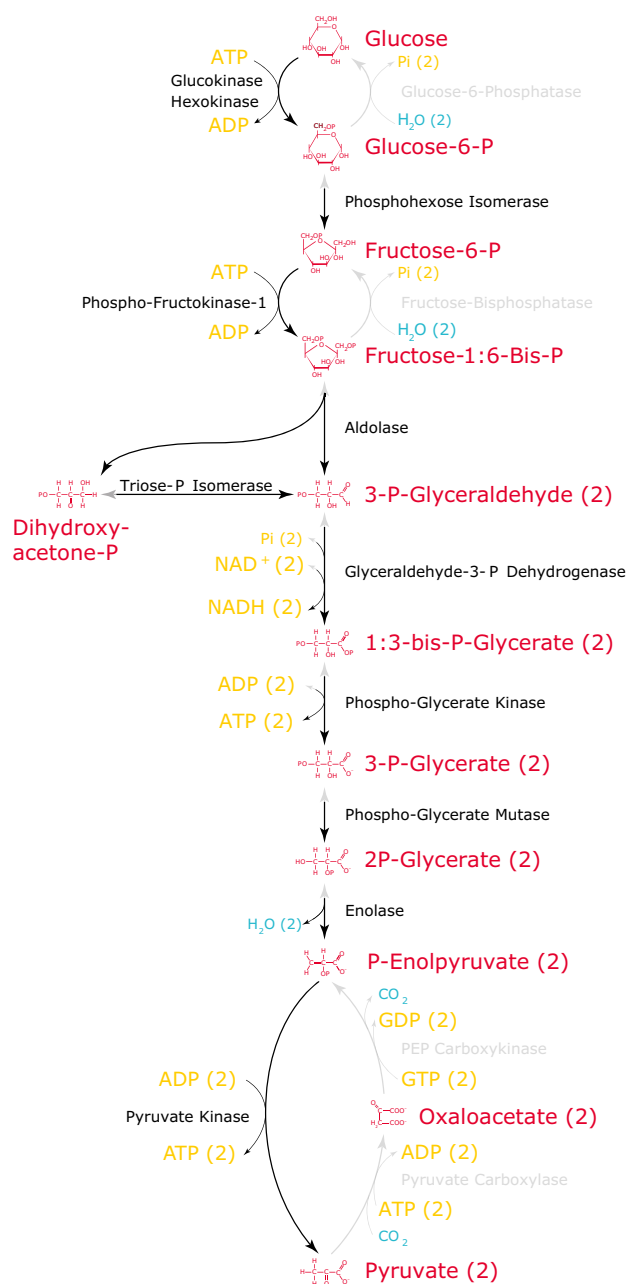
Metabolites, Standards, and Enzymes

Glycolysis Pathway

Glycolysis is the primary pathway that converts glucose into pyruvate. The glycolytic pathway is highly up regulated in rapidly-growing malignant tumor cells, a phenomenon first described by Otto Warburg in 1930. This phenomenon, commonly referred to as the Warburg effect, is a preference for highly proliferatively active cells to shift to aerobic glycolysis even in the presence of adequate oxygen. In aerobic glycolysis, NADH is regenerated through the reduction of pyruvate to lactic acid by lactate dehydrogenase. Enzymes of the glycolytic pathway are potential therapeutic targets for the treatment of cancer.

Glycolysis Metabolites

Description	Cat. No.
2,3-Diphospho-D-glyceric acid pentasodium salt glycolysis metabolite	D5764
D-(-)-3-Phosphoglyceric acid disodium salt ≥ 93%, powder	P8877
D-(+)-Glucose ≥ 99.5% (GC)	G8270
D-(+)-Glucose BioXtra, ≥ 99.5% (GC)	G7528
D-Fructose 1,6-bisphosphate trisodium salt hydrate ≥ 98% (TLC)	F6803
D-Fructose 6-phosphate disodium salt hydrate ≥ 98%, amorphous powder	F3627
D-Glucose 6-phosphate dipotassium salt hydrate Sigma Grade, 98 – 100%	G7375
D-Glucose 6-phosphate disodium salt hydrate Sigma Grade, ≥ 98%	G7250
D-Glucose 6-phosphate potassium salt ≥ 95%	G6526
D-Glucose 6-phosphate sodium salt Sigma Grade, crystalline	G7879
D-Glyceraldehyde 3-phosphate solution 8 – 13 mg/mL in H ₂ O	39705
DL-Glyceraldehyde 3-phosphate solution 45 – 55 mg/mL in H ₂ O	G5251
D-(+)-2-Phosphoglyceric acid sodium salt hydrate ≥ 75% (calc. on dry substance, enzymatic)	79470
Phospho(enol)pyruvic acid monopotassium salt ≥ 97% (enzymatic)	P7127
Phospho(enol)pyruvic acid tri(cyclohexylammonium) salt ≥ 98% (enzymatic)	P7252
Phospho(enol)pyruvic acid trisodium salt hydrate ≥ 97% (enzymatic)	P7002
Sodium pyruvate ReagentPlus®, ≥ 99% (Sigma-Aldrich)	P2256
α-D-Glucose 1-phosphate dipotassium salt hydrate ≥ 97%	G6875
α-D-Glucose 1-phosphate dipotassium salt hydrate BioXtra, ≥ 98%	G6750
α-D-Glucose 1-phosphate disodium salt hydrate ≥ 95%	G1259
α-D-Glucose 1-phosphate disodium salt hydrate ≥ 97%	G7000
α-D-Glucose 1-phosphate disodium salt hydrate ≥ 98%, BioXtra, lyophilized powder	G7018
α-D-Glucose 1-phosphate disodium salt hydrate 98 – 99%	G9380
β-D-Glucose 1-phosphate bis(cyclohexylammonium) salt	G7920



Key Glycolytic Enzymes

Description	Cat. No.
Aldolase from rabbit muscle ammonium sulfate suspension, 10–20 units/mg protein	A8811
Creatine Phosphokinase from rabbit muscle Type I, salt-free, lyophilized powder, ≥ 150 units/mg protein	C3755
Enolase from baker's yeast (<i>S. cerevisiae</i>) lyophilized powder, ≥ 50 units/mg protein	E6126
Fructose-6-phosphate Kinase from <i>Bacillus stearothermophilus</i> Type VII, lyophilized powder, ≥ 50 units/mg protein	F0137
Glyceraldehyde-3-phosphate Dehydrogenase from rabbit muscle lyophilized powder, ≥ 75 units/mg protein	G2267
α-Glycerophosphate Dehydrogenase-Triosephosphate Isomerase from rabbit muscle Type III, ammonium sulfate suspension, TPI 750–2,000 units/mg protein, GDH 75–200 units/mg protein (biuret)	G1881
Hexokinase from <i>Saccharomyces cerevisiae</i> Type F-300, lyophilized powder, ≥ 130 units/mg protein (biuret)	H4502
Invertase from baker's yeast (<i>S. cerevisiae</i>) Grade VII, ≥ 300 units/mg solid	I4504
L-Lactic Dehydrogenase from rabbit muscle Type II, ammonium sulfate suspension, 800–1,200 units/mg protein	L2500
L-Lactic Dehydrogenase from rabbit muscle Type XI, lyophilized powder, 600–1,200 units/mg protein	L1254
Phosphoglucose Isomerase from baker's yeast (<i>S. cerevisiae</i>) Type III, ammonium sulfate suspension, ≥ 400 units/mg protein (biuret)	P5381
3-Phosphoglyceric Phosphokinase from baker's yeast (<i>S. cerevisiae</i>) ammonium sulfate suspension, ≥ 1,000 units/mg protein	P7634
Pyruvate Kinase from rabbit muscle Type III, lyophilized powder, 350–600 units/mg protein	P9136
Triosephosphate Isomerase from rabbit muscle Type X, lyophilized powder, ≥ 3,500 units/mg protein	T6258

Tricarboxylic acid (TCA) Cycle

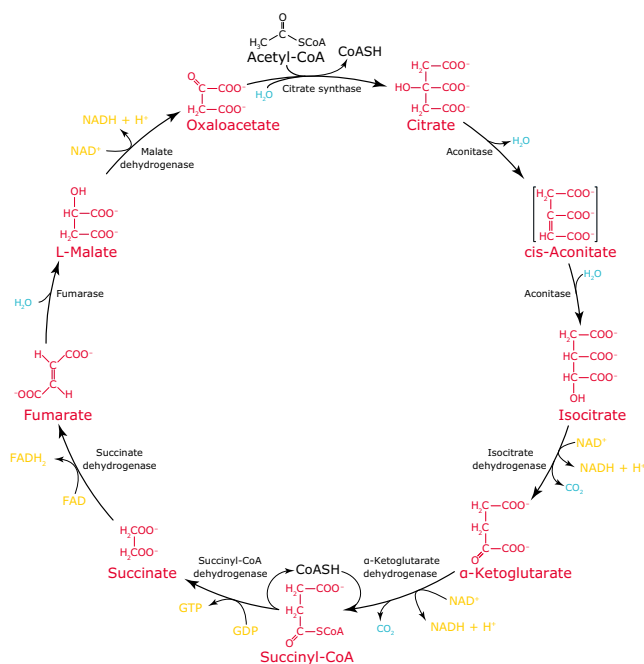
The Citric acid (TCA or Krebs) Cycle is the origin and the termination of many Metabolic Pathways. It harnesses the potential energy of Acetyl-CoA into the reducing power of NADH.

TCA Cycle Metabolites

Description	Cat. No.
TCA Cycle Metabolite Library	ML0010
Acetyl coenzyme A sodium salt, ≥ 93% (HPLC)	A2056
Citric acid monohydrate, reagent grade, ≥ 98% (GC/titration)	C7129
Sodium fumarate dibasic, ≥ 99%	F1506
DL-Isocitric acid trisodium salt hydrate, ≥ 93%	I1252
L-(–)-Malic acid, 95–100% (enzymatic)	M1000
Oxaloacetic acid, ≥ 97%	O4126
Sodium pyruvate, ReagentPlus®, ≥ 99%	P2256
Succinyl coenzyme A sodium salt, ≥ 85%	S1129
Sodium succinate dibasic hexahydrate, ReagentPlus®, ≥ 99%	S2378
α-Ketoglutaric acid disodium salt hydrate, analytical standard	K3752

Key TCA Cycle Enzymes

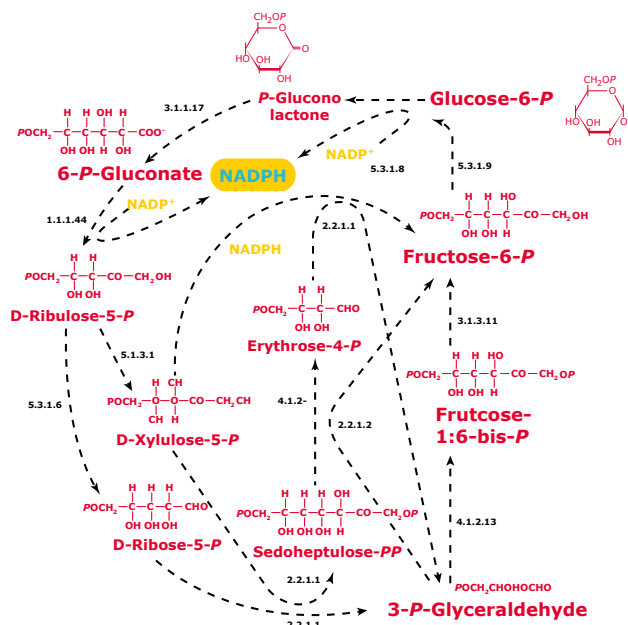
Description	Cat. No.
Malic Dehydrogenase from porcine heart buffered aqueous glycerol solution, 600–1,000 units/mg protein (biuret)	M2634
α-Ketoglutarate Dehydrogenase from porcine heart buffered aqueous glycerol solution, 0.1–1.0 units/mg protein (Lowry)	K1502
Citrate Synthase from porcine heart ammonium sulfate suspension, ≥ 100 units/mg protein	C3260
Fumarase from porcine heart ammonium sulfate suspension, 300–500 units/mg protein (biuret)	F1757
Aconitase from porcine heart	A5384



Pentose Phosphate Pathway

While glucose metabolism by glycolysis occurs where energy is needed quickly, e.g. in brain and muscle cells, a second pathway for glucose metabolism, called pentose phosphate pathway, operates in tissues that synthesize fatty acids and steroids.

Description	Cat. No.
D-Glyceraldehyde 3-phosphate solution	39705
D-Sedoheptulose 7-phosphate lithium salt	78832
Adenosine 5'-triphosphate disodium salt hydrate	A2383
Adenosine 5'-diphosphate sodium salt	A2754
Dihydroxyacetone phosphate dilithium salt	D7137
D-Erythrose 4-phosphate sodium salt	E0377
D-Fructose 6-phosphate disodium salt hydrate	F3627
D-Fructose 1,6-bisphosphate trisodium salt hydrate	F6803
D-Glucose 6-phosphate sodium salt	G7879
β -Nicotinamide adenine dinucleotide phosphate sodium salt hydrate	N0505
β -Nicotinamide adenine dinucleotide 2'-phosphate reduced tetrasodium salt hydrate	N7505
6-Phosphogluconic acid trisodium salt	P7877
5-Phospho-D-ribose 1-diphosphate pentasodium salt	P8296
D-(-)-Ribose	R7500
D-Ribose 5-phosphate disodium salt hydrate	R7750
D-Ribulose 5-phosphate sodium salt	R9875
D-Xylulose 5-phosphate sodium salt	X0754



Key Pentose Phosphate Pathway Enzymes

Description	Cat. No.
6-Phosphogluconic Dehydrogenase from yeast lyophilized powder, 3.0–6.0 units/mg solid	P4553
Glucose-6-phosphate Dehydrogenase from baker's yeast (<i>S. cerevisiae</i>) Type XV, lyophilized powder, 200–400 units/mg protein (modified Warburg-Christian)	G6378
Transketolase from <i>E. coli</i> ≥ 0.1 units/mg	68138
Transaldolase from baker's yeast (<i>S. cerevisiae</i>) lyophilized powder, 10–30 units/mg protein (biuret)	T6008
Hexokinase from <i>Saccharomyces cerevisiae</i> Type F-300, lyophilized powder, ≥ 130 units/mg protein (biuret)	H4502
Aldolase from rabbit muscle ammonium sulfate suspension, 10–20 units/mg protein	A8811
D-Ribulose-5-phosphate 3-Epimerase from baker's yeast (<i>S. cerevisiae</i>) lyophilized powder, 50–100 units/mg protein (modified Warburg-Christian)	R3251
Triose-phosphate isomerase/Triosephosphate Isomerase from rabbit muscle Type X, lyophilized powder, $\geq 3,500$ units/mg protein	T6258
Phosphoriboisomerase from spinach Type I, partially purified powder, ≥ 75 units/mg protein (biuret)	P9752
Phosphoglucose Isomerase from baker's yeast (<i>S. cerevisiae</i>) Type III, ammonium sulfate suspension, ≥ 400 units/mg protein (biuret)	P5381

For a comprehensive list of pathway metabolites, visit SigmaAldrich.com/metpath

Metabolite Libraries and Kits

The **ML0100 TCA Cycle Metabolite Library** provides all 10 components of the Krebs's Cycle in one convenient format.

TCA Cycle Metabolite Library

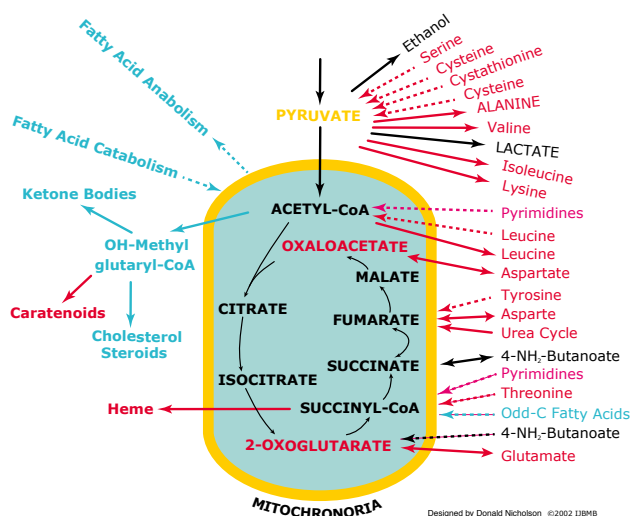
All components are directly water soluble at ≥ 50 mg/mL.

Components

Acetyl coenzyme A (Sigma A2056) 10 mg
 Citric acid (Sial C7129) 10 mg
 Sodium fumarate dibasic (Sigma F1506) 10 mg
 DL-Isocitric acid (Sigma I1252) 10 mg
 L-(-)-Malic acid (Sigma M1000) 10 mg
 Oxaloacetic acid (Sigma O4126) 10 mg
 Sodium pyruvate (Sial P2256) 10 mg
 Succinyl coenzyme A (Sigma S1129) 10 mg
 Sodium succinate (Sial S2378) 10 mg
 store at: -20°C

ML0100-1KT

1 kit



Name	Description	Cat. No.
Vitamins Kit ~98% (Components, TLC)	11 Vitamins in quantities as indicated: p-Aminobenzoic acid, 5 g; d-Biotin, 100 mg; Folic acid, 1 g; Niacinamide, 100 g; D-Pantothenic acid, hemicalcium salt, 5 g; Pyridoxal hydrochloride, 500 mg; Pyridoxamine dihydrochloride, 250 mg; Pyridoxine hydrochloride, 5 g; Riboflavin, 5 g; Thiamine hydrochloride, 5 g; DL-6,8-Thioctic acid, 500 mg	V1

Carbohydrate Metabolite Kits

Name	Description	Cat. No.
Carbohydrates Kit	Ten carbohydrates, 5 g of each, contains: Arabinose, Fructose, Galactose, Glucose, α -Lactose, Maltose, Mannose, Ribose, Sucrose and Xylose	CAR10
Sugar Alcohol Kit	Nine sugar alcohols, 500 mg of each, contains: D-(+)Arabitol, Dulcitol (Galactitol), iso-Erythritol, Glycerol, Maltitol, D-Mannitol, Ribitol (Adonitol), D-Sorbitol, and Xylitol	47266
Monosaccharides Kit	Seven monosaccharides, 500 mg of each, contains: D-(+)Glucose, mixed anomers, D-(-)Arabinose, Fructose, D-(+)Galactose, D-(+)Mannose (mixed anomers), D-(-)Ribose, and D-(+)Xylose	47267
Disaccharides Kit	Contains disaccharides in quantities indicated: Maltose 500 mg, Sucrose 500 mg, Isomaltose (mixed anomers) 100 mg, and α -Lactose 500 mg	47268-U

Amino Acids Kits

Name	Description	Cat. No.
L-Amino Acids analytical standard	Contains 21 L-Amino Acids plus glycine, 1 g of each	LAA21
L-Amino Acids analytical standard	Contains the 10 Essential Amino Acids, 1 g of each	LAA10
Amino acid Standard analytical standard	Amino Acids in this standard are 2.5 µmoles per mL in 0.1 N HCl, except L-cystine at 1.25 µmoles per mL	AAS18
Amino acid standards, physiological analytical standard, acidics and neutrals	Amino Acids in this standard are 2.5 µmoles per mL except L-cystine at 1.25 µmoles per mL	A6407
Amino acid standards, physiological analytical standard, acidics, neutrals, and basics	Amino Acids and related compounds are 0.5 µmole/mL in 0.2 N lithium citrate, pH 2.2 containing 0.1% phenol and 2% thiodiglycol	A9906
Amino acid standards, physiological analytical standard, basics	This solution contains physiological, basic Amino Acids and related compounds for calibration of amino acid analyzers. Amino Acids and related compounds are at 2.5 mmols/mL ± 4% in 0.1 N HCl	A6282

Fatty Acids & Lipid Metabolite Kits

Name	Cat. No.
Fatty Acid Kit (individually packaged, quantities indicated), analytical standard	EC10A-1KT
Fatty Acids, Odd Carbon Straight Chains Kit (individually packaged in quantities indicated), analytical standard	OC9-1KT
Fatty Acids Unsaturated Kit (individually packaged in quantities indicated), analytical standard	UN10-1KT
Triglycerides Kit (individually packaged in quantities indicated), analytical standard	TRI19-1KT
Triglycerides, Saturated, Even Carbon Kit (individually packaged in quantities indicated), analytical standard	TRI11-1KT

LC-MS Certified Spiking Solutions and Reference Materials

Single and multi-component solution standards (both stable-labeled and unlabeled) designed, manufactured and tested specifically for use as reference standards for laboratories performing bioanalysis, therapeutic drug monitoring, diagnostic and toxicology testing.

Cerilliant®'s products address the stringent and complex requirements of forensic toxicology, clinical toxicology, clinical chemistry/immunoassay, therapeutic drug monitoring, pain management and pharmaceutical analysis. Products manufactured at Cerilliant® are fully documented through the use of batch records to provide traceability of materials used, traceability of equipment utilized, calibration records, and detail of all work performed and staff utilized, all backed by a comprehensive Certificate of Analysis. Cerilliant®'s quality credentials include accreditations to ISO Guide 34, ISO/IEC 17025 and certification to ISO 13485 and ISO 9001. Cerilliant®'s quality system incorporates cGMP and GLP requirements.

Cerilliant® CRM portfolio includes:

Catalog and Custom

- Metabolites including P450 and Glucuronides
- Impurities/Degradants
- Internal Standards
- Many analyte classes, including
 - Drugs/Drugs of Abuse
 - TDM Drugs/Immunosuppressants/Catecholamines
 - Hormones including Thyroid/Steroids – Alcohol/Ethanol
 - Vitamins (A, B, D and E)
 - Natural Products/Phytochemicals



For a complete listing of Cerilliant® certified standards, visit [SigmaAldrich.com/cerilliant](https://www.sigmaaldrich.com/cerilliant)

Mass Spectrometry Metabolite Library

Supplied by IROA Technologies

MSMLS™ (Mass Spectrometry Metabolite Library of Standards) and LSMLS™ (Large Scale Metabolite Library of Standards) are a collection of high quality small biochemical molecules that span a broad range of primary metabolism. These are high purity (>95%) compounds supplied in an economical, ready-to-use format. The library of standards are most commonly used to provide retention times and spectra for key metabolic compounds, help optimize mass spectrometry analytical protocols, qualify and quantify mass spectrometry sensitivity and NMR, functional cellular assays, phenotypic screening and limit of detection.

Features and Benefits

Compounds

Unique small molecule metabolites organized in a 96-well format according to solubility. Broad metabolite spectrum, key primary metabolites and intermediates covering key metabolic pathways, including the following classes of compounds:

- Carboxylic acids, amino acids
- Biogenic amines, polyamines
- Nucleotides, coenzymes and vitamins
- Mono- and disaccharides
- Fatty acids, lipids, steroids, and hormones

MSMLS™ features 619 unique metabolites as 5 µg dried weight

LSMLS™ features 504 unique metabolites as 1 mg dried weight

Convenient

- High purity metabolites, pre-weighed, solubilized in either water, 40 % aqueous methanol or 100 % ethanol and supplied dried
- The library is intended to be used for mass spectrometry metabolomics applications and provides a broad representation of primary metabolites
- Suitable for manual and automated work flow

MSMLSDiscovery™ software tool is provided to support the extraction, manipulation, and storage of the data generated when using the MSMLS™ and LSMLS™ Library of Metabolite Standards.



Ordering Information

Description	Cat. No.
Mass Spectrometry Metabolite Library	MSMLS-1EA
Large Scale Metabolite Library	LSMLS-1EA

For more information, visit SigmaAldrich.com/MSMLS



Lipid Sample Preparation Kits

Isolate, Methylate, and Purify

Lipid and Sterol Extraction Kits

The Folch method of lipid and sterol extraction is an effective but time-consuming procedure. Our Lipid Extraction Kit and Sterol Extraction Kit provide an isolation method that is high-throughput, simpler, faster, and less costly than conventional techniques, such as the Folch method, but still yield the same high-quality results.

Features and Benefits

- **No centrifugation or pipetting required** – Extract compounds in two steps: Pour and Push
- **Solvents and internal standards come pre-mixed** – Eliminate the need to prepare solvents and standards
- **Less than 30 seconds per sample** – Reduce your labor costs and save your valuable time
- **High-throughput** – Cut cost and time without sacrificing yield

Ordering Information

Description	Cat. No.
Fatty acid Extraction Kit	MAK174-1KT
Sterol Extraction Kit	MAK175-1KT

Get the Same High-quality Results in Less Time

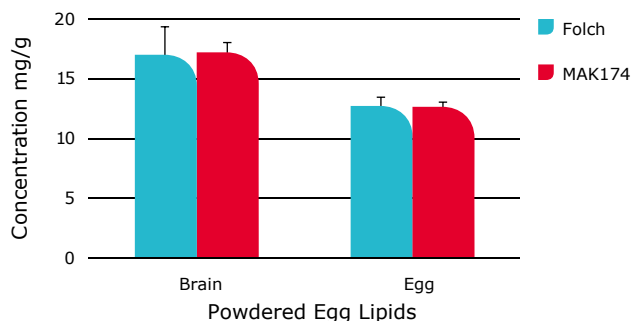


Figure 1: Rat brain fatty acid concentrations (mg/g)
Lipids were extracted from rat brain with the Folch or MAK174 kit method, transesterified, and quantified with GC-FID.

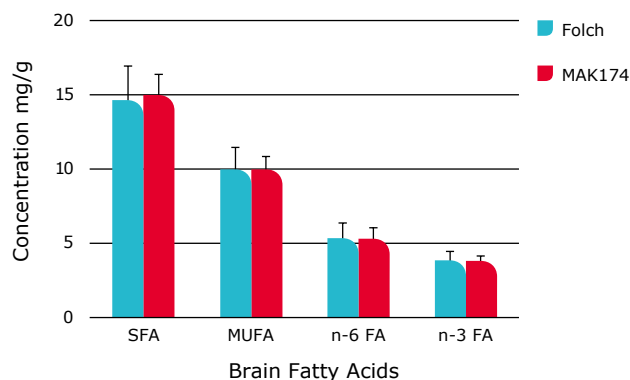


Figure 2: Rat brain and powdered egg cholesterol concentrations (mg/g)
Lipids were extracted with the Folch or MAK175 kit method, saponified, derivitized, and quantified with GC-FID.

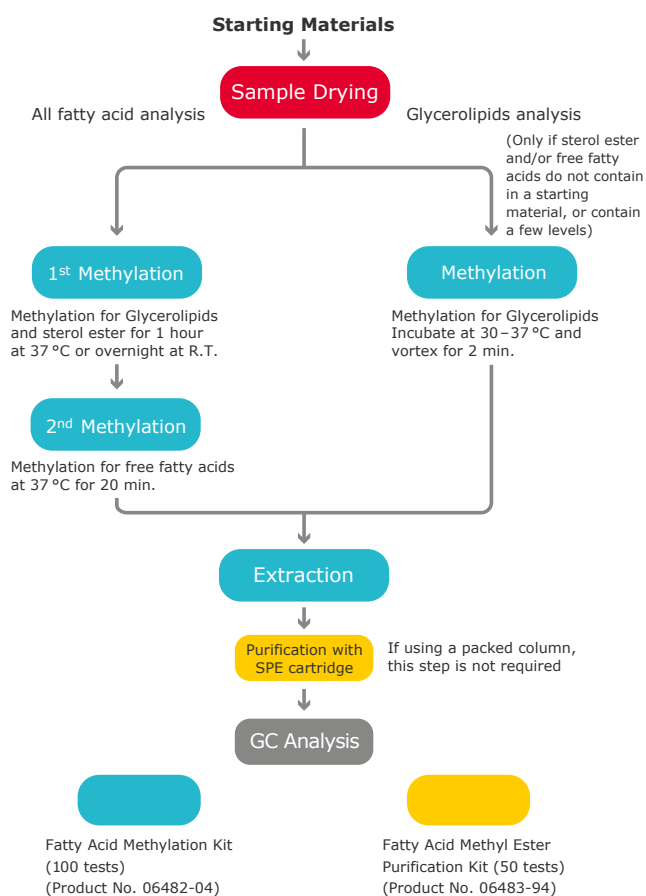
Fatty acid Methylation and Purification Kits

Manufactured by Nacalai Tesque, Inc.

Methyl esterification of fatty acids is commonly performed prior to gas chromatography analysis to prevent peak tailing and to increase sample volatility. However, the conventional esterification procedure requires specialized equipment and high technical skill. Preparation of methyl ester derivatives is often poorly understood and unnecessarily vigorous reaction conditions are often employed.

By using the Fatty acid Methylation Kit (MAK224) that utilizes a new reaction technique, followed by the Fatty acid Methyl Ester Purification Kit (MAK225), fatty acid methyl esterification is greatly simplified.

General Procedure



Features and Benefits

No excessive heating – Can be performed safely and easily

Reaction is conducted at 37 °C

Detects long-chain and short-chain fatty acids

Applicable for free fatty acids and glycerolipids, such as triglycerides, phospholipids, glycolipids and sterol esters

Ordering Information

Description	Cat. No.
Fatty acid Methylation Kit	MAK224-1KT
Fatty acid Methyl Ester Purification Kit	MAK225-1KT

Comparison of Methylation Efficiency Rate

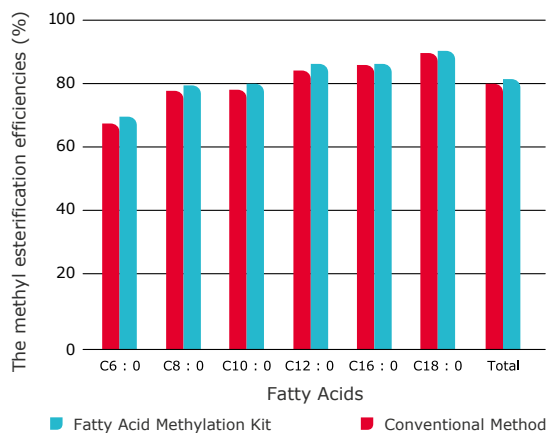


Figure 1: The methyl esterification efficiencies between the Fatty acid Methylation Kit and a conventional method using different fatty acid side-chains.

Supel™ Select Polymeric SPE Products

Key Features and Benefits

- Hydrophilic-modified styrene resin extracts and recovers a broad range of analytes (polar to nonpolar, acidic to basic) using a single sorbent
- Generic methodology saves time, money, and headaches during method development
- Greater capacity allows for smaller bed weights = smaller elution volumes = time savings in sample processing
- Resistant to over-drying allowing for more robust methodology

Versatile and Simple Sample Cleanup by SPE

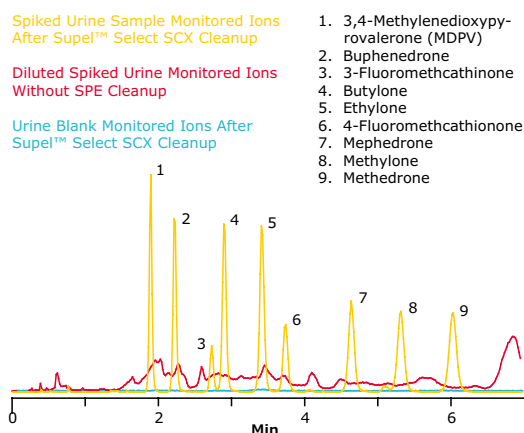
Supel™ Select SPE phases are ideal for the solid phase extraction (SPE) of a broad range of compounds from aqueous samples. While reversed-phase interactions dominate retention on the Supel™ Select HLB, and the retention mechanisms of the Supel™ Select SAX and SCX are predominately based on ion-exchange, the hydrophilic modifications of the styrene-based polymer backbone allow for retention and recovery of more polar compounds.

Supel™ Select Properties	
HLB Phase Chemistry	Hydrophilic-modified styrene polymer
SAX Phase Chemistry	Quaternary amine-functionalized hydrophilic-modified styrene polymer
SCX Phase Chemistry	Sulfonic acid-functionalized hydrophilic modified styrene polymer
Suitable for MS Detection?	Yes
pH Compatibility	0 – 14
Particle Size	50 – 70 µm
Surface Area	160 – 420 m ² /g
Pore Volume	0.8 – 1.2 mL/g
Pore Size	80 – 200 Å

Name	Description	Quantity	Cat. No.
Supel™ Select HLB 96-well SPE	10 mg/well	1	Inquire
	30 mg/well	1	575661-U
	60 mg/well	1	575662-U
Supel™ Select SAX 96-well SPE	10 mg/well	1	Inquire
	30 mg/well	1	575660-U
	60 mg/well	1	575663-U
Supel™ Select SCX 96-well SPE	10 mg/well	1	Inquire
	30 mg/well	1	575664-U
	60 mg/well	1	575665-U

LC-MS Analysis of Illicit Bath Salts in Urine on Ascentis® Express HILIC with and without Supel™ Select SCX SPE Cleanup

SPE tube: Supel™ Select SCX, 30 mg/1 mL (54240-U)
 column: Ascentis® Express HILIC, 10 cm × 2.1 mm I.D., 2.7 µm (53939-U)
 mobile phase: (A) 5 mM ammonium formate acetonitrile; (B) 5 mM ammonium formate water; (98:2, A:B) (solvents and additives LC-MS Ultra CHROMASOLV® grade)
 flow rate: 0.6 mL/min
 pressure: 127 bar
 column temp: 35 °C
 detector: MS, ESI+, 100 – 1,000 m/z
 injection: 1 µL
 sample: 200 ng/mL in acetonitrile (standards from Cerilliant®)



Name	Description	Quantity	Cat. No.
Supel™ Select HLB SPE	30 mg/1 mL	100	54181-U
	60 mg/3 mL	50	54182-U
	200 mg/6 mL	30	54183-U
	500 mg/12 mL	20	54184-U
	1 g/20 mL	20	54186-U
Supel™ Select SAX SPE	30 mg/1 mL	100	54231-U
	60 mg/3 mL	50	54233-U
	200 mg/6 mL	30	54235-U
	500 mg/12 mL	20	54236-U
	1 g/20 mL	20	54237-U
Supel™ Select SCX SPE	30 mg/1 mL	100	54240-U
	60 mg/3 mL	50	54241-U
	200 mg/6 mL	30	54242-U
	500 mg/12 mL	20	54243-U
	1 g/20 mL	20	54245-U

For more information, visit [SigmaAldrich.com/supel-select](https://www.sigmaaldrich.com/supel-select)

HybridSPE®-Phospholipid Products for Consistent LC-MS Ionization

Key Features and Benefits

- Maximize sensitivity by minimizing ion-suppression
- 100 % removal of phospholipids and precipitated proteins
- 2 – 3 step generic procedure
- Ideal for high-throughput pre-clinical and clinical studies

Ion-Suppression and Phospholipid Contamination

When analyzing a compound and its metabolites in biological fluids, such as plasma or serum, one frequently deals with interference from the complex sample matrix. Ion-suppression of the mass spec signal due to contaminants in the matrix often limits our ability to properly identify and quantify the analytes of interest. The presence of phospholipids in biological fluids is one of the major causes of ion-suppression in LC-MS when using positive ion electrospray mode (+ESI). Removing phospholipids with HybridSPE®-Phospholipid is a rapid and reliable means to improve identification and quantification of compounds in biological matrices using LC-MS.

How Does HybridSPE®-Phospholipid Work?

Sample preparation with HybridSPE®-Phospholipid is a very rapid and simple procedure. Proteins in the

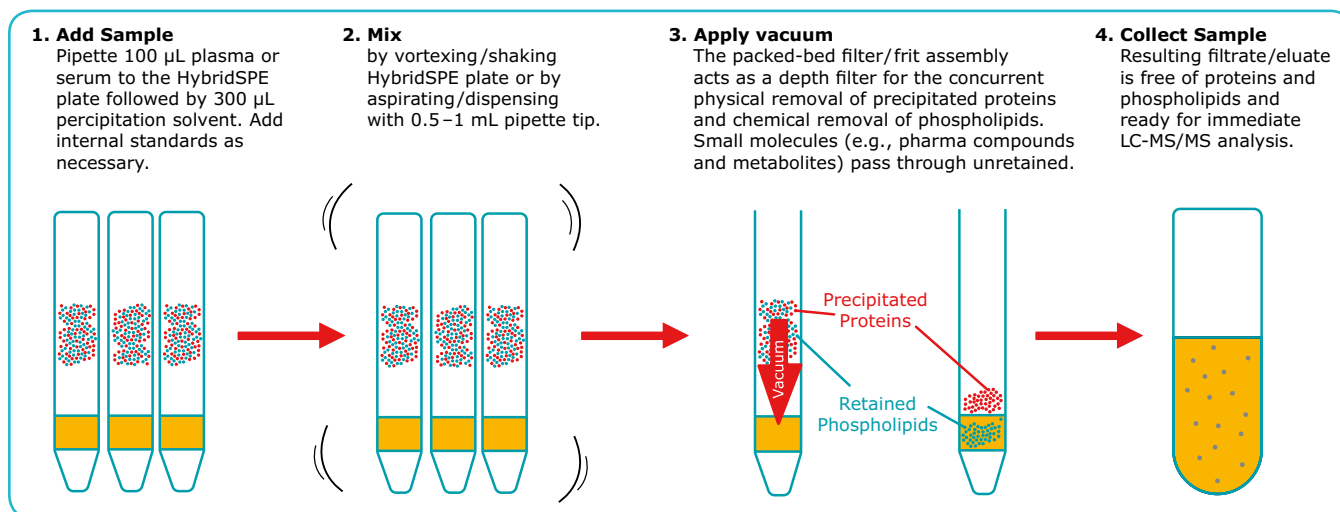
sample are precipitated by addition of acetonitrile containing 1 % formic acid. The sample is then added to the HybridSPE®-Phospholipid packed bed, either well plate or tube format. As shown in the accompanying figure, the bed consists of proprietary zirconia-coated silica particles. The zirconia sites exhibit Lewis acid (electron acceptor) properties that will interact strongly with Lewis bases (electron donors).

Phospholipids structurally consist of a polar head group (zwitterionic phosphonate moiety) and a large hydrophobic tail (two hydrophobic fatty acyl groups). The phosphonate group acts as a very strong Lewis base that interacts strongly with zirconia. Formic acid in the precipitation solvent is a critical modifier used to improve the recovery of many analytes of interest (particularly acidic compounds) by preventing analyte retention, while not affecting phospholipid removal.

The HybridSPE®-Phospholipid sample preparation products are available in several configurations.

- Two 96-well plate formats for sample volumes of ~100 µL and 20 – 40 µL. Both formats allow for in-well precipitation.
- Three SPE tube formats; the ultra version allows for in-tube protein precipitation.

For more information and to view a video of HybridSPE®-Phospholipid in operation, visit SigmaAldrich.com/hybridspe

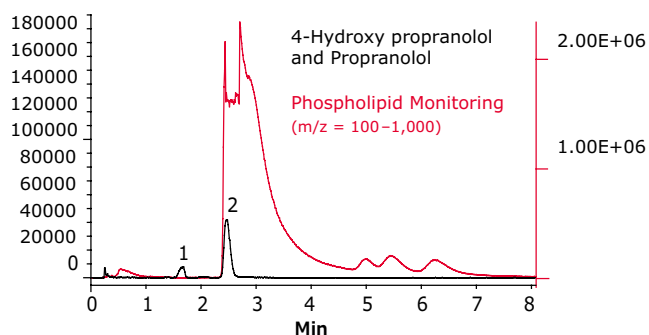


Ion-Suppression from Phospholipids: Standard Protein Precipitation vs. HybridSPE®-Phospholipid

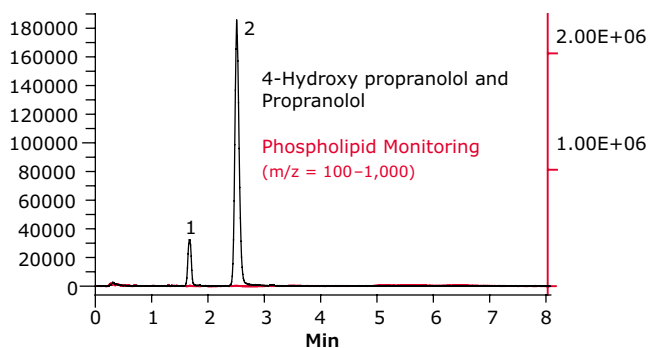
Sample prep	standard protein precipitation or HybridSPE®-Phospholipid (575656-U)
Column	Ascentis® Express F5, 5 cm × 2.1 mm I.D., 2.7 μm (53567-U)
Mobile phase	(A) 2 mM ammonium formate in acetonitrile; (B) 2 mM ammonium formate in water; (90:10, A:B)
Flow rate	0.4 mL/min
Pressure	1073 psi
Column temp	35 °C
Detector	MS, ESI(+) TOF, m/z = 100–1,000
Injection	2 μL
Sample	Agilent® 1200SL Rapid Resolution; 6210 Time of Flight (TOF) MS
System	Agilent® 1200SL Rapid Resolution; 6210 Time of Flight (TOF) MS

Standard Protein Precipitation Technique

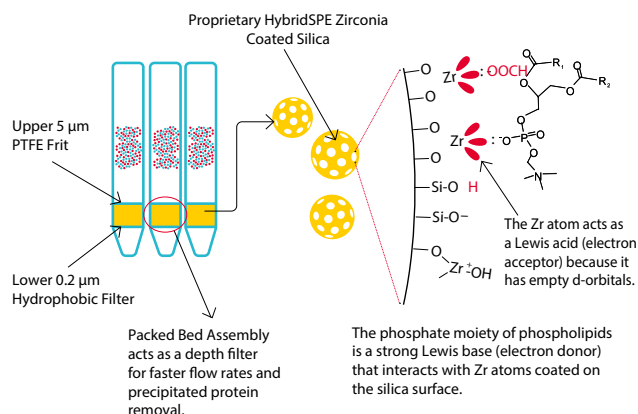
(Note suppression of propranolol signal)



HybridSPE®-Phospholipid Technique



Interaction of Phospholipids with HybridSPE®-Phospholipid



Featured Products

Name	Qty.	Cat. No.
HybridSPE®-Plus Plate Essentials Kit		
Includes HybridSPE®-Plus 96-well plate (575659-U), plate cap mat (as in 575680-U), sealing film (as in Z721581) and collection plate (as in Z717266)	1	52818-U
HybridSPE®-Plus 96-Well Plates		
50 mg/well	1	575659-U
	20	575673-U
HybridSPE®-Phospholipid Small Volume 96-Well Plates		
5 mg/well	1	52794-U
	20	52798-U
HybridSPE®-Phospholipid Cartridges		
HybridSPE®-Phospholipid Ultra Cartridge, 30 mg/1 mL	100	55269-U
HybridSPE®-Phospholipid Cartridge, 500 mg/6 mL	30	55267-U
HybridSPE®-Phospholipid Cartridge, 30 mg/1 mL	100	55261-U
	200	55276-U

Protein Precipitation

96-Well Protein Precipitation Filter Plate The 96-well protein precipitation filter plate is ideal for removing precipitated proteins from biological plasma/serum. The plate consists of a 0.2 μm hydrophobic graded filter/frit. Biological plasma is first added to the 96-well plate followed by a protein precipitating agent (e.g., acetonitrile). After a brief mixing step, vacuum is applied to the plate, and the filter/frit removes precipitated proteins from the sample. The resulting filtrate is ready for further processing and/or analysis.

Description	Qty.	Cat. No.
2 mL	1 ea.	55263-U

SupelMIP® Molecularly Imprinted Polymers

Key Features and Benefits

- Achieve lower detection limits through superior selectivity
- Reduce ion-suppression
- Save time and reduce cost via robust and rapid sample prep methodology
- Minimal to no method development required

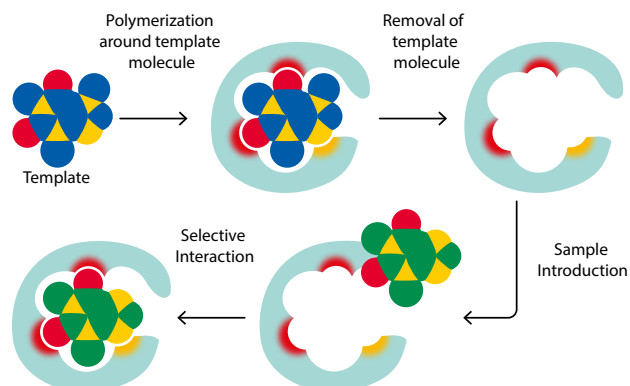
Highly Selective Extraction of Trace Analytes from Complex Matrices

Molecularly imprinted polymers (MIPs) are a class of highly crosslinked polymer-based molecular recognition elements engineered to bind one target compound or a class of structurally related target compounds with high selectivity. Selectivity is introduced during MIP synthesis in which a template molecule, designed to mimic the analyte, guides the formation of specific cavities or imprints that are sterically and chemically complementary to the target analyte.

SupelMIPs® are available for these analyte and matrix combinations

Analytes	Matrix
Chloramphenicol	Milk, plasma, honey, urine, and shrimp/prawns
Clenbuterol	Urine
Fluoroquinolones	Bovine kidney, honey, and milk
PAHs	Edible oils
Riboflavin (Vitamin B2)	Milk
β-Agonists and/or β-Blockers	Tissue, urine and wastewater
TSNAs (4 Different Tobacco-Specific Nitrosamines: NNK, NNN, NAB, NAT)	Urine and tobacco
NNAL (4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol)	Urine

Formation of MIPs



SupelMIP® Molecularly Imprinted Polymer SPE Tubes

Description	Pack Sizes	Cat. No.
SupelMIP® SPE – β-agonists, bed wt. 25 mg, volume 3 mL	50	53225-U
SupelMIP® SPE – β-agonists, bed wt. 25 mg, volume 10 mL	50	53202-U
SupelMIP® SPE – Chloramphenicol, bed wt. 25 mg, volume 3 mL	50	53209-U
SupelMIP® SPE – Chloramphenicol, bed wt. 25 mg, volume 10 mL	50	53210-U
SupelMIP® SPE – Clenbuterol, bed wt. 25 mg, volume 10 mL	50	53201-U
SupelMIP® SPE – Fluoroquinolones, bed wt. 25 mg, volume 3 mL	50	53269-U
SupelMIP® SPE – Full β-receptor (β-blockers and β-agonists), bed wt. 25 mg, volume 3 mL	50	53224-U
SupelMIP® SPE – Full β-receptor (β-blockers and β-agonists), bed wt. 25 mg, volume 10 mL	50	53223-U
SupelMIP® SPE – Riboflavin (vitamin B ₂), bed wt. 25 mg, volume 10 mL	50	53207-U
SupelMIP® SPE – TSNAs, bed wt. 50 mg, volume 3 mL	50	53222-U
SupelMIP® SPE – TSNAs, bed wt. 50 mg, volume 10 mL	50	53221-U
SupelMIP® SPE – NNAL, bed wt. 25 mg, volume 3 mL	50	53203-U

ZipTip® Pipette Tips: Proteomics Sample Prep in Seconds

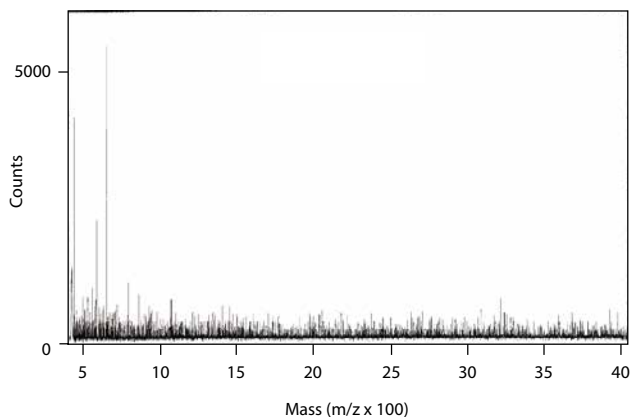


A staple of every mass spectrometry lab, ZipTip® is a 10 µL pipette tip with a 0.6 or 0.2 µL bed of chromatography media fixed at its end with no dead volume. It is ideal for concentrating and purifying peptides or proteins in seconds prior to mass spectrometry, HPLC, and capillary electrophoresis. The ZipTip® pipette tip provides a reproducible, high recovery method for concentrating, purifying or even fractionating femtomoles to picomoles of peptides, proteins and oligonucleotides for improved data quality.

ZipTip® Advantages:

- Single-step desalting, concentration, and purification
- Fractionate complex samples for more meaningful data
- Ideal for peptides, proteins, nucleic acids, and more
- No dead volume for maximum recovery
- Eliminates time-consuming chromatography

A. Direct Spotting



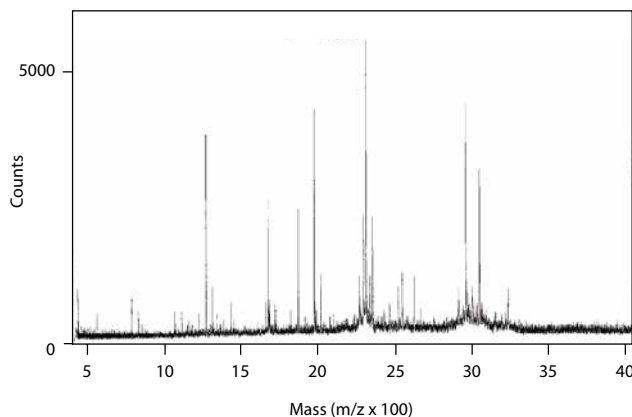
The ZipTip® pipette tip is simple and easy to use

- Place the tip on a single- or multi-channel pipettor, standard 22-gauge blunt-end HPLC needle, or compatible automated liquid handling/sample preparation station
- For sample binding, aspirate and dispense through the media several times
- Similarly, aspirate and dispense appropriate wash solvent to remove contaminants
- The concentrated, purified sample is eluted in 1–4 µL of compatible solvent with direct transfer to a mass spectrometer target, vial, or other analysis step

For applications requiring smaller elution volumes (e.g., < 1 µL), a micro-bed format containing 0.2 µL of media is available

Description	Qty / Pkg	Cat. No.
ZipTip® Pipette Tips		
ZipTip® with 0.6 mL strong cation resin	8	ZTSCXS008
ZipTip® with 0.6 mL strong cation resin	96	ZTSCXS096
ZipTip® with 0.6 mL C4 resin	8	ZTC04S008
ZipTip® with 0.6 mL C4 resin	96	ZTC04S096
ZipTip® with 0.6 mL C4 resin	960	ZTC04S960
ZipTip® with 0.6 mL C18 resin	8	ZTC18S008
ZipTip® with 0.6 mL C18 resin	96	ZTC18S096
ZipTip® with 0.6 mL C18 resin	960	ZTC18S960
ZipTip® with 0.2 mL C18 resin	8	ZTC18M008
ZipTip® with 0.2 mL C18 resin	96	ZTC18M096
ZipTip® with 0.2 mL C18 resin	960	ZTC18M960

B. After ZipTip®µ-C18



ZipTips® increase sensitivity of mass spectrometric analysis. MALDI MS spectra of a tryptic peptide digest from an in-gel 2D digest. The top spectrum represents a contaminated sample prior to sample clean-up. The lower spectrum represents the sample after treatment with a ZipTip®C18 prior to MALDI-ToF MS analysis.

MS-Compatible Millex® LCR Syringe Filters

Obtain immaculate, particle-free samples for LCMS with the peace of mind that you will have minimum interference from impurities introduced from your sample preparation device. Our MS-compatible Hydrophilic polytetrafluoroethylene (PTFE) Millex® LCR Filters have been shown to minimize extractable impurities in mass spectrometry, as shown in Table 1.

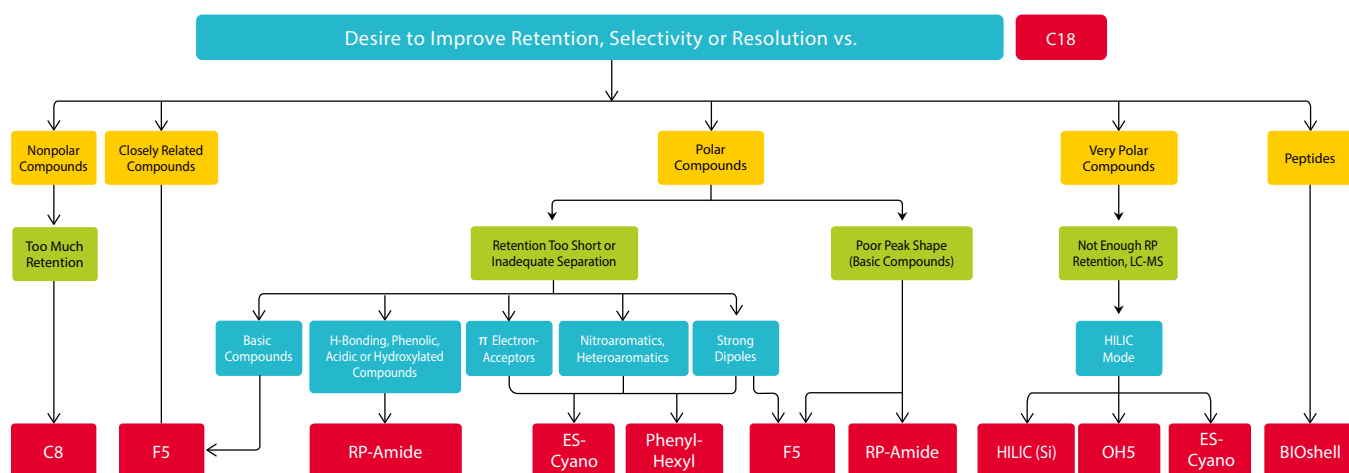
Description	Cat. No.
Millex®-LCR Filter, 13 mm, Hydrophilic PTFE, 0.45 µm, 100/pk	SLCR013NL
Millex®-LCR Filter, 13 mm, Hydrophilic PTFE, 0.45 µm, 1,000/pk	SLCR013NK
Millex®-LCR Filter, 25 mm, Hydrophilic PTFE, 0.45 µm, 250/pk	SLCR025NB
Millex®-LCR Filter, 25 mm, Hydrophilic PTFE, 0.45 µm, 1,000/pk	SLCR025NK

	Millex® Hydrophilic PTFE	Polypropylene (Vendor A)	Polypropylene (Vendor B)	Nylon (Vendor A)	Nylon (Vendor B)
Reproducibility	Good	Medium	Good	Poor	Poor
Extractable Level	Low	High	Medium	High	High
Nature of Extractables	100–400	Polymeric	Variable	Polymeric – Variable	Polymeric – Variable

Table 1. Across all solvents tested, Millex® Hydrophilic PTFE Filters outperformed syringe filters from other suppliers. We tested our filters with eight commonly used mobile phase solvents, such as water, methanol, acetonitrile, tetrahydrofuran in water, and isopropanol in water. After collecting 1st and 2nd mL filtrates, we analyzed them using infusion mass spectrometry (electrospray positive ion mode, 15-minute runs on average).

Selecting The Right HPLC Phase Chemistry for Your Application

C18 column is the standard first choice when starting a new LC-MS method. You can consider selecting another stationary phase when C18 doesn't give the desired separation, or the sample contains compounds difficult to retain or resolve on C18. The Ascentis® Express and BIOshell™ product lines offer a wide range of selectivities for making an effective choice. This decision tree will help you to select an alternative phase based on the particular compound type or separation challenge. All options displayed are relative to the C18 column that started your separation journey.



Key product features for LC-MS and (U)HPLC applications

Primary Application	Product Line	Particle Size (µm)	Pore Size (Å)	Surface Area (m ² /g)	Max Temperature	Pressure (bar)
Small molecules, metabolites and low molecular weight peptides	Titan	1.9	80	410	60	1,000
	Ascentis® Express	2.0	90	120	60	1,000
		2.7	90	150	60	600
		5.0	90	100	60	600
Proteins, Peptides and large Biomolecules	BIOshell™	2.7	160	90	90	600
		3.4	400	15	90	600
		5.0	160	60	60	600

For a complete listing of LC-MS columns, visit [SigmaAldrich.com/hplc](https://www.sigmaaldrich.com/hplc)

Available in a variety of analytical and capillary column dimensions

Column I.D	Column Length (cm)						
	2	3	5	7.5	10	15	25
75 µm			•			•	
100 µm			•			•	
200 µm			•			•	
2.1 mm	•	•	•	•	•	•	•
3 mm	•	•	•	•	•	•	•
4.6 mm	•	•	•	•	•	•	•

For Part Numbers, visit [SigmaAldrich.com/hplc](https://www.sigmaaldrich.com/hplc)

LC-MS & (U)HPLC Columns

Ascentis® Express & BIOshell™ Fused-Core® U/HPLC & LC-MS Columns

Key Features and Benefits

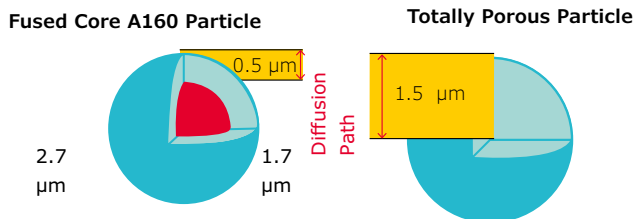
- Maximize speed with sharp peaks even at ultra-high flow rates
- Stable low-bleed for LC-MS and LC-UV
- Suitable for any HPLC, UHPLC, and LC-MS instruments
- Achieve UHPLC performance on a traditional HPLC system
- Available in both 2.0, 2.7 and 5 µm particles
- Wide variety of pore sizes, ranging from 90–1,000 Å, for small to large molecules

Ascentis® Express Fused-Core® Columns

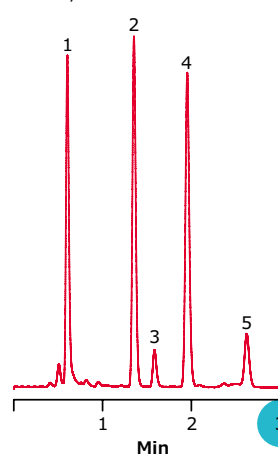
Ascentis® Express columns provide a breakthrough in (U)HPLC and LC-MS column performance. Based on Fused-Core® particle technology, Ascentis® Express columns provide the benefits of high speed and high efficiency. The Fused-Core® particle consists of a solid core and a porous shell, allowing for a shorter diffusion path compared to conventional fully porous particles. Compared to totally porous particles typically used in HPLC, Ascentis® Express Fused-Core® particles generate approximately half the backpressure without loss of resolution. This permits for more resolving power, and faster flow rates, for higher throughput. Ascentis® Express Fused Core Columns are now available in 2.0, 2.7 and 5 µm particle sizes with 8 different phase chemistries. Available in pore size of 90 Å, Ascentis® Express are ideal for LC-MS and (U)HPLC separations of small molecules, metabolites and low molecular weight peptides.

For more information, visit SigmaAldrich.com/express

Comparison of Fused-Core® and Standard HPLC Particle

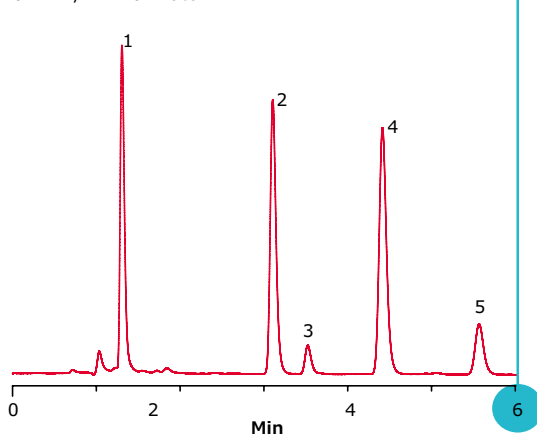


Ascentis Express C18
0.4 mL/min flow rate



1. Estriol (Cerilliant E-074)
2. 17β-Estradiol (Cerilliant E-061)
3. Unknown
4. Estrone (Cerilliant E-075)
5. Estrone degradant

C18 Sub-2 µm
0.2 mL/min flow rate



Particle Size	I.D.	Length	C18	C8	OH5
Capillary Dimensions Columns					
2.7 µm	75 µm	5 cm	53982-U	53983-U	-
2.7 µm	75 µm	15 cm	54219-U	54229-U	-
2.7 µm	100 µm	5 cm	53985-U	53987-U	-
2.7 µm	100 µm	15 cm	54256-U	54260-U	-
2.7 µm	200 µm	5 cm	53989-U	53991-U	-
Ascentis® Express Columns					
2.0 µm	2.1 mm	2 cm	50805-U	51652-U	50951-U
2.0 µm	2.1 mm	3 cm	50809-U	51654-U	50952-U
2.0 µm	2.1 mm	5 cm	50811-U	51656-U	50957-U
2.0 µm	2.1 mm	7.5 cm	50812-U	51657-U	50958-U
2.0 µm	2.1 mm	10 cm	50813-U	51658-U	50959-U
2.0 µm	2.1 mm	15 cm	50814-U	51661-U	50962-U
2.0 µm	3.0 mm	3 cm	50815-U	51663-U	50963-U
2.0 µm	3.0 mm	5 cm	50816-U	51664-U	50964-U
2.0 µm	3.0mm	7.5 cm	50817-U	51672-U	50965-U
2.0 µm	3.0 mm	10 cm	50819-U	51673-U	50967-U
2.0 µm	3.0 mm	15 cm	50821-U	51674-U	50968-U
2.7 µm	2.1 mm	2 cm	53799-U	53795-U	53779-U
2.7 µm	2.1 mm	3 cm	53802-U	53839-U	53748-U
2.7 µm	2.1 mm	5 cm	53822-U	53831-U	53749-U
2.7 µm	2.1 mm	7.5 cm	53804-U	53843-U	53755-U
2.7 µm	2.1 mm	10 cm	53823-U	53832-U	53757-U
2.7 µm	2.1 mm	15 cm	53825-U	53834-U	53764-U
2.7 µm	3.0 mm	3 cm	53805-U	53844-U	53766-U
2.7 µm	3.0 mm	5 cm	53811-U	53848-U	53767-U
2.7 µm	3.0 mm	7.5 cm	53812-U	53849-U	53768-U
2.7 µm	3.0 mm	10 cm	53814-U	53852-U	53769-U
2.7 µm	3.0 mm	15 cm	53816-U	53853-U	53771-U
2.7 µm	4.6 mm	3 cm	53818-U	53857-U	53772-U
2.7 µm	4.6 mm	5 cm	53826-U	53836-U	53774-U
2.7 µm	4.6 mm	7.5 cm	53819-U	53858-U	53775-U
2.7 µm	4.6 mm	10 cm	53827-U	53837-U	53776-U
2.7 µm	4.6 mm	15 cm	53829-U	53838-U	53778-U
5 µm	2.1 mm	10 cm	50517-U	50368-U	50322-U
5 µm	2.1 mm	15 cm	50518-U	50372-U	50327-U
5 µm	2.1 mm	2 cm	50507-U	50362-U	50313-U
5 µm	2.1 mm	25 cm	50521-U	50373-U	50328-U
5 µm	2.1 mm	3 cm	50508-U	50363-U	50314-U
5 µm	2.1 mm	5 cm	50509-U	50364-Y\U	50317-U
5 µm	2.1 mm	7.5 cm	50511-U	50367-U	50321-U
5 µm	3.0 mm	10 cm	50526-U	50381-U	50338-U
5 µm	3.0 mm	15 cm	50527-U	50382-U	50339-U
5 µm	3.0 mm	25 cm	50528-U	50385-U	50341-U
5 µm	3.0 mm	3 cm	50522-U	50376-U	50329-U

Particle Size	I.D.	Length	C18	C8	OH5
5 µm	3.0 mm	5 cm	50523-U	50377-U	50335-U
5 µm	3.0 mm	7.5 cm	50525-U	50378-U	50336-U
5 µm	4.6 mm	10 cm	50536-U	50391-U	50346-U
5 µm	4.6 mm	15 cm	50537-U	50392-U	50347-U
5 µm	4.6 mm	25 cm	50538-U	50394-U	50348-U
5 µm	4.6 mm	3 cm	50529-U	50386-U	50343-U
5 µm	4.6 mm	5 cm	50530-U	50389-U	50344-U
5 µm	4.6 mm	7.5 cm	50533-U	50390-U	50345-U
Ascentis® Express Guard Cartridges, Package of 3					
2.0 µm	2.1 mm	0.5 cm	50822-U	51676-U	-
2.0 µm	3.0 mm	0.5 cm	50823-U	51679-U	-
2.7 µm	2.1 mm	-	53501-U	53509-U	53780-U
2.7 µm	3.0 mm	-	53504-U	53511-U	53781-U
2.7 µm	4.6 mm	-	53508-U	53512-U	53782-U
5 µm	2.1 mm	-	50539-U	-	-
5 µm	3.0 mm	-	50541-U	-	-
5 µm	4.6 mm	-	50542-U	-	-
Titan U/HPLC columns					
1.9 µm	2.1 mm	2 cm	577120-U	-	-
1.9 µm	2.1 mm	3 cm	577121-U	-	-
1.9 µm	2.1 mm	5 cm	577122-U	-	-
1.9 µm	2.1 mm	7.5 cm	577123-U	-	-
1.9 µm	2.1 mm	10 cm	577124-U	-	-
1.9 µm	3.0 mm	3 cm	577125-U	-	-
1.9 µm	3.0 mm	5 cm	577126-U	-	-
Titan U/HPLC columns					
1.9 µm	2.1 mm	-	577127-U	-	-
1.9 µm	3.0 mm	-	577128-U	-	-

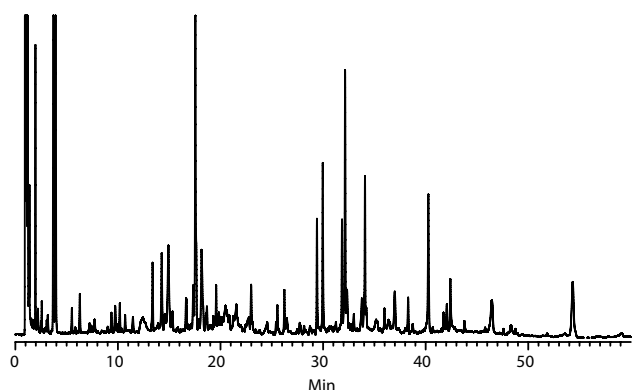
Guard Cartridge Holder

Description	Pack Sizes	Cat. No.
Universal Guard Holder		
Holder w/EXP Titanium Hybrid Ferrule (cartridge not included)	1	53500-U



Analysis of Tryptic Digests on BIOshell™ A160 Peptide ES-C18

Column	BIOshell™ A160 Peptide C18, 10 cm × 4.6 mm I.D.
(66915-U)	
Mobile phase	A 0.1% (w/v) TFA in water
Mobile phase	B 0.1% TFA (w/v) in 40:60
Water	acetonitrile
Gradient	initial = 3% B to 100% B in 53 min.
Flow	rate 1.0 mL/min
Temp.	30 °C
Det.	UV at 215 nm
Injection	20 µL



Titan UHPLC Columns

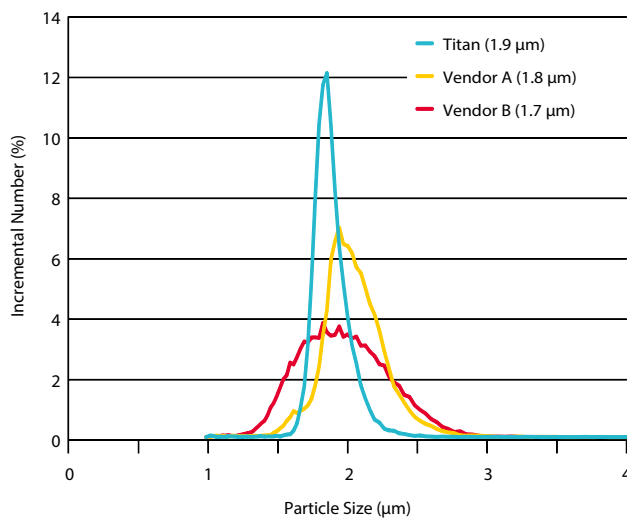
Titan C18 is based on a silica particle platform that has the narrowest particle size distribution available of any totally porous particles. This provides performance advantages in the A-term of the van Deemter equation and in the elimination of fines associated with broader particle size distributions. Monodisperse particles, owing to their narrow particle size distributions, are one of the key reasons that core-type particles achieve higher efficiencies than comparative porous particles.

Key Features

These monodisperse particles offer:

- Minimized voiding and channeling in silica bed compared to higher PSD particles
- A positive influence on column permeability, as evident from a Titan UHPLC column's low pressure drop compared to other traditional porous particle columns
- A profound affect on separation impedance or kinetic performance, resulting in more robust and rugged LC-MS columns

Particle Size Distribution (PSD) Comparison for Different Silica



Poor Retention of Polar Compounds?

SeQuant® ZIC®-HILIC Columns solve your problem

From small peptides to ions, complex carbohydrates and metabolites — all types of hydrophilic compounds can be separated with ZIC®-HILIC Columns.

What is HILIC?

HILIC or Hydrophilic Interaction Liquid Chromatography is a straight-forward chromatographic technique for separation of many types of polar and hydrophilic compounds. To put it simply, one can say that HILIC is a normal-phase (NPLC) type of separation but uses reversed-phase (RPLC) type eluents.

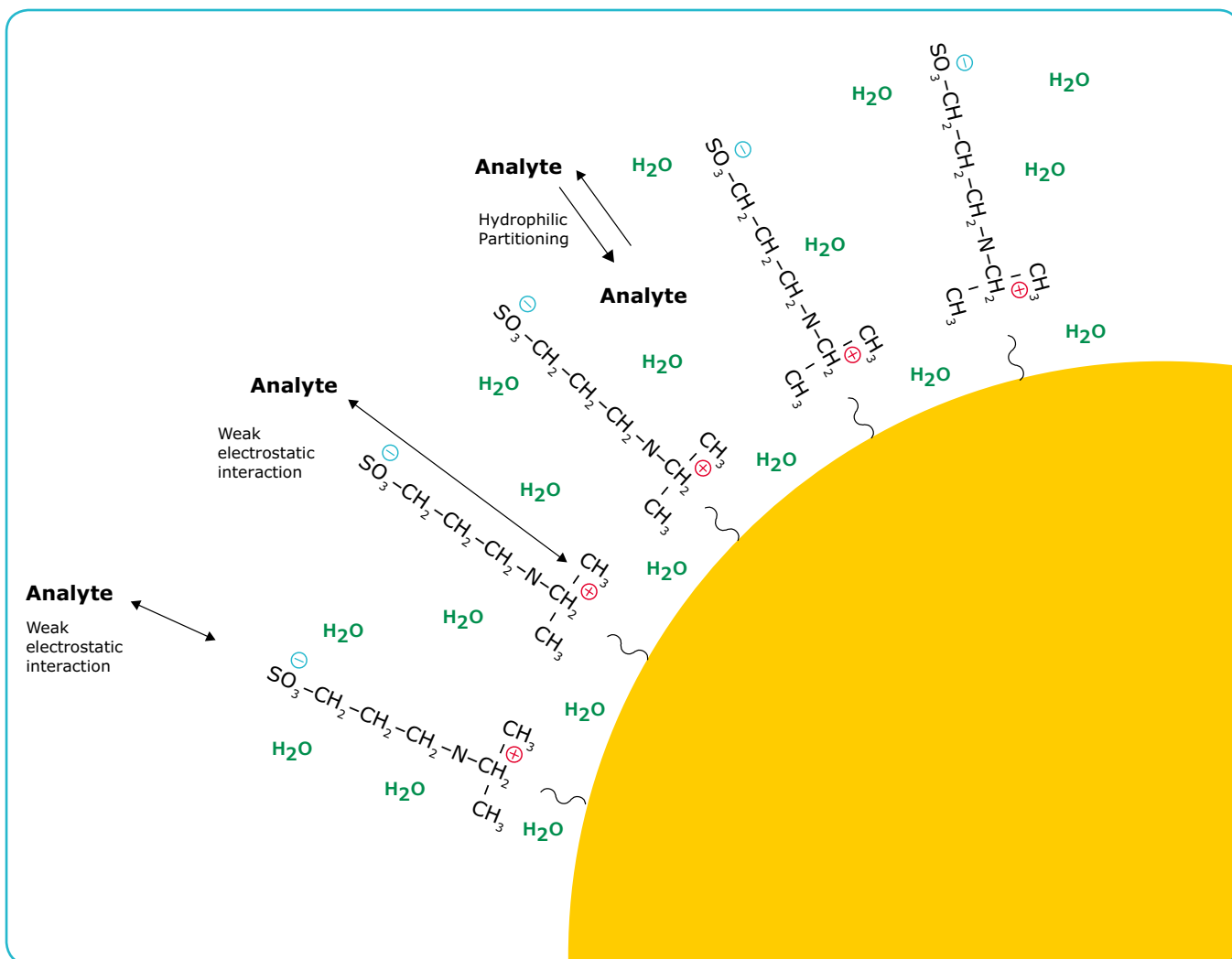
HILIC provides:

- A column with a hydrophilic stationary phase
- An eluent with water, buffer and a high concentration of water-miscible organic solvent

A typical HILIC application uses an eluent with 50-85% organic solvent in an aqueous buffer that has a high solubility in the solvent, for example acetonitrile in ammonium acetate.

The elution order in HILIC is roughly the opposite of that in RPLC and retention increases with hydrophilicity and charge of the analyte. This enables straightforward separation of compounds that would otherwise elute in the void volume on RPLC columns.

Retention of the ZIC®-HILIC Column increases with hydrophilicity and charge of the analyte.



Chiral LC-MS Columns

Astec® CHIROBIOTIC® CSPs

Key Features and Benefits

- Versatile, robust chiral HPLC and LC-MS separations
- Amenable to aqueous samples and mobile phases
- Wide applicability, especially suited to polar and ionizable compounds
- Covalently bonded chiral selector for rugged operation

Ideally Suited for LC-MS of Polar, Ionizable and Neutral Drugs and Biomolecules

Highly enantioselective Astec® CHIROBIOTIC® CSPs (chiral stationary phases) are based on macrocyclic glycopeptides that have been bonded through multiple covalent linkages to high-purity silica particles. CHIROBIOTIC® columns separate the enantiomers of many drugs and biochemical compounds, like amino acids, that cannot be separated by other CSPs. Their most relevant attribute to bioanalysis is the presence of ionic interactions. This allows CHIROBIOTIC® columns to be used with polar ionic (polar organic solvents containing salts) and reversed-phase mobile phases for sensitive LC-MS operation, where analyte ionization and detection sensitivity are of critical concern. Due to the fact that the stationary phase is covalently bonded to the silica surface means CHIROBIOTIC® columns have exceptional stability and long column life, even with repeated injections of biological samples.

Astec® CHIROBIOTIC® Columns

Many more dimensions are available. Please call or consult our website SigmaAldrich.com/chiral

Particle Size	I.D. (mm)	Length (cm)	V	V2	T	T2	TAG	R
5 µm	2.1	10	11018AST	15018AST	12018AST	16018AST	14018AST	13018AST
5 µm	2.1	15	11019AST	15019AST	12019AST	16019AST	14019AST	13019AST
5 µm	2.1	25	11020AST	15020AST	12020AST	16020AST	14020AST	13020AST
5 µm	4.6	10	11022AST	15022AST	12022AST	16022AST	14022AST	13022AST
5 µm	4.6	25	11024AST	15024AST	12024AST	16024AST	14024AST	13024AST

Method Development Kit

Contains one column each of Astec® CHIROBIOTIC® V2, T, TAG and R

Particle Size	I.D.	Length	Cat. No.
5 µm	4.6	10	10300AST
5 µm	4.6	25	10305AST

Astec® CHIROBIOTIC® Application Areas

- **Drug Discovery** – High enantioselectivity, fast screening protocols, scalability to prep, reproducibility for reliable methods, effective for both polar and nonpolar analytes
- **Clinical, Bioanalytical, Drug Metabolism** – High throughput, MS-compatibility, aqueous samples, short run times, rugged columns
- **Amino Acid and Peptide Analysis** – Resolves underivatized natural and synthetic chiral amino acids and peptides

Chiral Column Selection

Astec® CHIROBIOTIC® CSPs are based on 5, 10 or 16 µm, high purity, porous silica gel. They differ in the nature of the bonded macrocyclic glycopeptide and resulting enantioselectivity.

- Astec® CHIROBIOTIC® V and V2 – Vancomycin
- Astec® CHIROBIOTIC® T and T2 – Teicoplanin
- Astec® CHIROBIOTIC® R – Ristocetin
- Astec® CHIROBIOTIC® TAG – Teicoplanin Aglycone

For additional information, request our “Chiral Method Development Wall Chart” at SigmaAldrich.com/chiral

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. However, in today's advanced research and analytical areas, such as metabolomics, clinical and forensics analytics, such methods are sometimes insufficiently sensitive to deliver the solution to a particular analytical problem¹. Therefore, derivatization is used in mass spectrometry to increase ionization efficiency, and thus enhance the sensitivity of the ionization used, to result in lower analyte detectability². The derivatization reagents have functional groups with high proton (cation) affinity that stabilize positive charge. Of similar importance in derivatization is the improvement of qualitative analysis by modifying fragmentation behavior to form unique product ions, and shifting them to a specific, unique mass ("fingerprinting"), as well as precise quantitative analysis to profile comparatively small analyte molecules, particularly in metabolomics.

For more information, visit

SigmaAldrich.com/derivatization

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Description	Analyte Functional Group	Typical Application	Reference	Cat. No.
4-(Dimethyl-d ₆ -amino)benzoyl chloride	Hydroxy	Deuterium mass shift	3	00721
Dansylhydrazine	Carbonyl	-	2c	03334
Dansyl chloride	Hydroxy	-	2c	03641
<i>N,N</i> -Dimethylglycine	Hydroxy	Cholesterol	11	05022
Diethyl ethoxymethylenemalonate	Amine	Amino acids	12	05689
3-Amino-9-ethylcarbazole	Hydroxy	Sugars	13	06696
4-(Diethylamino)benzhydrazide	Carbonyl	-	3	06963
2-Hydrazinopyridine	Carbonyl	Steroids	14	08843
(<i>N</i> -Succinimidylloxycarbonylmethyl) tris (2,4,6-trimethoxyphenyl) phosphonium bromide	Amine	Protein sequence analysis	15	29208
4-Phenyl-1,2,4-triazoline-3,5-dione	Diene	Vitamin D	16	42579
4-(Diethylaminomethyl) benzhydrazide	Carbonyl	-	3	59799
<i>N</i> -Succinimidyl 4-(dimethylamino) benzoate	Amine	Glycerophosphoethanol-amine lipids	4	61224
2-Picolylamine	Carbonyl	Steroids	14	65562
4-(Dimethylamino) benzoyl chloride	Hydroxy	17β-Estradiol	3	67954
6-Bromo-3-pyridinylboronic acid	1,2-Dihydroxy	Brassinosteroids	5	69706
3,5-Dinitrobenzoyl chloride	Hydroxy	Tetrahydrocorticosterones	6	72702
1-Fluoro-2,4-dinitrobenzene	Amine	Prim./sec. aliphatic amines	7	73177
9-Anthracenemethanol	Carboxylic acid, amine, alcohol	-	17	74905
1,2-Benzo-3,4-dihydrocarbazole-9-ethyl-ptoluenesulfonate	Carboxylic acid	Fatty-/bile acids	8	75821
4-[2-(<i>N,N</i> -Dimethylamino)ethylaminosulfonyl]-7-(2-aminoethylamino)-2,1,3-benzoxadiazole	Carboxylic acid	Fatty acids	9	79291
Girard's reagent T	Carbonyl	Nucleosides	18	89397
4-(Dimethylamino)benzohydrazide	Carbonyl	-	3	92989

Description	Analyte Functional Group	Typical Application	Reference	Cat. No.
Pentafluorophenylhydrazine	Carbonyl	Oligosaccharides	10	93742
{1-[2-(Diethylamino)ethoxy]-2-isothiocyanatoethyl} benzene	Amine	-	3	94076
2-Mercaptoethanol	Double bond	Microcystins	19	97622

N-Methyl-N-trimethylsilylfluoroacetamide (MSTFA) is also an important TMS reagent. It has similar reactivity as BSA and BSTFA. However, because the reaction byproducts are more volatile, MSTFA is particularly useful for GC analysis of early-eluting compounds that would otherwise be obscured in the chromatogram. Silylation is also valuable for MS applications where introducing the silyl group produces either more interesting diagnostic

fragments or particular characteristic ions used for SIM (Selected Ion Monitoring). The product table below features selected silylation reagents for GC derivatization. To request the 100 page guide "Derivatization Reagents for Selective Response and Detection in Complex Matrices", you can search for T407138.

To learn more, visit

[SigmaAldrich.com/derivatization](https://www.sigmaaldrich.com/derivatization)

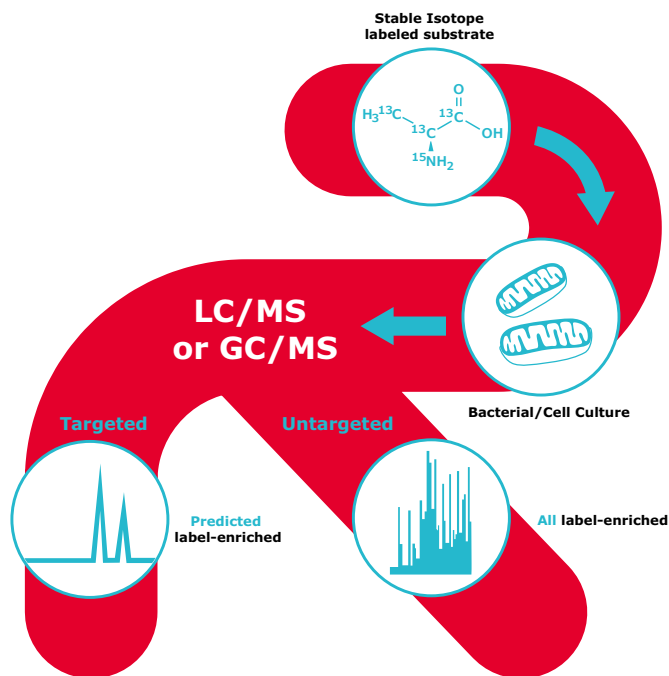
Description	Cat. No.
1,1,3,3-Tetramethyl-1,3-diphenyldisilazane	43340
4-(Trimethylsiloxy)-3-penten-2-one	69649
Bis(dimethylamino)dimethylsilane	14755
BSA + TMCS	15256
Chlorodimethyl(pentafluorophenyl)silane	76750
Chlorotriethylsilane	90383
Chlorotrimethylsilane	89595
Hexamethyldisilazane	52619
Hexamethyldisiloxane	01565
N-(Trimethylsilyl)acetamide	91566
N,N-Bis(trimethylsilyl)methylamine	15235
N,O-Bis(tert-butyl)dimethylsilyl)trifluoroacetamide	89539
N,O-Bis(trimethylsilyl)acetamide	15269
N,O-Bis(trimethylsilyl)trifluoroacetamide	15222
N,O-Bis(trimethylsilyl)trifluoroacetamide with trimethylchlorosilane	15209, 15238
N-Methyl-N-(trimethylsilyl)trifluoroacetamide	69479
N-Methyl-N-(trimethylsilyl)trifluoroacetamide with 1% trimethylchlorosilane	69478
N-tert-Butyldimethylsilyl-N-methyltrifluoroacetamide with 1% tert-Butyldimethylchlorosilane	00942
BSA Derivatization Grade	33036, 33035-U, 33037-U
BSA + TMCS + TMSI	33030, 33151, 33031-U
BSTFA + TMCS	33149-U, 33154-U, 33155-U, 33148
BSTFA, Derivatization Grade	33024, 33027, 33084
Chlorotrimethylsilane	33014
HMDS, Derivatization Grade	33350-U
HMDS + TMCS + Pyridine	33038, 33039
Silica Column Regeneration Solution	33175
Silylation Sampler Kit	505846
Sylon CT	33065-U
tert-Butyldimethylsilylimidazole solution	33092-U
TMSI, Derivatization Grade	33068-U
TMSI + Pyridine	33156-U, 33159-U

Metabolic Labeling with Stable Isotopes

Introducing heavy isotopologs into the metabolome enables detection of resulting metabolites by mass spectrometry. Growing cells or bacteria with labeled substrates allows for incorporation of heavy isotopes, such as deuterium, ^{13}C , and ^{15}N , into metabolites, assisting in the understanding of metabolic pathways and identification of metabolites of interest. Both steady-state and flux analysis benefit from the use of heavy isotope labeled compounds.

Specifically-labeled nutrients and metabolites allow for a detailed understanding of mechanistic features. Refer to SigmaAldrich.com/isotec for a complete list stable isotope labeled metabolic labeling compounds.

Amino Acids	Cat. No.
L-Alanine-2,3,3,3-d ₄	485845
L-Alanine-2- ¹³ C	486779
L-Alanine-1- ¹³ C	489867
L-Alanine- ¹³ C ₃	489875
L-Alanine-3,3,3-d ₃	489921
L-Alanine-3- ¹³ C	489948
L-Alanine-2,3- ¹³ C ₂	604682
DL-Alanine-2,3,3,3-d ₄	488917
L-Alanine- ¹⁵ N	332127
L-Alanine-d ₇	774820
L-Arginine-(guanidineimino- ¹⁵ N ₂) hydrochloride	609080
L-Arginine- ¹⁵ N ₄ hydrochloride	600113
L-Asparagine- ¹⁵ N ₂	641960
L-Asparagine-4- ¹³ C monohydrate	579866
L-Asparagine- ¹⁵ N ₂ monohydrate	485918
L-Asparagine-1- ¹³ C	750824
L-Aspartic acid-2,3,3,3-d ₃	489980
L-Aspartic acid-1,2- ¹³ C ₂	579793
L-Aspartic-3,4- ¹³ C ₂ acid	586161
L-Aspartic-2- ¹³ C acid	604895
L-Aspartic-3- ¹³ C acid	617539
L-Aspartic acid-d ₇	673021
L-Aspartic- ¹⁵ N acid	332135
L-Cysteine-1- ¹³ C	676128
L-Cystine-1,1'- ¹³ C ₂	676136
L-Glutamic-4- ¹³ C acid	587672
D-Glutamic-5- ¹³ C acid	605255
DL-Glutamic-2,3,3,4,4-d ₅ acid	631973
L-Glutamic-2- ¹³ C acid	605123
L-Glutamic- ¹⁵ N acid	332143
L-Glutamine-2,3,3,4,4-d ₅	616303
L-Glutamine-2- ¹³ C	605085
L-Glutamine-4- ¹³ C	750506
L-Glutamine- ¹⁵ N ₂	490032
Glycine-1- ¹³ C	279420
Glycine-2- ¹³ C	279439
Glycine- ¹³ C ₂	283827
Glycine- ¹⁵ N, 98+ ATOM % ¹⁵ N	299294
Glycine-2,2-d ₂	336459
L-Isoleucine-1- ¹³ C	604771
L-Leucine- ¹⁵ N	340960



Amino Acids	Cat. No.
L-Leucine-2- ¹³ C	486817
L-Leucine-5,5,5-d ₃	486825
L-Leucine-1- ¹³ C	490059
L-Leucine-2,3,3,4,5,5,5,5',5'-d ₁₀	492949
L-Leucine-3- ¹³ C	604828
L-Leucine-4-d	615978
L-Leucine-(isopropyl-d ₇)	615986
L-Leucine-2-d	704504
L-Lysine-2- ¹⁵ N dihydrochloride	592900
L-Lysine-1- ¹³ C hydrochloride	604704
L-Lysine-2- ¹⁵ N hydrochloride	608963
L-Lysine-ε- ¹⁵ N hydrochloride	608971
L-Lysine- ¹⁵ N ₂ hydrochloride	609021
L-Methionine-1- ¹³ C	490083
L-Methionine-(methyl- ¹³ C)	299146
L-Methionine-(methyl-d ₃)	300616

Amino Acids	Cat. No.	Carbohydrates	Cat. No.
D-Methionine-(<i>methyl</i> - ¹³ C)	589780	D-Fructose-2- ¹³ C	492140
L-Methionine-2-d	589802	D-Fructose-1,6- ¹³ C ₂	587613
L-Methionine- ¹⁵ N	609242	D-Fructose- ¹³ C ₆	587621
L-Phenylalanine-1- ¹³ C	490091	D-Fructose-6- ¹³ C	605395
L-Phenylalanine- ¹⁵ N	490105	D-Fructose-6,6-d ₂	488720
L-Phenylalanine-2- ¹³ C	490113	D-Fructose-d ₁₂	723908
L-Phenylalanine-3- ¹³ C	490121	L-Fucose-1- ¹³ C	605425
L-Phenylalanine-2,3,3-d ₃	490148	D-Galactose-1- ¹³ C	415545
L-Phenyl- ¹³ C ₆ -alanine	604879	D-Galactose-2- ¹³ C	454621
L-Phenyl-1- ¹³ C-alanine	605042	D-Galactose- ¹³ C ₆	605379
L-Phenyl-d ₅ -alanine	615870	D-Galactose-1-d	495077
L-Phenylalanine-3,3-d ₂	615889	D-Glucose-1- ¹³ C	297046
L-Phenylalanine- ¹³ C ₉	795844	D-Glucose-4- ¹³ C	668648
L-Phenylalanine-2-d	589438	D-Glucose-1,6- ¹³ C ₂	453196
L-Proline-1- ¹³ C	589497	D-Glucose-2- ¹³ C	310794
L-Proline-2,5,5-d ₃	791261	D-Glucose-1,2- ¹³ C ₂	453188
L-Proline- ¹⁵ N	608998	D-Glucose-3- ¹³ C	605409
L-Selenomethionine-(<i>methyl</i> - ¹³ C)	634093	D-Glucose-1,2,3- ¹³ C ₃	720127
L-Serine-1- ¹³ C, 99 ATOM % ¹³ C	490156	D-Glucose-4,5,6- ¹³ C ₃	731501
L-Serine-2- ¹³ C	604712	D-Glucose-4,5- ¹³ C ₂	605468
L-Serine-3- ¹³ C	604720	D-Glucose-5- ¹³ C	717355
L-Serine-2,3- ¹³ C ₂	605174	D-Glucose-5,6- ¹³ C ₂	755893
L-Serine- ¹⁵ N	609005	D-Glucose- ¹³ C ₆	389374
L-Threonine-1- ¹³ C	605034	D-Glucose-6- ¹³ C	310808
L-Threonine- ¹³ C ₄	677604	D-Glucose-1-d	310816
L-Threonine-1,2- ¹³ C ₂	668060	D-Glucose-2-d	310824
L-Tryptophan-1- ¹³ C	604836	D-Glucose-3-d	615498
L-Tryptophan-(<i>indole ring</i> -2- ¹³ C)	604844	D-Glucose-6- ¹³ C,6,6-d ₂	734403
L-Tryptophan-(<i>indole</i> -d ₅)	615862	D-Glucose-6,6-d ₂	282650
L-Tyrosine-2,6-d ₂	485829	D-Glucose-d ₁₂	616338
L-Tyrosine-(<i>phenyl</i> - ¹³ C ₆)	489794	D-Glucose-1,2,3,4,5,6,6-d,	552003
L-Tyrosine-(<i>phenyl</i> -d ₄)	489808	Inulin- ¹³ C	900388
L-Tyrosine-(<i>phenyl</i> -3,5-d ₂)	489816	D-Mannose-1- ¹³ C	415537
L-Tyrosine-1- ¹³ C	489824	D-Mannose-2- ¹³ C	605344
L-Tyrosine-3- ¹³ C	489859	D-Mannose-3- ¹³ C	749419
L-Tyrosine-(<i>phenyl</i> -4- ¹³ C)	605093	D-Mannose-4- ¹³ C	733733
L-Tyrosine-2- ¹³ C	605107	D-Mannose-5- ¹³ C	749400
L-Tyrosine-(4- <i>hydroxy</i> - ¹⁸ O)	609919	D-Mannose-6- ¹³ C	605387
L-Tyrosine- ¹⁵ N	332151	D-(+)-Mannose- ¹³ C ₆	592994
L-Tyrosine-3,3-d ₂	489840	D-Ribose-1- ¹³ C	605352
L-Valine-1- ¹³ C, 99 ATOM % ¹³ C	490164	D-Ribose-2- ¹³ C	310840
L-Valine-2- ¹³ C	604917	D-Ribose-1,2- ¹³ C ₂	605476
L-Valine- ¹⁵ N	490172	D-Ribose-2,3,4,5- ¹³ C ₄	605484
		D-Ribose- ¹³ C ₅	798258
		Starch- ¹³ C from algae	605336
		Sucrose- ¹³ C ₁₂	605417
		Sucrose- ¹³ C-(<i>glucose</i> -1- ¹³ C)	705136
		Sucrose-(<i>glucose</i> - ¹³ C ₆)	738786
		D-Xylose- ¹³ C ₅	666378
		D-Xylose-1- ¹³ C	331104
Carbohydrates	Cat. No.		
D-Arabinose-1- ¹³ C	426415		
D-Arabinose- ¹³ C ₅	763802		
Cellulose- ¹³ C from maize	696498		
D-Fructose-1,1,3,4,5,6,6-d,	729051		
D-Fructose-1- ¹³ C	415553		

Fatty Acids and Lipids	Cat. No.
Behenic-d ₄₃ acid	586064
Butyric acid- ¹³ C ₄	723894
Sodium butyrate-2- ¹³ C	485357
Sodium butyrate- ¹³ C ₄	488380
Sodium butyrate-2,4- ¹³ C ₂	492000
Sodium butyrate-4- ¹³ C	492019
Decanoic-d ₁₉ acid	488666
Decanoic acid-1- ¹³ C	488658
Decanoic acid-1,2- ¹³ C ₂	587818
1,12-Dodecanedioic acid- ¹³ C ₁₂	659525
Glycerol tri(oleate-1,2,3,7,8- ¹³ C ₅)	772941
Glycerol- ¹³ C ₃ trioleate	605638
Glycerol tri(palmitate-d ₃₁)	616966
Glycerol tri(octanoate-d ₁₅)	617121
Glycerol tri(palmitate-1,2,3,4- ¹³ C ₄)	777862
Glycerol tri(octanoate-1,2,3,4- ¹³ C ₄)	808563
Glycerol tri(oleate-2,3,7,8- ¹³ C ₄)	722960
Methyl heptadecanoate-d ₃₃	733148
Heptadecanoic-d ₃₃ acid	807907
2-Ethylhexanoic-d ₁₅ acid	710709
Isovaleric-d ₉ acid	808997
Lauric-d ₂₃ acid	451401
Lauric acid-12- ¹³ C	486639
Linoleic acid- ¹³ C ₁₈	605735
Linoleic acid-d ₃₂	735124
Potassium linoleate- ¹³ C ₁₈	605816
Linolenic acid- ¹³ C ₁₈	605743
Algal fatty acid mixture- ¹³ C	487937
Myristic-d ₂₇ acid	366889
Myristic acid- ¹³ C ₁₄	605689
Sodium octanoate-2,4,6,8- ¹³ C ₄	657204
Octanoic-d ₁₅ acid	448214
Octanoic acid-1,2,3,4- ¹³ C ₄	493163
Octanoic acid- ¹³ C ₈	605727
Oleic acid-1,2,3,7,8- ¹³ C ₅	749079
Oleic acid- ¹³ C ₁₈	490431
Oleic acid-1,2,3,7,8,9,10- ¹³ C ₇	646458
Oleic acid-d ₃₄	683582
Oleic acid-d	900336
Potassium oleate- ¹³ C ₁₈	714313
Sodium oleate- ¹³ C ₁₈	798479
Potassium oleate-d ₃₃	736155
Potassium oleate-1,2,3,7,8- ¹³ C ₅	739693
Potassium oleate-15,15,16,16,17,17,18,18,18-d ₉	772399

Fatty Acids and Lipids	Cat. No.
Palmitoleic acid- ¹³ C ₁₆	724173
Palmitic acid-d ₃₁	366897
Palmitic acid- ¹³ C ₁₆	605573
Palmitic acid-1- ¹³ C	292125
Palmitic acid-1,2- ¹³ C ₂	485802
Palmitic acid-1,2,3,4- ¹³ C ₄	489611
Potassium palmitate- ¹³ C ₁₆	605751
Potassium palmitate-d ₃₁	614378
Potassium palmitate-1- ¹³ C	489646
Sodium palmitate- ¹³ C ₁₆	700258
Sodium pyruvate- ¹⁸ O ₃	700274
Stearic-d ₃₅ acid	448249
Stearic acid- ¹³ C ₁₈	605581
Stearic acid-d	900337
Valeric acid-1- ¹³ C	596442
Valeric acid-5- ¹³ C	605662
4-Methylvaleric-d ₁₁ acid	809004

Isotopically-Labeled Water	Cat. No.
Deuterium oxide- ¹⁸ O, 98 atom % D, 50 atom % ¹⁸ O	608548
Deuterium oxide- ¹⁸ O, 5 atom % D, 5 atom % ¹⁸ O	608556
Deuterium oxide- ¹⁸ O, 99 atom % D, 95 atom % ¹⁸ O	608572
Deuterium oxide- ¹⁸ O 99 atom % D, 75 atom % ¹⁸ O	609757
Water- ¹⁸ O, 99 atom % ¹⁸ O	487090
Water- ¹⁸ O, 98 atom % ¹⁸ O	603112
Water- ¹⁸ O, 97 atom % ¹⁸ O	329878
Water- ¹⁸ O, 10 atom % ¹⁸ O	332089
Deuterium oxide, filtered, 99.9 atom % D	756822

Other Isotopically-Labeled Products for Metabolic Labeling	Cat. No.
Ammonium- ¹⁵ N chloride	299251
Ammonium- ¹⁵ N,d ₄ chloride	366501
Ammonium- ¹⁵ N ₂ sulfate	299286
Ammonium- ¹⁵ N ₂ ,d ₈ sulfate	593990
ISOGRO®- ¹³ C powder growth medium	606863
ISOGRO®- ¹³ C, ¹⁵ N growth medium	606839
ISOGRO®- ¹⁵ N growth medium	606871
ISOGRO®- ¹³ C, ¹⁵ N,D growth medium	608297
ISOGRO®- ¹⁵ N,D growth medium	608300
ISOGRO®-D growth medium	616729

Solvents and Blends for LC-MS

LC-MS has become an important tool in today's analytical labs. In order to obtain accurate and reproducible results, high demands are made on the purity of chemicals. We offer high purity solvents specifically to meet the stringent requirements of LC-MS applications, ensuring high UV transmittance, baseline stability and lowest impurity levels. We have developed and introduced high purity solvents pre-blended with acetic acid (HA), formic acid (FA) or trifluoroacetic acid (TFA) to provide ready-to-use mobile phases for LC-MS. With this comprehensive portfolio, we set the standard for accurate, reproducible and high-resolution analytical separations.

Features:

- Ready-to-use
- LC-MS suitability
- Minimal metal adduct formation
- Minimal ionization suppression
- Batch to batch consistency
- Filtered through 0.2 µm

Benefits:

- Time- & cost-saving
- Reliable LC-MS application
- Less laborious mixing procedure
- Reduced contamination danger
- Safer – less exposure to hazardous chemicals
- No glassware cleaning
- Reduced solvent/acid excess
- Less storage room needed

Name	Description	Pack Sizes	Cat. No.
Acetonitrile + 0.1% Acetic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L	1.59004.2500
Acetonitrile + 0.1% Formic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L	1.59002.2500
Acetonitrile + 0.1% Trifluoroacetic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L	1.59014.2500
		4 L	1.59014.4000
Water + 0.1% Acetic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L	1.59007.2500
Water + 0.1% Formic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L	1.59013.2500
Water + 0.1% Trifluoroacetic acid (v/v)	Hypergrade for LC-MS LiChrosolv®	2.5 L	4.80112.2500
		4 L	4.80112.4000
Acetonitrile	Hypergrade for LC-MS LiChrosolv®	1 L GL*	1.00029.1000
		2.5 L GL*	1.00029.2500
		10 L ST	1.00029.9010
		30 L ST	1.00029.9030
Methanol	Hypergrade for LC-MS LiChrosolv®	1 L GL*	1.06035.1000
		2.5 L GL*	1.06035.2500
Water	Hypergrade for LC-MS LiChrosolv®	1 L GL*	1.15333.1000
		2.5 L GL*	1.15333.2500
		4 L GL*	1.15333.4000
		10 L ST	1.15333.9010
		30 L ST	1.15333.9030
Ethyl acetate	Hypergrade for LC-MS LiChrosolv®	1 L	1.03649.1000
		2.5 L	1.03649.2500
Hexane	Hypergrade for LC-MS LiChrosolv®	1 L	1.03701.1000
		2.5 L	1.03701.2500
Heptane	Hypergrade for LC-MS LiChrosolv®	1 L	1.03654.1000
		2.5 L	1.03654.2500
2-Propanol	Hypergrade for LC-MS LiChrosolv®	1 L	1.02781.1000
		2.5 L	1.02781.2500

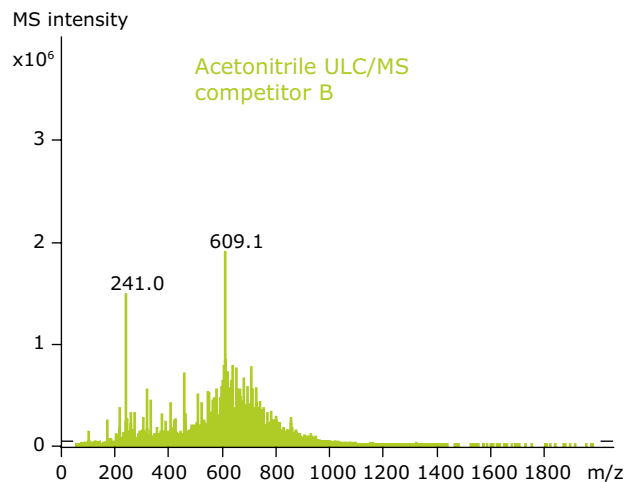
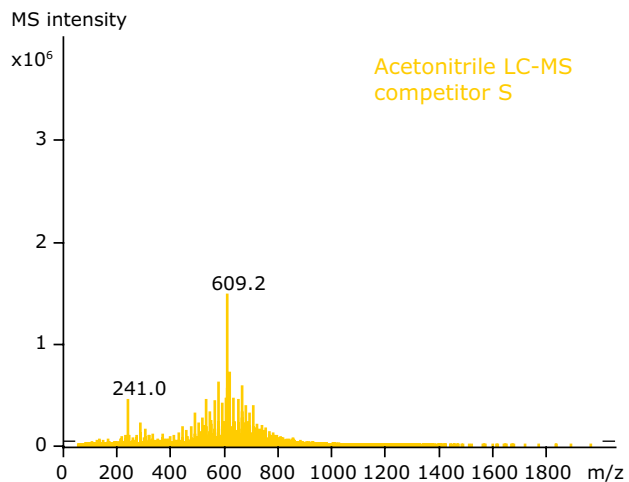
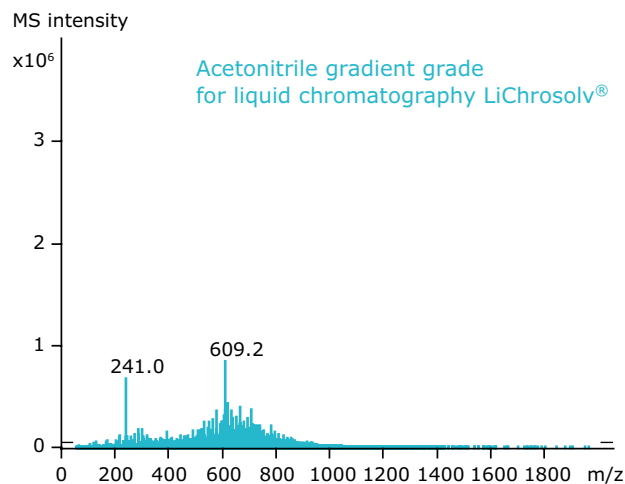
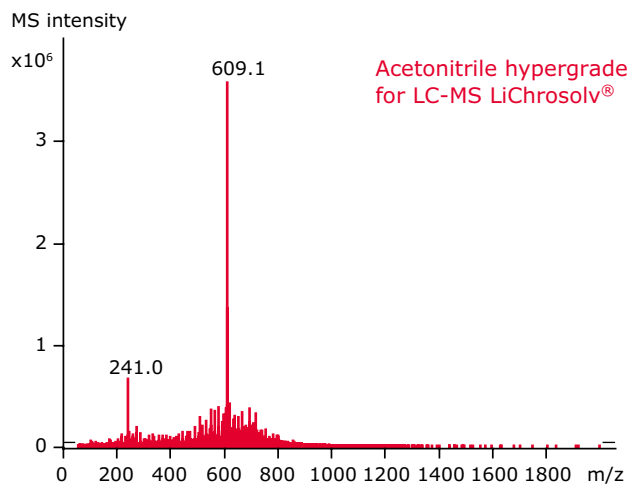
*special treated amber glass bottle

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

MS conditions

System	Bruker Esquire 3,000+ ion trap MS
Detection	Pos. ESI-MS, m/z range 50 – 2,000
Flow rate	0.2 mL/min via syringe pump
Temperature	25 °C
Sample	Reserpine (m/z 609.1), internal standard (m/z 241.0)

The mass spectra of four different acetonitrile grades clearly show 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.



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

LiChropur® LC-MS Reagents

It is common practice in LC-MS to add certain chemicals to the mobile phase or introduce them post-column prior to the interface to influence analyte ionization. Most often, an improvement in the analyte signal is the goal. However, 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.

We offer a wide range of high purity mobile phase additives for LC-MS applications. Our offer includes the most commonly used acids, bases and volatile salts. All are of high purity and are rigorously tested for LC-MS application suitability, offering many advantages for both small and large molecule analysis.

Impurities, such as alkali ions, plasticizers and surfactants, found in lower-grade reagents are particularly problematic as they interfere strongly with LC-MS, resulting in higher background noise and formation of adducts. Only highly pure reagents allow high signal-to-noise ratios.

Features:

- LC-MS application tested for consistent quality
- Improves ionization and resolution
- Extremely low levels of inorganic and organic impurities
- Manufactured specifically for accurate and fast LC-MS
- Highest quality acids, bases & salts

For more information, visit

SigmaAldrich.com/lcms-reagents

Product Name	Description	Pack Sizes	Cat. No.
Acetic acid	100 % for LC-MS LiChropur®	50 mL	5.33001.0050
Formic acid	98 – 100 % for LC-MS LiChropur®	50 mL	5.33002.0050
Ammonia solution	25 % for LC-MS LiChropur®	50 mL	5.33003.0050
Ammonium acetate	for LC-MS LiChropur®	50 mL	5.33004.0050
Ammonium hydrogen carbonate	for LC-MS LiChropur®	50 mL	5.33005.0050

Tools for Metabolite Analysis by GC-MS

Strategies to analyze small biological compounds in a metabolome range from analyzing a particular class of metabolites (targeted analysis) to separating and detecting as many metabolites as possible of a particular developmental stage (metabolite profiling or metabolomics). When gas chromatography (GC) is used as the separation technique, the analyst benefits from the high resolving power of capillary GC, but the task is complex, as not all compounds are volatile and therefore need to be derivatized before analysis. This and other pages in this publication list selected product options for the analysis of volatile and semivolatile metabolites, including metabolite standards, derivatization reagents, solid-phase microextraction (SPME), and selected GC columns and accessories. For detailed

information, references 1 and 2 look at the role of GC and MS in metabolite analysis, while references 3 and 4 discuss compound identification and sample throughput, respectively.

References

1. D. Wishart, Chapter 10, "Metabolomics in Humans and Other Mammals", in *Metabolome Analysis: An Introduction*, SG Villas-Boas, J. Nielsen, J. Smedsgaard, M. Hansen, U. Roessner-Tunali, eds., John Wiley & Sons, 2007.
2. Villas-Bôas S.G., et al., *Mass Spectrom Rev.* 2005, 24 (5):613-46.
3. Applying In-Silico Retention Index and Mass Spectra Matching for Identification of Unknown Metabolites in Accurate Mass GC-TOF Mass Spectrometry, Kumari, S., et al., *Anal. Chem.* 2011, 83, 5895-5902.
4. Fast, High Peak Capacity Separations in Gas Chromatography–Time-of-Flight Mass Spectrometry, Wilson, R.B., et al., *Anal. Chem.* 2012, 84, 4167-4173.

SLB®-5ms An MS-Grade Capillary GC Column for Metabolomics Research

The 5% phenyl equivalent phase provides a boiling point elution order with a slight increase in selectivity, especially for aromatic compounds. The low bleed characteristics, inertness, and durable nature make it the column of choice for the analysis of semivolatiles or, in general, any application that requires a low bleed non-polar column. Temp. Limits for ≤ 0.25 mm I.D. are -60 °C to 340 °C (isothermal) or 360 °C (programmed).

I.D. (mm)	df (μ m)	Length (m)	Beta Value	Qty.	Cat. No.
0.10	0.10	10	250	1 ea.	28465-U
-	0.10	15	250	1 ea.	28466-U
0.18	0.18	20	250	1 ea.	28564-U
-	0.30	12	150	1 ea.	28566-U
-	0.30	30	150	1 ea.	28575-U
-	0.36	20	125	1 ea.	28576-U
0.20	0.20	30	250	1 ea.	28513-U
0.25	0.10	30	625	1 ea.	28467-U
-	0.25	15	250	1 ea.	28469-U
-	0.25	30	250	1 ea.	28471-U
-	0.25	60	250	1 ea.	28472-U
-	0.50	15	125	1 ea.	28577-U
-	0.50	30	125	1 ea.	28473-U
-	0.50	60	125	1 ea.	28474-U
-	1.00	30	63	1 ea.	28476-U

Extend the Lifetime of Your Capillary Column

A guard column/retention gap is a short (1–5 m) piece of uncoated deactivated fused silica tubing which is placed in-line between the GC injection port and the capillary column. A guard column/retention gap consists of two parts: a short length of fused silica tubing and a connector. Match the deactivation of the fused silica tubing with the polarity of the injection solvent. In most cases, it is also recommended to match the I.D. of the capillary column.

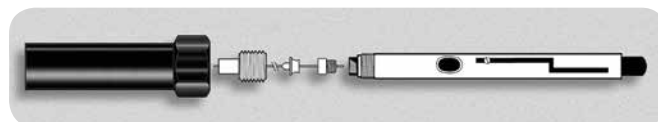
For more information about guard column selection, visit SigmaAldrich.com/gc-guard

SPME A Unique Sample Preparation Technique

Solid Phase Microextraction is the sample preparation technique of choice for analyzing volatile and semi-volatile metabolites by GC-MS. SPME eliminates most drawbacks to extracting organics by more traditional methods. It requires no solvents or complicated apparatus, and can concentrate volatile and nonvolatile compounds, in both liquid and gaseous samples, for analysis by GC and GC-MS. SPME reduces sample preparation time by 70%, minimizes the use of solvents and their disposal, is cost-effective, can be used with any GC system, and can be automated. An SPME fiber assembly consists of a length of fused silica fiber coated with a polymer material, in some cases mixed with a solid adsorbent. The fiber is attached to a stainless steel plunger sheathed by a protective needle. Fiber holders are available for manual injection as well as for use with autosamplers. The holder protects the coated fiber, and controls exposure of the fiber during analyte adsorption and desorption. The holder is reusable indefinitely and accepts the replaceable fiber assembly. First time users must order both a holder and a fiber assembly. Fiber holders for use with an autosampler are also available.

Fiber Holder for Manual Sampling

An adjustable depth guide positions the fiber for sampling and for correct placement in the heated zone of the GC injection port. The fiber can be locked in the exposed position.



Description	Qty.	Cat. No.
SPME Fiber Holder, for use with manual sampling	1 ea.	57330-U

SPME Fiber Assemblies

SPME fiber assemblies can be reused for ≥ 100 analyses, depending on the application and the care they are given. For reuse, simply condition with heat before and after every analysis. Each assembly has a color-coded or notched hub indicating the type of coating on the fiber. Choose the appropriate assembly for the holder: manual or autosampler. The key to proper SPME performance is fiber selection.

For information on how to select a fiber, visit SigmaAldrich.com/spme

SPME Fiber Assortment Kit for Volatiles and Semivolatiles

Recommended starter kit for the extraction of volatile and semivolatile metabolites contains one fiber each of 85 µm polyacrylate coating, 100 µm polydimethylsiloxane coating, and 7 µm polydimethylsiloxane coating.

Description	Qty.	Cat. No.
Manual holder 24 ga	1 kit	57306
Autosampler 24 ga	1 kit	57307
Autosampler 23 ga	1 kit	57285-U

Achieve Sharper Peaks with SPME-GC Analyses Using Supelco® Inlet Liners

GC injection port liners are designed for optimal sample introduction for specific injection techniques. When using SPME, a 0.75 mm I.D. inlet liner increases linear velocity, compared to a conventional, larger volume 2 mm I.D. liner, and rapidly introduces analytes onto the column in a narrow band. To minimize sample loss or peak tailing, the inlet liner must be inert to minimize adsorption of active sample components. An inlet liner, in conjunction with efficient, solvent-free, SPME sample introduction, helps to achieve excellent chromatographic results. An inlet liner for several Agilent® GC systems is available.

For Agilent® (5890, 6890, and 7890)

Inlet Liner, Direct (SPME) Type, Straight Design (unpacked)

L × O.D. × I.D. _____ 785 mm × 65 mm × 0.75 mm

Qty.	Cat. No.
1 ea.	2637501

To select the appropriate inlet liner for your GC, visit SigmaAldrich.com/inletliners

GC Derivatization Reagents

A large number of reagents are used to prepare derivatives for gas chromatography. Derivatives are used for the following reasons:

- To improve resolution and reduce tailing of polar compounds (-OH, -COOH, =NH, -NH₂, -SH, and other functional groups)
- To analyze relatively nonvolatile compounds
- To improve analytical efficiency and increase detectability
- To improve stability of compounds

The following table lists the silylation reagents most commonly used together with acylation and alkylations.

Description	Cat. No.
1,1,3,3-Tetramethyl-1,3-diphenyldisilazane	43340
4-(Trimethylsiloxy)-3-penten-2-one	69649
Bis(dimethylamino)dimethylsilane	14755
BSA + TMCS	15256
Chlorodimethyl(pentafluorophenyl)silane	76750
Chlorotriethylsilane	90383
Chlorotrimethylsilane	89595
Hexamethyldisilazane	52619
Hexamethyldisiloxane	01565
<i>N</i> -(Trimethylsilyl)acetamide	91566
<i>N,N</i> -Bis(trimethylsilyl)methylamine	15235
<i>N,O</i> -Bis(tert-butyltrimethylsilyl)trifluoroacetamide	89539
<i>N,O</i> -Bis(trimethylsilyl)acetamide	15269
<i>N,O</i> -Bis(trimethylsilyl)trifluoroacetamide	15222
<i>N,O</i> -Bis(trimethylsilyl)trifluoroacetamide with trimethylchlorosilane	15209 15238
<i>N</i> -Methyl- <i>N</i> -(trimethylsilyl)trifluoroacetamide	69479
<i>N</i> -Methyl- <i>N</i> -(trimethylsilyl)trifluoroacetamide with 1% trimethylchlorosilane	69478
<i>N-tert</i> -Butyldimethylsilyl- <i>N</i> -methyltrifluoroacetamide with 1% <i>tert</i> -Butyldimethylchlorosilane	00942
BSA Derivatization Grade	33036 33035-U 33037-U
BSA + TMCS + TMSI	33030 33151 33031-U
BSTFA + TMCS	33149-U 33154-U 33155-U 33148
BSTFA, Derivatization Grade	33024 33027 33084
Chlorotrimethylsilane	33014
HMDS, Derivatization Grade	33350-U
HMDS+TMCS+Pyridine	33038 33039
Silica Column Regeneration Solution	33175
Silylation Sampler Kit	505846
Sylon CT	33065-U
<i>tert</i> -Butyldimethylsilylimidazole solution	33092-U
TMSI, Derivatization Grade	33068-U
TMSI + Pyridine	33156-U 33159-U

To learn more, view the Derivatization Reagents for Selective Responses Guide at SigmaAldrich.com/derivatization

MALDI Matrices Selection Table

Matrix-assisted laser desorption/ionization (MALDI) has expanded MS into the analysis of high molecular mass, non-volatile, and thermally labile compounds, such as intact proteins and oligonucleotides. Moreover, it has become an important technique in proteomics research.¹⁻³ Further significant applications of MALDI-MS include the analysis of polymers, glycans, lipids, and metabolites.

A typical MALDI matrix substance is an aromatic acid with a chromophore that absorbs strongly at the wavelength of the incident laser. The MALDI technique generally involves mixing the sample with a matrix substance, followed by crystallization by different techniques on the MALDI sample plate. The crystallized sample-matrix mixture is irradiated by laser light, usually UV. As the matrix absorbs the light energy, it vaporizes into the gas phase, resulting in an indirect ionization of the sample molecules.⁴⁻⁶

Choosing a suitable matrix of high quality is the key to the success of a MALDI-MS experiment. Organic impurities can lead to extraneous peaks, especially in the low mass range. Trace levels of ions, especially Na⁺ and K⁺, form adducts with sample molecules. These adducts differ in mass according to the number of positive ions and complicate the MS spectrum. Since the matrix substance is generally applied in large excess to the sample,

a very high purity is even more crucial. The MALDI Matrices Selection Table below facilitates choosing the appropriate matrix for the use in proteomics and metabolomics.


Features and Benefits

- High chemical purity
- Low trace metal content to minimize adduct formation and simplify the resulting MS spectrum
- Ultra pure grades of the most popular matrix substances with extremely strict specifications concerning purity, trace metal content, appearance, and solubility

References

1. Karas, M., et al., Matrix-assisted ultraviolet laser desorption of nonvolatile compounds. *Int. J. Mass Spectrom. Ion Proc.*, 78, 53-68 (1987).
2. Hillenkamp, F., and Peter-Katalinic, J. (eds.), *MALDI MS. A Practical Guide to Instrumentation, Methods and Applications*, Wiley-VCH (2007).
3. Aebersold, R., and Mann, M., Mass spectrometry-based proteomics. *Nature*, 422, 198-207 (2003).
4. Dreisewerd, K., The desorption process in MALDI. *Chem. Rev.*, 103, 395-425 (2003).
5. Karas, M., and Krüger, R., Ion formation in MALDI. *Chem. Rev.*, 103, 427-439 (2003).
6. Knochenmuss, R., and Zenobi, R., MALDI ionization: The role of in-plume processes. *Chem. Rev.*, 103, 441-452 (2003).

Description	Purity	Abbreviation							Other Analytes	Note	Pack Sizes	Cat. No.
			Proteins	Peptides	Glycans	Oligonucleotides	Polymers	Lipids				
9-Aminoacridine	≥ 99.5%	9-AA							• Metabolites		1 g	92817
4-Bromo- α -cyanocinnamic acid	≥ 95%	BrCCA		•					• Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS		100 mg	89063
4-Bromo- α -cyanocinnamic acid-4-Chloro- α -cyanocinnamic acid mixture	≥ 95%	BrCCA:CICCA		•					• Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS		100 mg	68914
4-Aminoquinoline	≥ 99.0%					•			amino acids		1 g	05851
9-Nitroanthracene	≥ 98.5%	9-NA						•	fullerenes, humic acids		100 mg 1 g	56229
4-Phenyl-acyanocinnamamide	≥ 98.5%							•	MALDI imaging		100 mg	69028
Anthranilamide	≥ 99.0%		•	•	•						1 g	76884
Curcumin	≥ 99.5%							•	pharmaceuticals, drugs, MALDI imaging		100 mg	78246
(2E)-3-(9-Anthryl)-2-cyanoacrylic acid	≥ 97.0%								low molecular weight compounds		100 mg	83788
trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene] malononitrile	≥ 99.0%				•			•	Gold nanoparticles, fullerenes, organometallics, macrocycles		250 mg 1 g	87884
(E)-2-Cyano-3-(2-naphthyl) acrylic acid	≥ 98.0%								low molecular weight compounds		100 mg	94477

Description	Purity	Abbreviation							Other Analytes	Note	Pack Sizes	Cat. No.
			Proteins	Peptides	Glycans	Oligonucleotides	Polymers	Lipids				
4-Bromo- α -cyanocinnamic acid – α -Cyano-2,4-difluorocinnamic acid mixture	$\geq 95\%$	BrCCA:DiFCCA		•					•	Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	55841
Caffeic acid	$\geq 99.0\%$		•	•							1 g 5 g	60018
4-Chloro- α -cyanocinnamic acid	$\geq 95\%$	CICCA		•					•	Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	94141
4-Chloro- α -cyanocinnamic acid – α -Cyano-2,4-difluorocinnamic acid mixture	$\geq 95\%$	CICCA:DiFCCA		•					•		100 mg	39379
α -Cyano-2, 4-difluorocinnamic acid	$\geq 95\%$	DiFCCA		•						Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	77646
α -Cyano-4-fluorocinnamic acid	$\geq 95\%$	FCCA		•						Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	77081
α -Cyano-4-hydroxycinnamic acid	$\geq 99.0\%$	CHCA	•	•	•						250 mg 1 g	70990
α -Cyano-4-hydroxycinnamic acid	$\geq 99.5\%$, Ultra pure	CHCA	•	•	•						10 × 10 mg	39468
α -Cyano-4-hydroxycinnamic acid – α -Cyano-2, 4-difluorocinnamic acid – α -Cyano-2, 3, 4, 5, 6-pentafluorocinnamic acid mixture	$\geq 95\%$	CHCA:DiFCCA: PentaFCCA		•						Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	03841
α -Cyano-2, 3, 4, 5, 6-pentafluorocinnamic acid	$\geq 95\%$	PentawFCCA		•						Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	38419
1,5-Diamino naphthalene	$\geq 99.0\%$			•		•				1,5-DAN In-Source-Decay	250 mg	56451
2', 6'-Dihydroxy acetophenone	$\geq 99.5\%$	2,6-DHAP	•	•	•				•		1 g 5 g	37468
2, 5-Dihydroxybenzoic acid	$\geq 99.0\%$	DHB	•	•	•				•	Organic molecules	10 mg 250 mg 1 g	85707
2, 5-Dihydroxybenzoic acid	$\geq 99.5\%$, Ultra pure	DHB	•	•	•				•	Organic molecules	10 × 10 mg	39319
trans-Ferulic acid	$\geq 99.0\%$	FA	•	•							1 g 5 g	46278
2-(4-Hydroxy phenylazo) benzoic acid	$\geq 99.5\%$	HABA	•	•	•				•		1 g 5 g	54793
3-Hydroxypicolinic acid	$\geq 99.0\%$	3-HPA					•			Oligosaccharides	250 mg 1 g	56197
3-Nitrobenzyl alcohol	$\geq 99.5\%$										5 g	73148
3-Nitrobenzotrile	$\geq 99.0\%$	3-NBN								Tissues via MAIV	1 g	80362
Salicylamide	$\geq 99.0\%$						•				1 g	84228
Sinapic acid	$\geq 99.0\%$	SA	•	•						Dendrimers, Fullerenes	1 g 5 g	85429
Sinapic acid	$\geq 99.5\%$	SA	•	•						Dendrimers, Fullerenes	10 × 10 mg	49508
Super-DHB BioReagent		Super-DHB	•	•	•						10 × 10 mg 1 g 5 g	50862
2', 4', 6'-Trihydroxy acetophenone monohydrate	$\geq 99.5\%$	THAP	•	•	•	•					1 g 5 g	91928

Stable Isotope Labeled Bioactive Compounds

ISOTEC® Products for Use as Internal Standards

Stable isotope labeled compounds are used as internal standards for various MS techniques and within many applications. With chemical and ionization properties nearly identical to their unlabeled counterparts, stable isotope labeled compounds are often considered the top choice for an internal standard. Furthermore, the labeled standard and the analyte of interest can be easily differentiated by the mass shift between the two compounds, which is ideally three or more units.¹ ISOTEC® Stable Isotopes offers a large selection of labeled products suitable for this purpose. Labeled standards have been utilized within numerous applications, including quantification of cholesterol in a clinical setting,² vitamin D within baby formula,³ and B vitamins in human milk.⁴ Labeled internal standards have also been employed in research on the diagnosis of Graves disease⁵ and hypertension,⁶ the study of fatty acid oxidation,⁷ and the analysis of androgenic steroids in wastewater.⁸

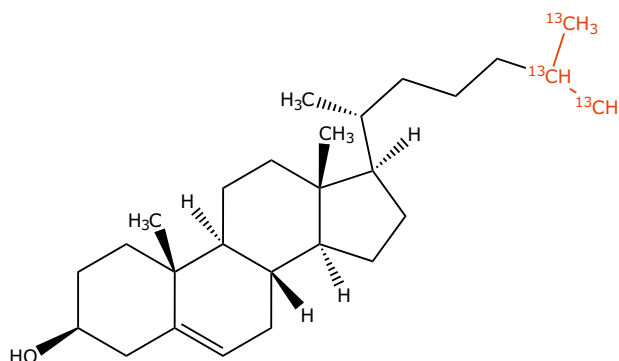
MS standards from ISOTEC® have high chemical and isotopic purities with labeling patterns including ¹³C, ¹⁵N, and deuterium. The ¹³C and/or ¹⁵N labels do not exchange within the mass spectrometer source, providing further advantage.⁹

ISOTEC® is also able to custom-synthesize labeled compounds upon request. Custom compounds can be designed with specific isotopes in specific locations. Whether a fully labeled or specifically labeled compound is of interest, let our expert team evaluate your needs.

Amino acids

Description	Cat. No.
DL-Alanine-2,3- ¹³ C ₂	485578
L-Arginine-2,3,3,4,4,5,5-d ₇ hydrochloride	776408
L-Arginine- ¹³ C ₆ hydrochloride	643440
DL-aspartic acid-2- ¹³ C, ¹⁵ N	492353
L-Citrulline-5- ¹³ C,4,4,5,5-d ₄	748935
L-Citrulline-4,4,5,5-d ₄	578886
L-Citrulline-5,5-d ₂	741833
DL-Cysteine-3,3-d ₂	900206
DL-Glutamic acid- ¹³ C ₅	604984
DL-Histidine-1- ¹³ C	588644
L-Leucine- ¹³ C ₆	605239
L-Lysine- ¹³ C ₆ hydrochloride	643459
L-Ornithine-3,3,4,4,5,5-d ₆ hydrochloride	749443
DL-Serine-1- ¹³ C	489107
DL-Valine-2- ¹³ C amine	592048

Additional products and labeling patterns are available.



References

1. Vogeser, M. and Seger, C., Pitfalls associated with the use of liquid chromatography-tandem mass spectrometry in the clinical laboratory. *Clin. Chem.*, 56, 1234-1244 (2010).
2. Edwards, S.H., et al., Proposed serum cholesterol reference measurement procedure by gas chromatography-isotope dilution mass spectrometry. *Clin. Chem.*, 57, 614-622 (2011).
3. Sullivan, D., Infant formula and adult/pediatric nutritional methods approved First Action using the AOAC voluntary consensus standards process. *J. AOAC Int.*, 95, 1-4 (2012).
4. Hampel, D., et al., Ultra-performance liquid chromatography tandem mass-spectrometry (UPLC-MS/MS) for rapid, simultaneous analysis of thiamin, riboflavin, flavin adenine dinucleotide, nicotinamide and pyridoxal in human milk. *J. Chromatogr. B*, 903, 7-13 (2012).
5. Higashi, T., et al., Stable isotope-dilution liquid chromatography/tandem mass spectrometry method for determination of thyroxine in saliva. *J. Chromatogr. B*, 879, 1013-1017 (2011).
6. Taylor, P.J., et al., Measurement of aldosterone in human plasma by semiautomated HPLC-tandem mass spectrometry. *Clin. Chem.*, 55, 1155-1162 (2009).
7. Mohammad, M.A., et al., Galactose promotes fat mobilization in obese lactating and nonlactating women. *Am. J. Clin. Nutr.*, 93, 374-381 (2011).
8. Backe, W.J., et al., Analysis of androgenic steroids in environmental waters by large-volume injection liquid chromatography tandem mass spectrometry. *Anal. Chem.*, 83, 2622-2630 (2011).
9. Ciccimaro, E. and Blair, I.A. Stable-isotope dilution LC-MS for quantitative biomarker analysis. *Bioanalysis*, 2(2), 311-341(2010).

To find additional stable isotope labeled standards, visit SigmaAldrich.com/isotec

To inquire about Stable Isotopes pricing and availability, email us at isosales@sial.com

Fatty acids

Description	Cat. No.
Arachidonic-5,6,8,9,11,12,14,15-d ₈ acid	735000
Decanoic-10,10,10-d ₃ acid	616125
cis-4,7,10,13,16,19-Docosahexaenoic-21,21,22,22,22-d ₅ acid	733326
cis-5,8,11,14,17-Eicosapentaenoic acid-19,19,20,20,20-d ₅	734322
Heptanoic-d ₁₃ acid	617040
trans-9-Hexadecenoic acid-1,2,3,7,8- ¹³ C ₅	722774
Lauric-d ₂₃ acid	451401
Linoleic acid- ¹³ C ₁₈	605735
Methyl heptadecanoate-d ₃₃	733148
Myristic acid-1,2- ¹³ C ₂	490865
Myristic acid-13,13,14,14,14-d ₅	614165
trans-6-Octadecenoic acid-1,2,3,4,5- ¹³ C ₅	722847
trans-9-Octadecenoic acid-1,2,3,7,8- ¹³ C ₅	722790
trans-11-Octadecenoic acid-1,2,3,9,10- ¹³ C ₅	722855
Octanoic acid- ¹³ C ₈	605727
Octanoic-d ₁₅ acid	448214
Oleic acid- ¹³ C ₁₈	490431
Palmitic acid- ¹³ C ₁₆	605573
Palmitic acid-d ₃₁	366897

Additional products and labeling patterns are available.

Glycerides & Lipids

Description	Cat. No.
Cholesteryl linoleate- ¹³ C ₁₈	729663
Cholesteryl-26,26,26,27,27,27-d ₆ oleate-1,2,3,7,8,9,10- ¹³ C ₇	729671
Glyceryl tri(palmitate-d ₃₁)	616966
Glyceryl tri(octanoate-d ₁₅)	617121
Glyceryl- ¹³ C ₃ trioleate	605638
Cholesteryl oleate- ¹³ C ₁₈	729523
Glyceryl tri(palmitate-1,2,3,4- ¹³ C ₄)	777862
2-Oleoyl-1-palmitoyl-rac-glycero-3-phosphocholine-(trimethyl-d ₉)	730041
Glyceryl-d ₅ trilinoleate	729507
Cholesteryl-26,26,26,27,27,27-d ₆ linoleate	729515
rac-Glyceryl-1,1,2,3,3-d ₅ -1,2-dioleate	723703
Glyceryl tri(oleate-1,2,3,7,8,9,10- ¹³ C ₇)	646253
1-Palmitoyl-rac-glycero-3-phosphocholine-(trimethyl-d ₉)	757438
Glyceryl tri(oleate-1- ¹³ C)	489514
Glyceryl tri(oleate-9,10- ¹³ C ₂)	646245
1-Palmitoyl-rac-glycero-3-phosphocholine-(trimethyl-d ₉)	757438
Glyceryl tri(stearate-1- ¹³ C)	492663

For a full listing of labeled lipid and fatty acid products, visit [SigmaAldrich.com/lipid](https://www.sigmaaldrich.com/lipid)
To inquire about Stable Isotopes pricing and availability, email us at isosales@sial.com

Steroids and Hormones

Description	Cat. No.
Aldosterone-2, 2, 4, 6, 6, 21, 21-d ₇	706035
Aldosterone-9,11,12,12-d ₄ solution	802883
4-Androstene-3, 17-dione-2, 3, 4- ¹³ C ₃ solution	730645
Cholesterol-2,3,4- ¹³ C ₃	749478
Cholesterol-2, 2, 3, 4, 4, 6-d ₆	488577
Cholesterol-25, 26, 27- ¹³ C ₃	707678
Corticosterone-9,11,12,12-d ₄	802905
Hydrocortisone-2,3,4- ¹³ C ₃ solution	803146
Cortisone-2, 3, 4- ¹³ C ₃ solution	803154
Dehydroepiandrosterone-2, 2, 3, 4, 4, 6-d ₆	709549
Dehydroepiandrosterone-2, 2, 3, 4, 4, 6-d ₆ sulfate sodium salt	723266
11-Deoxycortisol-2, 2, 4, 6, 6-d ₅	710784
Dihydrotestosterone-2, 3, 4- ¹³ C ₃ solution, 0.1 mg/mL	730637
17β-Estradiol-2, 3, 4- ¹³ C ₃	719552
17β-Estradiol-2, 4, 16, 16, 17-d ₅	613967
Estriol-2, 3, 4- ¹³ C ₃	731668
Estrone-2, 3, 4- ¹³ C ₃	719544
Estrone-2,3,4- ¹³ C ₃ solution	802921
18-Hydroxycorticosterone	710806
Hydrocortisone-9, 11, 12, 12-d ₄	705594
17-α-Hydroxypregnenolone-20, 21- ¹³ C ₂ -16,16-d ₂	803081
Pregnenolone-20, 21- ¹³ C ₂ -16, 16-d ₂	739545
Pregnenolone-20, 21- ¹³ C ₂ -16, 16-d ₂ sulfate sodium salt	740985
Progesterone-2, 3, 4- ¹³ C ₃	737143
Progesterone-2, 3, 4- ¹³ C ₃ solution	803065
Testosterone-2, 3, 4- ¹³ C ₃ solution	730610
3α, 5β-Tetrahydroaldosterone	750026
3, 3', 5'-Triiodothyronine-(diiodophenyl- ¹³ C ₆) hydrochloride	709719
3, 3', 5'-Triiodothyronine-(tyrosine ring- ¹³ C ₆) hydrochloride	709611
Chenodeoxycholic-2,2,3,4,4,6,6,7,8-d ₉ acid	809667
Cholesterol-23,24,25,26,27- ¹³ C ₅	809837
Pregnenolone-2,2,4,4-d ₄	809845
Allopregnanolone-2,2,3,4,4-d ₅ solution	809853
Etiocolanolone-2,2,3,4,4-d ₅ solution	809861
Cortisone-2,3,4- ¹³ C ₃ 21-sulfate sodium salt solution	900079
Hydrocortisone-9,11,12,12-d ₄ 21-sulfate sodium salt	900080
L-Thyroxine-1",1",2,2",6-d ₅ hydrochloride solution	900067
Cortisone-2,2,4,6,6,9,12,12-d ₈	900170
Tetrahydrocortisol-2,2,3,4,4-d ₅	900182
Tetrahydrocortisone-2,2,3,4,4-d ₅	900183

For a full listing of labeled vitamins, steroids and hormones, visit [SigmaAldrich.com/sibio](https://www.sigmaaldrich.com/sibio)
To inquire about Stable Isotopes custom synthesis or pricing and availability, email us at isosales@sial.com

Vitamins

Description	Cat. No.
Biotin-(ring-6, 6-d ₂)	705268
Coenzyme Q10-(ring-d ₉)	802891
Folic acid-(glutamic acid- ¹³ C ₅ , ¹⁵ N)	803162
Folic acid-(glutamic acid- ¹³ C ₅)	803049
25-Hydroxyvitamin D ₃ -(26,26,26,27,27,27-d ₆)	803030
(24R), 24,25-Dihydroxyvitamin D ₃ -26,26,26,27,27,27-d ₆ solution	802913
25-Hydroxyvitamin D ₃ -(23-24-25-26-27- ¹³ C ₅) solution	803103
25-Hydroxyvitamin D ₂ solution	740217
25-Hydroxyvitamin D ₂ (6, 19, 19-d ₃) solution	740071
25-Hydroxyvitamin D ₂ (6, 19, 19-d ₃)	705497
25-Hydroxyvitamin D ₃ solution	739650
25-Hydroxyvitamin D ₃ (6, 19, 19-d ₃)	705888
Nicotinamide-2, 4, 5, 6-d ₄	762970
Pyridoxal-(methyl-d ₃) hydrochloride	705187
Pyridoxamine-(methyl-d ₃) dihydrochloride	705322
Riboflavin-dioxypyrimidine- ¹³ C ₄ , ¹⁵ N ₂	705292
Thiamine-(4-methyl- ¹³ C-thiazol-5-yl- ¹³ C ₃) hydrochloride	731188
α-Tocopherol-(ring-5, 7-dimethyl-d ₆)	731234
Vitamin B ₅ (di-β-alanine- ¹³ C ₆ , ¹⁵ N ₂) calcium salt	705837
Vitamin B ₁₂ -(dimethylbenzimidazole- ¹³ C ₇) solution	803170
Vitamin D ₂ (6,19,19-d ₃)	705489
Vitamin D ₂ (6,19,19-d ₃) solution	739839
Vitamin D ₃ (6,19,19-d ₃) solution	740284
	731285
Vitamin E acetate-(trimethyl-d ₉)	615366
Vitamin K-d ₄ -(5,6,7,8-d ₄ , 2-methyl-d ₃)	705470
Vitamin K ₃ -d ₈	737836
Biotin-2',2',3',3'-d ₄	809608
Pyridoxine-(methyl-d ₃) hydrochloride	809659
1α,25-Dihydroxyvitamin D ₃ -26,26,26,27,27,27-d ₆ solution	809926
(24R)-24,25-Dihydroxyvitamin D ₃ solution	809748
Vitamin D ₃ -25,26,27- ¹³ C ₃ solution	809756
Vitamin D ₃ -23,24,25,26,27- ¹³ C ₅ solution	900234
Vitamin D ₃ -23,24,25,26,27- ¹³ C ₅ solution	809772
Nicotinamide-2,6,7- ¹³ C ₃ -(pyridyl- ¹⁵ N)	809799
Vitamin K ₁ -4a,5,6,7,8,8a- ¹³ C ₆	809888
Vitamin K ₂ (MK-4)-(5,6,7,8-d ₄ ,2-methyl-d ₃)	809896
Vitamin K ₂ (MK-4)-4',5,6,7,8,8'- ¹³ C ₆	809918
Vitamin K ₂ (MK-7)-(5,6,7,8-d ₄ ,2-methyl-d ₃)	900074
Vitamin K ₂ (MK-9)-(5,6,7,8-d ₄ ,2-methyl-d ₃)	900076
Vitamin K ₂ (MK-7)-4',5,6,7,8,8'- ¹³ C ₆	900075
Vitamin K ₂ (MK-9)-4',5,6,7,8,8'- ¹³ C ₆	900077

Metabolites

Description	Cat. No.
5-Hydroxyindole-3a,4,5,6,7,7a- ¹³ C ₆ -3-acetic acid	809616
Sodium taurochenodeoxycholate-2,2,4,4-d ₄	809683
Sodium taurochenodeoxycholate-2,2,3,4,4,6,6,7,8-d ₉	809691
Sodium taurocholate-2,2,4,4-d ₄	900036
Sodium taurodeoxycholate-2,2,4,4,11,11-d ₆	900078
Sodium taurodeoxycholate-2,2,4,4-d ₄	900073
Sodium tauroolithocholate-2,2,4,4-d ₄	809713
Sodium tauroursodeoxycholate-2,2,4,4-d ₄	809721
Indoxyl-3a,4,5,6,7,7a- ¹³ C ₆ sulfate potassium salt	809780

Other Bioactive Compounds

Description	Cat. No.
L-Arbrine-(methyl-d ₃)	750913
Aldicarb-(N-methyl- ¹³ C ₃ , d ₃ , carbomoyl- ¹³ C)	733865
Aldicarb-(N-methyl- ¹³ C ₃ , d ₃ , carbomoyl- ¹³ C) sulfone	733873
(±)-Catechin-2,3,4- ¹³ C ₃	719579
Chenodeoxycholic acid-2,2,4,4-d ₄	614122
Cholic acid-2,2,4,4-d ₄	614149
Deoxycholic acid-2,2,4,4-d ₄	614130
Desethylamodiaquine-(ethyl-d ₅)	705349
3, 3'-Diiodo-L-thyronine-(phenoxy- ¹³ C ₆) (T2)	719528
3, 3'-Diiodo-L-thyronine (T2)	719536
4, 6-Dioxoheptanoic acid-3,4,5,6,7- ¹³ C ₅	749001
Ferulic acid-1,2,3- ¹³ C ₃	722820
Glycocholic-2,2,4,4-d ₄ acid	739723
Histamine-α, α, β, β-d ₄ dihydrochloride	762962
Kynurenic acid-3,5,6,7,8-d ₅	793477
Spermidine-(butane-d ₈) trihydrochloride	709891
Spermidine-(butane- ¹³ C ₄) trihydrochloride	740780
Spermine-(butane-d ₈) tetrahydrochloride	705330
Vinblastine- ¹³ C ₃	746274
Yohimbine-(methyl- ¹³ C ₃ ester)	731242
(±)-Epicatechin-2,3,4- ¹³ C ₃ gallate	900368
(±)-Epigallocatechin-2,3,4- ¹³ C ₃	900369
(±)-Epigallocatechin-2,3,4- ¹³ C ₃ gallate	900376
(±)-Catechin-2,3,4- ¹³ C ₃ gallate	900370
(±)-Gallocatechin-2,3,4- ¹³ C ₃	900371
(±)-Gallocatechin-2,3,4- ¹³ C ₃ gallate	900372
α-Tocopherol-(phenyl- ¹³ C ₆)	900374
11-Deoxycortisol-2,3,4- ¹³ C ₃ solution	809594
11-Deoxycorticosterone-2,3,4- ¹³ C ₃ solution	809586
Dehydroepiandrosterone-2,2,3,4,4-d ₅	809640
Exemestane-(3,4- ¹³ C ₂ -6-methylidene- ¹³ C)	809802
Clodinafop-propargyl-(phenoxy- ¹³ C ₆)	809810
Atrazine-(triazyl- ¹³ C ₃ , ¹⁵ N ₃)	809829

Metabolism Assay Kits

We offer a wide range of kits for analyzing both critical metabolites and the activity of key metabolic enzymes. These kits offer convenient, simple, and highly-dependable assays for monitoring metabolic pathways.

- Amino acid Metabolism Assay Kits
- Carbohydrate Metabolism Assay Kits
- Cholesterol Metabolism Assay Kits
- Coenzymes and Cofactors Metabolism Assay Kits
- Fatty acid and Lipid Metabolism Assay Kits
- Glycolysis Metabolism Assay Kits
- Nutritional Analysis and Quantitation
- Oxidative Stress Assay Kits
- TCA Cycle Metabolism Assay Kits
- Inorganic Ions Metabolism Assay Kits
- Blood and Urine Chemistry Assay Kits
- Enzymatic Activity Assay Kits



Features and Benefits

- Convenient, simple and highly-dependable assays for monitoring metabolic pathways
- Assay kits utilize spectrophotometric, fluorometric, and/or gravimetric detection methods
- Kits contain all necessary components and reagents for analysis
- Most assay kits are suitable for high-throughput assays

General Assay Design



For more information, visit [SigmaAldrich.com/assaykits](https://www.sigmaaldrich.com/assaykits)

BIOshell™ Glycan HPLC Columns

Empowering the Analysis of Glycoproteins with Exceptional Reproducibility

Characterizing and monitoring the glycosylation pattern of a biotherapeutic protein is required by regulatory authorities due to the fact that safety, efficacy and the serum half-life of therapeutic proteins can be affected by differences in their glycosylation pattern. Analysis and identification of glycoproteins can be challenging, however, because of the structural complexity of N-linked and O-linked sugar molecules. Hydrophilic interaction liquid chromatography (HILIC) is a proven technique for the separation and quantitation of isolated glycans under native conditions or after their derivatization with fluorescent labels.

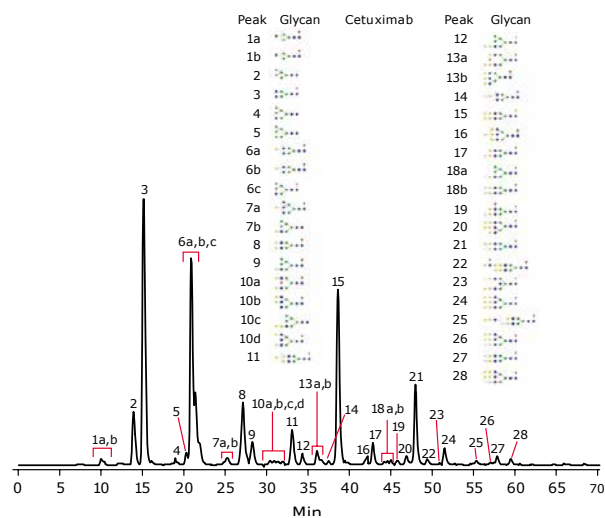
BIOshell™ Glycan HPLC columns are specifically engineered to deliver fast, high resolution, reproducible glycan separation using HILIC chromatography. There are many advantages to using Fused-Core® BIOshell™ Glycan HPLC columns for glycoprotein analysis:

- Increased resolution, faster separations, and lower back pressure – BIOshell™ HPLC columns utilize Fused-Core® particle technology which offers significant performance benefits over traditional columns based on totally porous particles
- Excellent reproducibility – Quality control testing requires tight retention time and peak width specifications ensuring lot-to-lot reproducibility
- Complimentary Sigma-Aldrich products – Sigma-Aldrich® supplies reagents and consumables needed for each step in glycoprotein analysis as indicated in Table 1.

Steps in Glycoprotein Analysis



Figure 1. BIOshell™ Glycan Column Separation of Procainamide Labeled Cetuximab Glycans

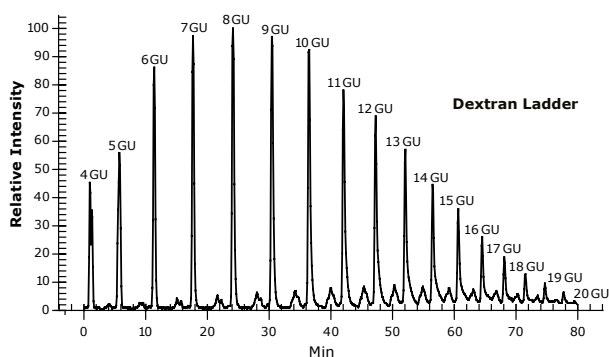


Cetuximab is a chimeric mouse-human IgG1 monoclonal antibody against the epidermal growth factor receptor. It is used to treat head, neck, and colorectal cancers. The antibody is N-glycosylated both in the Fc and Fab regions, which have been shown to impact safety and quality of the drug. Thus, characterizing its glycosylation pattern is exceptionally important. As shown in this application, the BIOshell™ Glycan column is able to elucidate the complex glycosylation of this biotherapeutic, allowing a better understanding of the drug's efficacy.

For a complete protocol detailing glycoprotein analysis, including testing conditions, visit SigmaAldrich.com/BIOshell

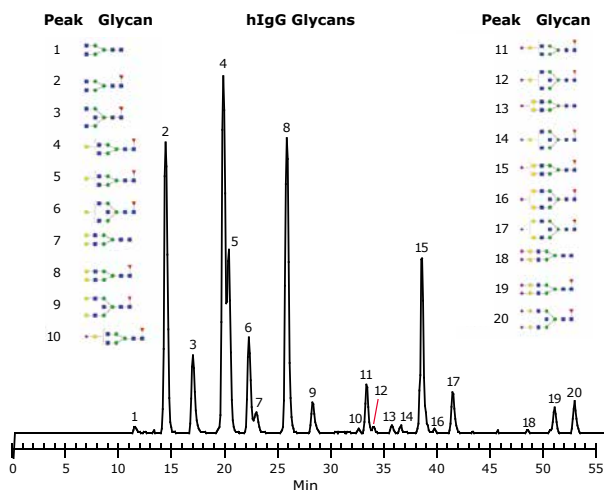
BIOshell™ Glycan Applications

Figure 2. BIOshell™ Glycan Column Separation of a Procainamide Labeled Dextran Ladder



The dextran ladder is used as an external standard for the analysis of glycans by HILIC mode HPLC after fluorescent labeling. When analyzed on the BIOshell™ Glycan HPLC column, this standard gives a characteristic ladder profile from monomeric glucose to a 20-mer glucose oligosaccharide. This ladder provides calibration reference points that can aid in identifying more complex glycans based upon retention characteristics.

Figure 3. BIOshell™ Glycan Column Separation of Procainamide Labeled Human IgG Glycans



A sample of human IgG glycans was analyzed on a BIOshell™ Glycan HPLC column resulting in the identification of 20 distinct peaks. Glycans were identified by mass spectrometry, which was coupled in line with the HPLC-fluorescence detector system. Excellent separation as well as symmetrical peak shape can be observed in the chromatogram.

Get Started

Additional resources are available for helping you implement BIOshell™ Glycan columns into your laboratory.

For product information, webinars, ordering and real time availability information, visit

SigmaAldrich.com/BIOshell

Table 1. Sigma-Aldrich Reagents and Consumables for Glycoprotein Analysis

Description	Cat. No.
Step 1: Glycan release	
IgG from human serum	I4506
Trizma® HCl	T5941
Urea	U0631
Ammonium bicarbonate	9830
PNGase F	7367
Step 2: Procainamide labeling	
Sodium cyanoborohydride	156159
Procainamide hydrochloride	P9391
Dimethyl sulfoxide	D8418
Acetic acid	320099
Water	39253
Dextran hydrolysate	31417
Step 3: Cleanup	
Acetonitrile	34851
DPA-6S 50 mg cartridges	52624-U
Step 4: LC-MS analysis	
BIOshell™ glycan, 15 cm × 2.1 mm I.D., 2.7 µm	50994-U
Ammonium formate	17843
Formic acid	94318

BIOshell™ Glycan Fused-Core® Silica Characteristics

- Pore Size – 90 Å
- Max Temp. – 65 °C
- Pressure – 1,000 bar (14,500 psi)
- Operating pH Range – 2–9
- Surface Area – 135 m²/g

BIOshell™ Glycan Fused-Core® HPLC Columns

Particle Size	I.D.	Length	Cat. No.
2.7 µm	2.1 mm	10 cm	50993-U
2.7 µm	4.6 mm	10 cm	50998-U
2.7 µm	2.1 mm	15 cm	50994-U
2.7 µm	4.6 mm	15 cm	50999-U
2.7 µm	2.1 mm	5 cm	50991-U
2.7 µm	4.6 mm	5 cm	50997-U

Our technical service staff is ready to answer questions

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Translation to Clinical Applications

The understanding of the genetic and environmental factors influencing health and disease remains a major challenge in the 21st century. The increasing utilization of molecular tools in medicine to analyze samples of body fluids or tissues, in vitro or in-vivo, requires new global standards relevant to patient biology at the individual and population level. Although metabolites have been used for diagnoses and treatments for centuries, the elucidation of biochemical pathways and the development of new analytical technologies have moved the frontiers to define variations of a person's physiological and pathological states. From its foundation Sigma-Aldrich's aim was to enable researchers to expand

the frontiers of metabolic pathways to elucidate biomarkers for drug development or clinical diagnostics.

The search for disease biomarkers in urine, breath or blood is highly attractive due to established metabolite analysis in routine clinical chemistry analysis. The focus has however been restricted to a small number of metabolites for which the corresponding rapid analytical methods have been highly automated. New methodologies in metabolomics research allowing the simultaneous analysis of a large number of metabolites enable new discoveries of disease-related metabolites.

Inborn Errors of Metabolism of Amino acids

Characteristic Metabolites for Inborn Errors of Amino acid Metabolism

Inborn errors of metabolism are caused by changes in specific enzymatic reactions and hundreds of different such alterations, which affect about 1 of every 5,000 new-borns, have been characterized thus far. The first inborn errors of metabolism, described in the beginning of the 20th century by Sir Archibald Garrod, dealt with alkaptonuria, pentosuria, cystinuria and albinism. Infants and children with treatable errors of metabolism can be identified by screening newborns for meaningful metabolite biomarkers. Several classic inborn errors of metabolism can be detected by the accumulation of certain amino acids in body-fluids like serum and urine. Phenylketonuria (PKU) is an inherited metabolic disorder in which individuals do not have the ability to further metabolize phenylalanine. Fortunately, this metabolic disorder can be analyzed by the urinary excretion of phenylalanine and successfully treated by dietary restriction.

Urinary excretion of the branched chain amino acids leucine, valine and isoleucine is an indicator for

maple syrup urine disease, N-acetylaspartic acid for Canavan disease and tyrosine and N-acetyltyrosine for tyrosinemia type I. The identification of new amino-acid biomarkers for amino-acid-related metabolic disorders is of major importance to biomedical research.

Newborns are not typically screened for other metabolic disorders and as a result, these disorders are often only detected in infants and children after damage has occurred and effects such as developmental delay and mental retardation become apparent. Early detection involving a blood sample analysis for a metabolic marker can reduce such consequences by nutritional adaptations and dietary restriction. Simultaneous enzyme and metabolite tests from a single patient sample are needed for the efficient diagnosis of inborn errors of metabolism in an individual.

Description	Cat. No.
<i>N</i> -Acetyl- <i>L</i> -aspartic acid, puriss., ≥ 99.0% (T)	00920
<i>N</i> -Acetyl- <i>L</i> -tyrosine, ≥ 98.0% (T)	01527
γ-Aminobutyric acid, SigmaUltra, ≥ 99%	A5835
Argininosuccinic acid disodium salt hydrate, ≥ 80%	A5707
<i>L</i> -Citrulline, ≥ 98% (TLC)	C7629
<i>L</i> -Cystathionine, ~ 90% (TLC)	C7505
Fumaric acid, purum, ≥ 99.0% (T)	47910
Glutaric acid, 99%	G3407
dl-Homocysteine, ≥ 95% (titration)	H4628
<i>L</i> -Homocystine, ≥ 98% (TLC)	H6010

Description	Cat. No.
Homogentisic acid	H0751
3-Hydroxy-3-methylglutaric acid, ≥ 95%	H4392
<i>L</i> -Isoleucine, ≥ 99.5% (NT)	58879
Isovaleric acid, 99%	129542
<i>L</i> -Leucine, ≥ 99.5% (NT)	61819
Melanin	M8631
Methylmalonic acid, 99%	M54058
<i>L</i> -Phenylalanine, ≥ 99.0% (NT)	78019
<i>L</i> -Tyrosine, ≥ 99.0% (NT)	93829
<i>L</i> -Valine, ≥ 99.5% (NT)	94619

Genotype-Phenotype Relationships in Inborn Errors of Metabolism

More than a century has passed since Archibald Garrod connected the excretion of homogentisic acid in normal and alkaptonuric members of families with an alternative course of metabolism and entitled his report specifically as a study in chemical individuality.¹ This concept was later generalized in his book on "Inborn Factors of Disease".² The tremendous work on the knowledgebase in human genetic disorders in "Mendelian Inheritance in Man" (MIM) by Victor A. McKusick published first in book form in twelve printed editions and various

translations and subsequently in its online version OMIM, is a great resource for the relationships between phenotype and genotype in teaching, research, applications and the clinic.^{3,4}

From the early days of the analysis of inborn errors of metabolism up to the present we are offering an ever increasing range of metabolites for research and applications in order to support the establishment of genotype-phenotype relationships and to decrease the gap between the known and the available metabolites.

Selected Metabolites for Genotype-Phenotype-Relationships in Inborn Errors of Metabolism

Genotypes			Phenotypes		Metabolites	
Chromosome	Gene/Locus	MIM No.	Phenotype	MIM No.	Description	Cat. No.
17q21.31	G6PC	613742	Glycogen storage disease (von Gierke Disease)	232200	D-Glucose 6-phosphate disodium salt hydrate	G7250
13q32.3	PCCA	606054	Propionic acidemia	232000	Trisodium (2RS,3RS)-2-methylcitrate	59464
3q22.3	PCCB	606054	Propionic acidemia	232050	Trisodium (2RS,3RS)-2-methylcitrate	59464
21q22.3	CBS		Homocystinuria (CBS deficiency)	236200	L-Homocystine	H6010
					L-Homocysteine	69453
2q37.3	D2HGDH	609186	D-2-Hydroxyglutaric aciduria 1	600721	D- α -Hydroxyglutaric acid disodium salt	H8378
15q26.1	IDH2	147650	D-2-Hydroxyglutaric aciduria 1	613657	D- α -Hydroxyglutaric acid disodium salt	H8378
14q21.3	L2HGDH	609584	L-2-Hydroxyglutaric aciduria	236792	L- α -Hydroxyglutaric acid disodium salt	90790

1. A.E.Garrod, The incidence of alkaptonuria: a study in chemical individuality, *Lancet* 2,1616-1620 (1902).

2. A.E.Garrod, The inborn factors in disease: an essay, Clarendon Press, Oxford, United Kingdom (1931).

3. V.A.McKusick, A 60-year tale of spots, maps, and genes, *Annual Review Genomics Human Genetics* 7, 1-27 (2006).

4. V.A.McKusick, Mendelian Inheritance in Man and Its Online Version OMIM, *The American Journal of Human Genetics*, 80, 588-604 (2007).

Characteristic Metabolites for Inborn Errors of Lipid Metabolism

Hereditary disorders in lipid metabolism include Tay-Sachs disease, Gaucher disease, Niemann-Pick disease, metachromatic leucodystrophy, Fabry disease, Refsum disease, and Tangier disease. These lipidoses are characterized by dysfunctional lipid metabolism and result in abnormal metabolite accumulations. One of the first disorders recognized as an inborn error of lipid metabolism was Refsum disease, which produces toxic levels of phytanic acid if untreated.

Gaucher disease is a progressive sphingolipid-degradation disease characterized by genetic mutations in the lysosomal enzyme glucocerebrosidase, which leads to decreased enzymatic activity. Measurements of the metabolites methylcholine, phosphatidylcholine, and sphingomyelin are important for studying the pathophysiology of Gaucher disease. The main therapy used to treat Gaucher disease is enzyme-replacement therapy in order to normalize sphingolipid degradation and to prevent tissue damage caused by sphingolipid accumulation. Another promising therapeutic approach to Gaucher disease is to decrease the tissue glucocerebrosidase level to a concentration which can be cleared by the existing glucocerebrosidase. A deficiency of the lysosomal enzyme α -galactosidase A results in the progressive accumulation of the glycosphingolipids globotriaosylceramide Gb3 and digalactosyl-ceramide in Fabry disease, which can cause early death from cardiac, renal, and cerebrovascular events.

Dimethylglycine dehydrogenase (DMGDH) deficiency is an inborn error of choline metabolism caused by a mutation in the gene hDMGDH and results in increased N,N-dimethylglycine concentrations of 100-fold in serum and 20-fold in urine.

Nine inborn errors of bile acid metabolism have been identified that result in enzyme deficiencies and damaged bile acid biosynthesis in infants, children, and adults. Since bile acids have several important physiological functions, such as emulsifying fats and fat-soluble vitamins, and involvement in cholesterol, bilirubin, xenobiotics, and drug metabolites elimination, a failure in the multistep enzymatic conversion of cholesterol to bile acids will accumulate unusual bile acids and metabolic intermediates.

Description	Cat. No.
O-Acetyl-L-carnitine hydrochloride	A6706
N,N-Dimethylglycine	D1156
N,N-Dimethylglycine hydrochloride	D6382
Globotriaosylsphingosine from porcine blood	G9534
dl-Hexanoylcarnitine chloride	H2132
3-Hydroxy-3-methylglutaric acid	H4392
Palmitoyl-L-carnitine chloride	P1645
Palmitoyl-dl-carnitine chloride	P4509
Phytanic acid, mixture of isomers	P4060
Pristanic acid solution, mixture of isomers	P6617

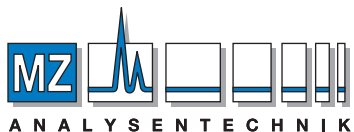


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