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

Sigma-Aldrich®
Lab & Production Materials

Navigate Toward

Metabolomic Discovery

Before testing new drugs, metabolomic pathways need to be thoroughly investigated. Our broad range of >1300 products, including metabolites, enzymes, separation tools, and metabolite analysis and labeling, help you navigate the metabolic pathways to biomarker discovery. Whether your metabolomics research involves targeted or untargeted metabolomics workflows, our integrated approach for profiling, pinpointing and designating compounds provides efficient and reliable results. This reference guide provides a brief overview of these products.

Stay on course with our metabolomics resources.

Our Learning Center supports your research endeavors with interactive metabolic charts to search, explore and expand pathways, as well as instructive webinars, explanatory technical notes and literature, Nicholson metabolic minimaps, and other useful tools.

For more information, please visit:
SigmaAldrich.com/Metabolomics

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International Union of Biochemistry and Molecular Biology (IUBMB)-Nicholson Interactive Metabolic Pathways Tool
Metabolites, Standards, and Enzymes
Metabolomics Workflow
Metabolite Analysis and Labeling
Metabolomics Applications

IUBMB-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.

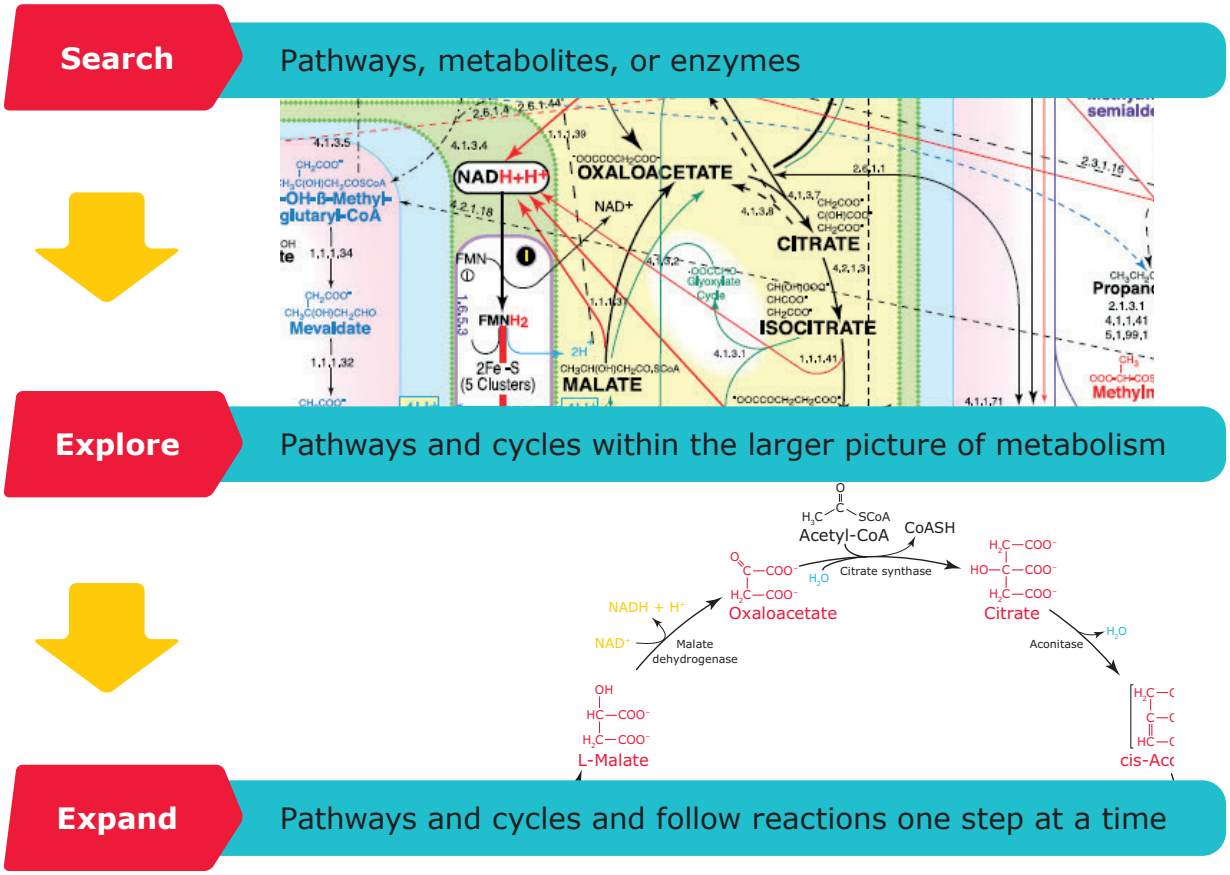
Key Features and Benefits

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"
- Colored pins differentiate metabolites from enzymes
- Pins drop upon searching any of 1,100 metabolites and enzymes and their associated pathways
- Click pins to view more information or see related products

Discover your pathway at
SigmaAldrich.com/metpath

TCA Cycle



Metabolic Pathway Map

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 product information via the catalog number links

Example of Product Information

Acetyl-Coa

Classication: Acyl CoAs

Pathway(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 (Krebs cycle). It is also a key precursor in lipid biosynthesis and the source of all fatty acid carbons.

Product Name: Acetyl coenzyme A sodium salt

Catalog No. A2056

Inborn Errors of Metabolism Chart

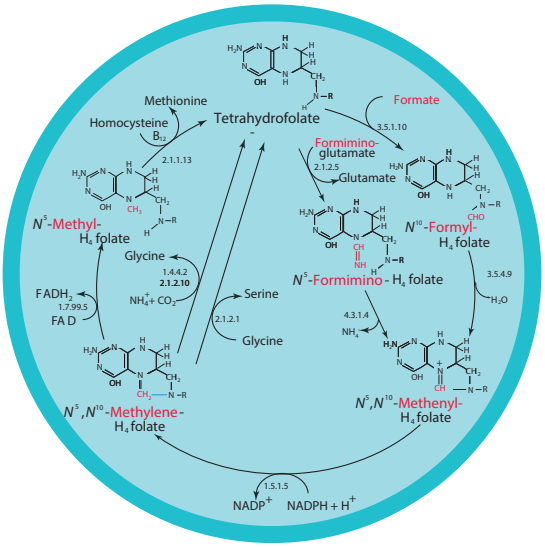
Every characteristic of human anatomy and physiology is determined by biochemical reactions catalyzed by enzymes. These in turn are determined by our genetic make-up. If a gene is defective or missing, it will result in a defective or missing enzyme, a so-called “inborn error of metabolism.” The Inborn Errors of Metabolism Map includes over 100 metabolic deficiency diseases that are named on the map.

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

IUBMB-Nicholson Minimaps

Look at selected individual pathways enlarged to illustrate aspects of metabolism, such as compartmentalization and regulation. Minimaps expand the information provided in the Metabolic Pathways Chart.

Find the interactive Metabolic Pathways Chart, minimaps, and animaps at **SigmaAldrich.com/metpath**



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 ($FADH_2$)
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-tetrahydofolate ligase

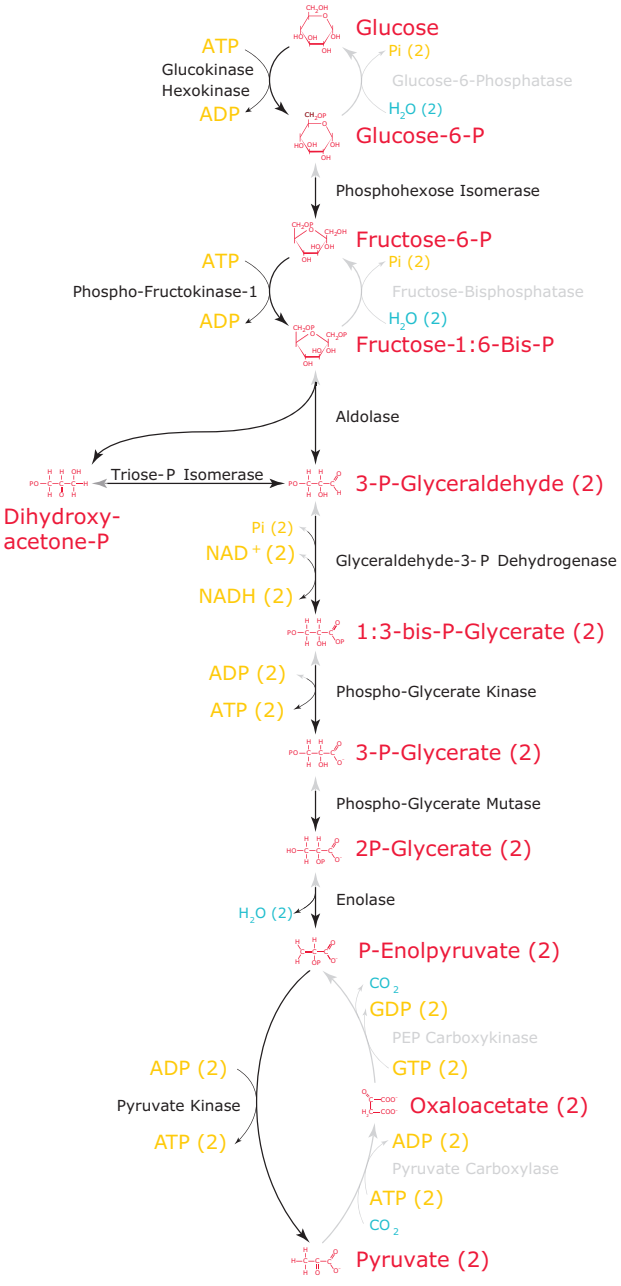
Metabolites, Standards, and Enzymes

Glycolysis Pathway

Glycolysis is the primary pathway that converts glucose into pyruvate. The glycolytic pathway is highly upregulated 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

Product 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_2O	39705
DL-Glyceraldehyde 3-phosphate solution 45–55 mg/mL in H_2O	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%	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

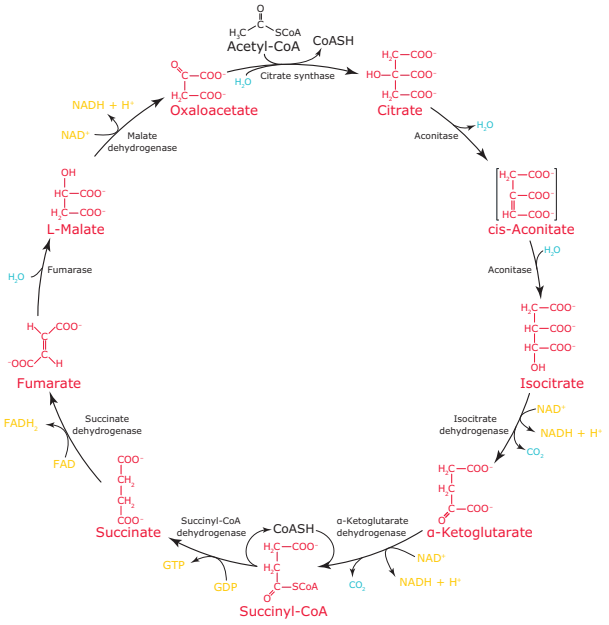
Product Description	Cat. No.
Aldolase from rabbit muscle ammonium sulfate suspension, 10 – 20 units/mg protein	**A8811**
Creatine Phosphokinase from rabbit muscle Type I, salt-free, lyophilized powder, ≥ 150 units/mg protein	**C3755**
Enolase from baker's yeast (S. cerevisiae) lyophilized powder, ≥ 50 units/mg protein	**E6126**
Fructose-6-phosphate Kinase from Bacillus stearothermophilus 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 Saccharomyces cerevisiae Type F-300, lyophilized powder, ≥ 130 units/mg protein (biuret)	**H4502**
Invertase from baker's yeast (S. cerevisiae) 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 (S. cerevisiae) Type III, ammonium sulfate suspension, ≥ 400 units/mg protein (biuret)	**P5381**
3-Phosphoglyceric Phosphokinase from baker's yeast (S. cerevisiae) 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

Product 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**



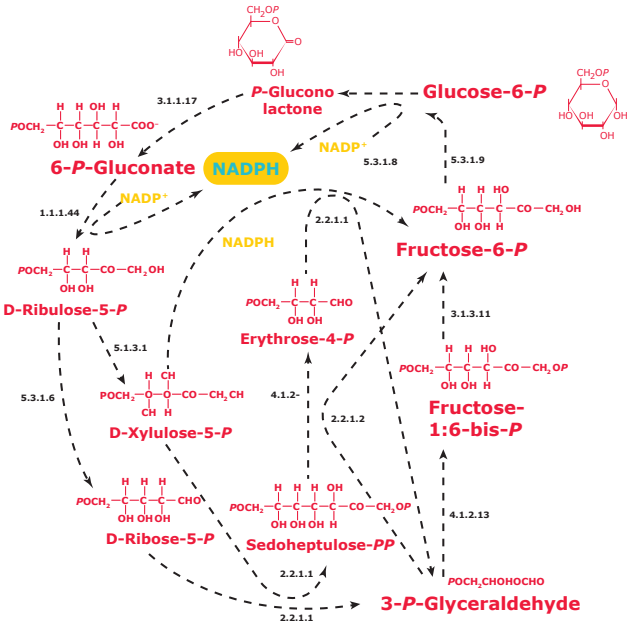
Key TCA Cycle Enzymes

Product 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 the pentose phosphate pathway, operates in tissues that synthesize fatty acids and steroids.

Product 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



Key Pentose Phosphate Pathway Enzymes

Product 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 (S. cerevisiae) Type XV, lyophilized powder, 200 – 400 units/mg protein (modified Warburg-Christian)	G6378
Transketolase from E. coli ≥ 0.1 units/mg	68138
Transaldolase from baker's yeast (S. cerevisiae) lyophilized powder, 10 – 30 units/mg protein (biuret)	T6008
Hexokinase from Saccharomyces cerevisiae 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 (S. cerevisiae) lyophilized powder, 50 – 100 units/mg protein (modified Warburg-Christian)	R3251
Triose-phosphate isomeraseTriosephosphate Isomerase from rabbit muscle Type X, lyophilized powder, ≥ 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 (S. cerevisiae) 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 cycle in one convenient format.

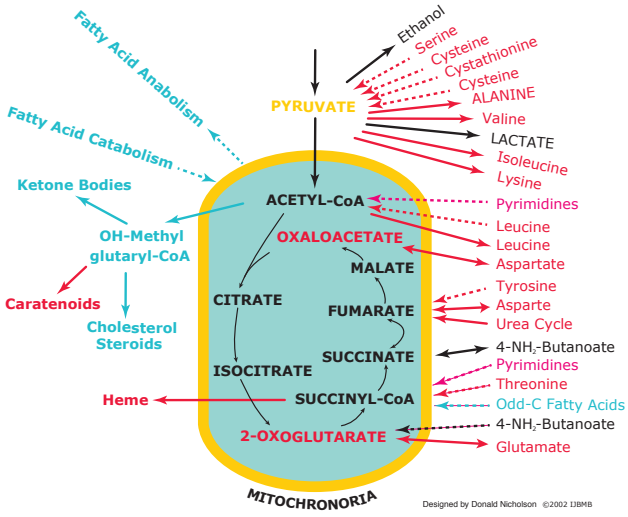
TCA Cycle Metabolite Library

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

Components

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

ML0100-1KT	1 kit



Product Description	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

Product Description	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 (Supelco)	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 (Supelco)	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 (Supelco)	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

Product Name	Product 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 mmoles/mL ±4% in 0.1 N HCl	**A6282**

Fatty Acids & Lipid Metabolite Kits

Individually packaged, quantities indicated, analytical standard

Product Name	Cat. No.
Fatty Acid Kit	**EC10A-1KT**
Fatty Acids, Odd Carbon Straight Chains Kit	**OC9-1KT**
Fatty Acids Unsaturated Kit	**UN10-1KT**
Triglycerides Kit	**TRI19-1KT**
Triglycerides, Saturated, Even Carbon Kit	**TRI11-1KT**

LC-MS Certified Spiking Solutions and Reference Materials

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

Cerilliant® 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® facilities are fully documented through 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® quality credentials include accreditations to ISO Guide 34, ISO/IEC 17025 and certification to ISO 13485 and ISO 9001. Cerilliant® quality systems incorporate 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**

Supelco®
Analytical Products

Mass Spectrometry Metabolite Library of Standards

Supplied by IROA Technologies

MSMLS™ (Mass Spectrometry Metabolite Library of Standards) and LSMLS™ (Large Scale Metabolite Library of Standards) collections of high-quality small biochemical molecules span a broad range of primary metabolism uses. These are high purity (>95%) compounds supplied in an economical, ready-to-use format. The library of standards is 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 perform NMR, functional cellular assays, phenotypic screening and limit of detection.

Features

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

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

MSMLS™ library feature 619 unique metabolites as 5 µg dried weight

LSMLS™ library features 504 unique metabolites as 1 mg dried weight

Benefits

- 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 flows

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

Fatty Acid Metabolite Library	**FAMLS-1EA**
Organic Acid Metabolite Library	**OAMLS-1EA**

For more information, visit
SigmaAldrich.com/IROA

IROA TECHNOLOGIES
...making metabolic profiling easy®

Ordering Information

Description	Cat. No.
Mass Spectrometry Metabolite Library	**MSMLS-1EA**
Large Scale Metabolite Library	**LSMLS-1EA**
Large Scale Metabolite Library (International)	**LSMLSINT-1EA**
MSMLS™ Plate 1 (Water Soluble)	**MSMLS01-1EA**
MSMLS™ Plate 2 (Water Soluble)	**MSMLS02-1EA**
MSMLS™ Plate 3 (Water Soluble)	**MSMLS03-1EA**
MSMLS™ Plate 4 (Water Soluble)	**MSMLS04-1EA**
MSMLS™ Plate 5 (Water Soluble)	**MSMLS05-1EA**
MSMLS™ Plate 6 (Lipophilic)	**MSMLS06-1EA**
MSMLS™ Plate 7 (Lipophilic)	**MSMLS07-1EA**
LSMLS™ Plate 1 (Water Soluble)	**LSMLS01-1EA**
LSMLS™ Plate 2 (Water Soluble)	**LSMLS02-1EA**
LSMLS™ Plate 3 (Water Soluble)	**LSMLS03-1EA**
LSMLS™ Plate 4 (Water Soluble)	**LSMLS04-1EA**
LSMLS™ Plate 5 (Water Soluble)	**LSMLS05-1EA**
LSMLS™ Plate 6 (Lipophilic)	**LSMLS06-1EA**
LSMLS™ Plate 7 (Lipophilic)	**LSMLS07-1EA**
Bile Acid/Carnitine/Sterol Metabolite Library	**BACSMLS-1EA**

Lipidomics

Connecting Lipids, Technology and Cellular Biology

Not available from MilliporeSigma within in the US.

The Avanti®Mission

Whether you specialize in lipidomics or are new to the field, you know the critical role lipids play and the inherent challenges they present. You don't need to be a lipid specialist to know that you should order from one.

Mass Spec Standards

Identifying the structure or determining the accurate concentration of each molecular species in mass spectrometry-based research requires well-defined internal standards. Whatever your application, Avanti® chemically pure synthetic lipid standards are available for your precise quantization or identification of major lipid classes, including glycerolipids, glycerophospholipids, sphingolipids, and sterols.

Quantitative standards are characterized and prepackaged in unit containers at defined concentrations. A detailed certificate of analysis accompanies each standard, and the stability is monitored by our QC staff.

Qualitative standards aid in the general identification of lipids by mass spec analysis.

Lipid Binding Antibodies

Studying the role of lipids as cofactors, agonists, or antagonists in cellular signaling events is increasingly common. Avanti® monoclonal antibodies are selected against bioactive lipids to detect the presence of these species or the downstream signals that they stimulate. Add them to your basic signaling and disease research.

E06 discriminates between native LDL and OxLDL by binding to the phosphocholine headgroup of oxidized phospholipid that is present in OxLDL but is absent from native LDL.

WR304 can be used to probe the presence of PIP and PIP2.

Lipid Toolbox

Build a Better Understanding of Lipid Functions

A lipid toolbox of integrated methodologies is essential in understanding the functional role of lipids in biological systems. Avanti® novel tools for probing protein-lipid interactions, enhanced systems for the cellular delivery of lipids, and robust assay kits are the perfect complement to your research.

Lipid Snoopers® nitrocellulose membranes or 8-well ELISA strips are ideal for investigating protein-lipid interactions.

Huzzah® improves the cellular delivery of lipid species through their conjugation with human serum albumin (HSA).

CerS Assay Kit is easy to use in measuring ceramide synthase (CerS) activity in biological samples.

And many more methodologiesto build your lipid toolbox including:

- Monoclonal antibodies
- LIPID MAPS® mass spec standards

Product Showcase

- Phospholipids
- Natural and synthetic lipids
- Sphingolipids
- Sterols
- Fluorescent lipids
- Detergents
- Lipidomics
- Bioactive lipids
- Fatty acid modified lipids
- Headgroup modified lipids
- Coenzyme A and derivatives
- Stable isotopes and ESR probes
- Polymers and polymerizable lipids
- Cationic lipids (transfection)
- Neutral lipids
- Aurora® gold probes

For a complete listing of Avanti® Polar Lipids, visit SigmaAldrich.com/Avanti

Avanti® Polar Lipids, Inc.

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 Cholesterol Extraction Kit and Fatty Acid Extraction Kits provide an isolation method that is high-throughput, simpler, faster, and less costly than conventional techniques, such as the Folch method, with the same high-quality results. These kits also use a significantly lower volume of chemical solvents, allowing laboratories to cut down on waste management costs while being environmentally friendly and socially responsible.

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 time
- **High-throughput** – Cut cost and time without sacrificing yield

Ordering Information

Product Description	Cat. No.
Fatty Acid Extraction Kit, Low Standard	MAK174-1KT
Cholesterol Extraction Kit	MAK175-1KT
Fatty Acid Extraction Kit, High Standard	MAK338-1KT

12 Principles of Green Chemistry

An icon has been added to identify our Greener alternative products. Products with this icon fulfill one of the three criteria.

- Products reengineered by our scientists to significantly improve their environmental footprint
- Products that align with the 12 Principles of Green Chemistry
- Products that help make greener alternatives possible through enabling technologies

For more information, visit
SigmaAldrich.com/extraction-kits

Get the Same High-Quality Results in Less Time

Lipids were extracted from rat brain with the Folch or MAK174 kit method, transesterified, and quantified with GC-FID.

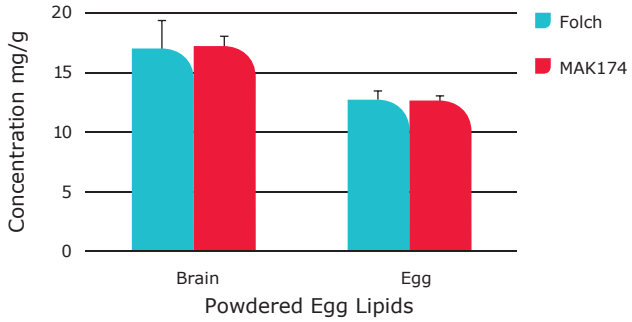


Figure 1: Rat brain fatty acid concentrations (mg/g)

Lipids were extracted with the Folch or MAK175 kit method, saponified, derivitized, and quantified with GC-FID.

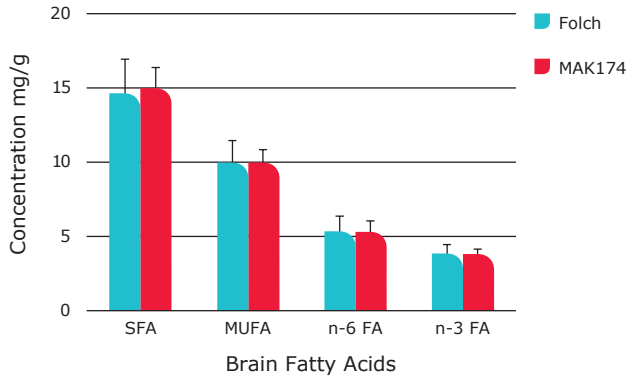


Figure 2: Rat brain and powdered egg cholesterol concentrations (mg/g)

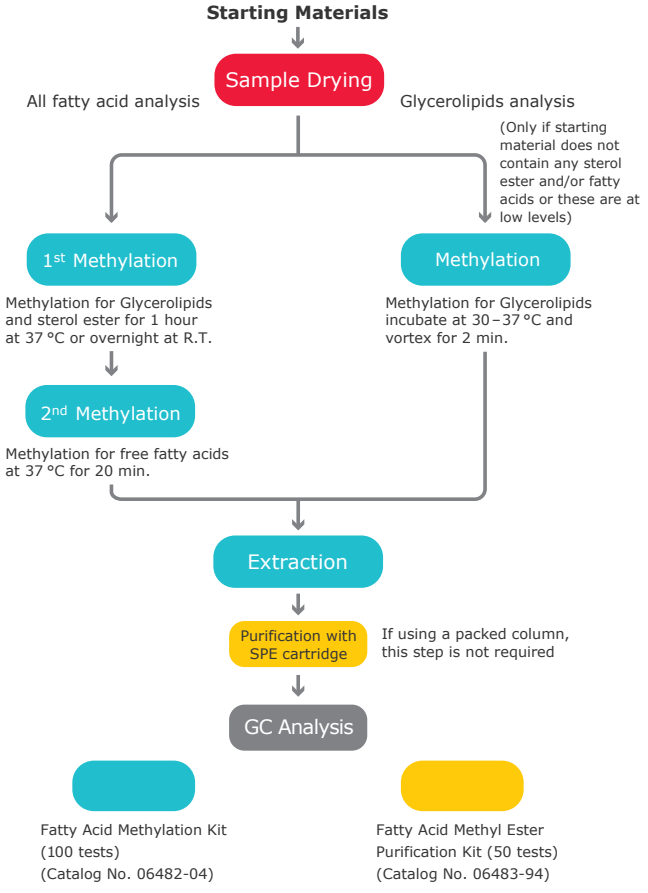
Fatty Acid Methylation and Purification Kits

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

Product Description	Cat. No.
Fatty Acid Methylation Kit	**MAK224-1KT**
Fatty Acid Methyl Ester Purification Kit	**MAK225-1KT**

Comparison of Methylation Efficiency Rate

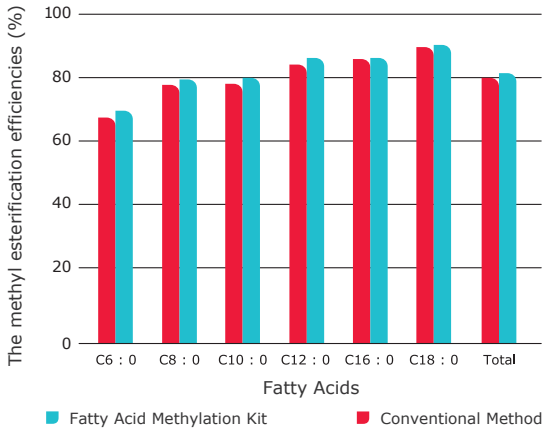


Figure 1: The methyl esterification efficiencies between the Fatty Acid Methylation Kit and a conventional method using different fatty Acid side-chains.

Supel™ Select Polymeric SPE Products

Key Features and Benefits

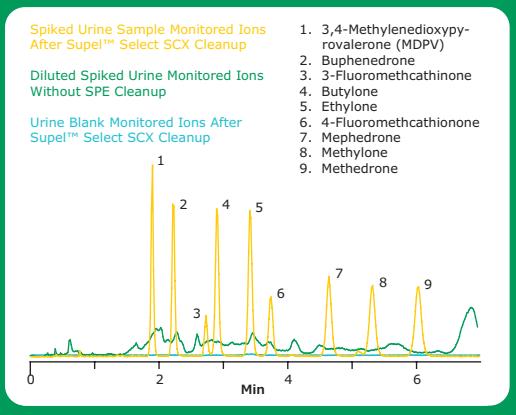
- Hydrophilic-modified styrene resin extracts and recovers a broad range of analytes (polar to nonpolar, acidic to basic) using a single sorbent
- Generic methodology saves time, money, and effort during method development
- Greater capacity allows for smaller bed weights = smaller elution volumes = 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, 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.

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 (Cerilliant® standards)



Supel™ Select Properties	
HLB Phase Chemistry	Hydrophilic-modified styrene polymer
SAX Phase Chemistry	Quanternary 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 m²/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**

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**

Supelco®
Analytical Products

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, researchers frequently deal 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 technology 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 rapid and simple. 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 in 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 without 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.

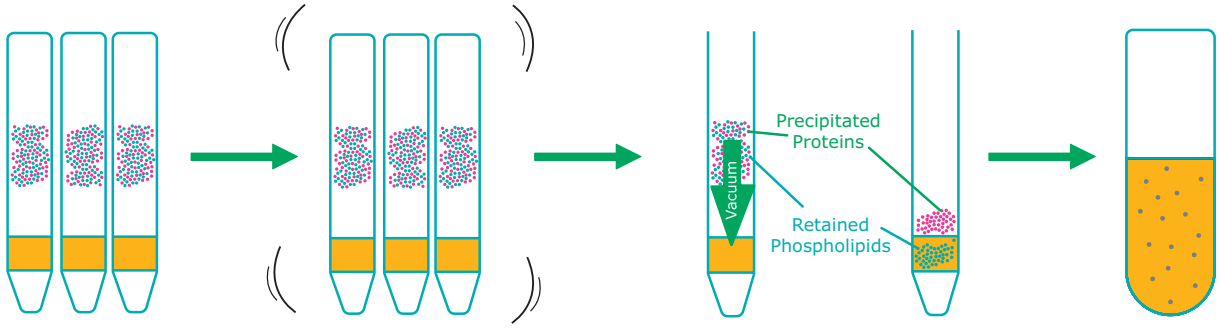
For more information and to view a video of HybridSPE®-Phospholipid technology in operation, visit **SigmaAldrich.com/hybridspe**

1. Add Sample
Pipette 100 µL plasma or serum to the HybridSPE plate followed by 300 µL percipitation solvent. Add internal standards as necessary.

2. Mix
by vortexing/shaking HybridSPE plate or by aspirating/dispensing with 0.5–1 mL pipette tip.

3. Apply vacuum
The packed-bed filter/frit assembly acts as a depth filter for the concurrent physical removal of precipitated proteins and chemical removal of phospholipids. Small molecules (e.g., pharma compounds and metabolites) pass through unretained.

4. Collect Sample
Resulting filtrate/eluate is free of proteins and phospholipids and ready for immediate LC-MS/MS analysis.



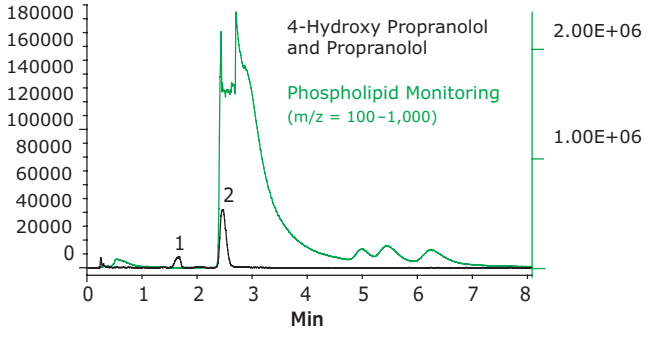
Supelco®
Analytical Products

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

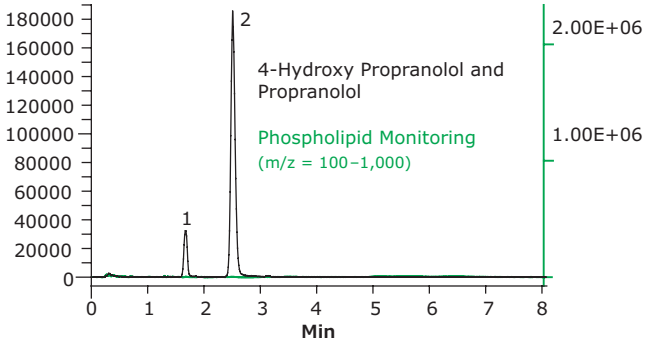
Sample prep	Standard protein precipitation or HybridSPE®-Phospholipid (575656-U)
Column	Ascentis® Express F5, 5 cm × 2.1 mm I.D., 2.7 µm (53567-U)
Mobile phase	(A) 2 mM ammonium formate in acetonitrile; (B) 2 mM ammonium formate in water; (90:10, A:B)
Flow rate	0.4 mL/min
Pressure	1073 psi
Column temp	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

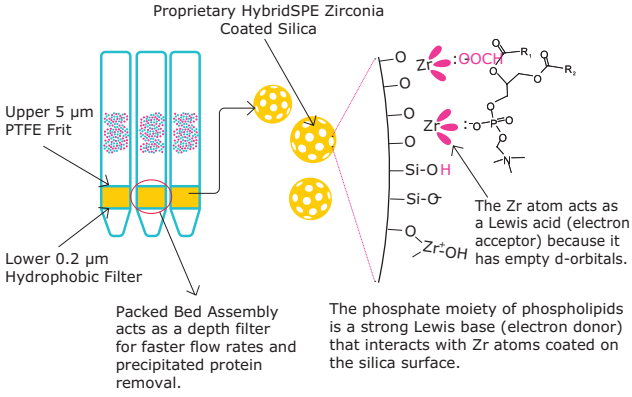
(Note suppression of propranolol signal)



HybridSPE®-Phospholipid Technique



Interaction of Phospholipids with HybridSPE®-Phospholipid Technology



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

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 or analysis.

Size	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

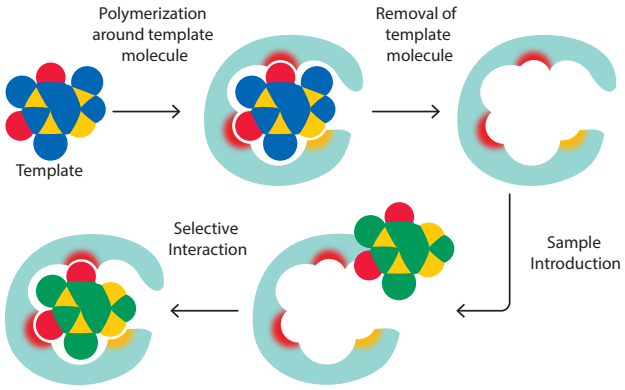
Molecularly imprinted polymers (MIPs) are a class of highly crosslinked polymer-based molecular recognition elements engineered to bind one target compound or a class of structurally related target compounds with high selectivity. Selectivity is introduced during MIP synthesis in which a template molecule,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

SupelMIP® products 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

For more information, visit
SigmaAldrich.com/SupelMIP

Formation of MIPs

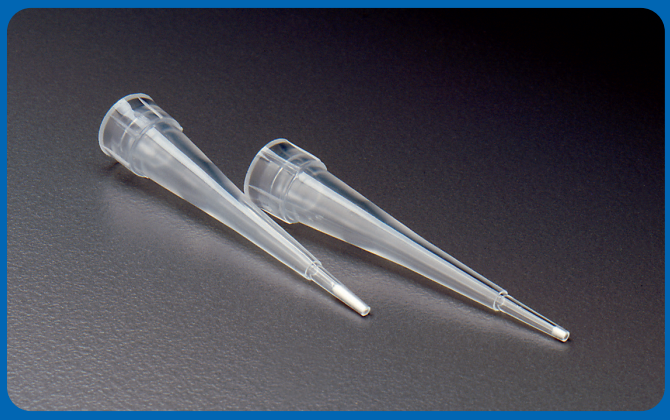


SupelMIP® Molecularly Imprinted Polymer SPE Tubes

Product 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**

Supelco®
Analytical Products

ZipTip® Pipette Tips: Proteomics Sample Prep in Seconds



A staple of every mass spectrometry lab, ZipTip® pipette tips hold 10 µL and have a 0.6 or 0.2 µL bed of chromatography media fixed at the end with no dead volume. They are 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.

Features and Benefits:

- 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

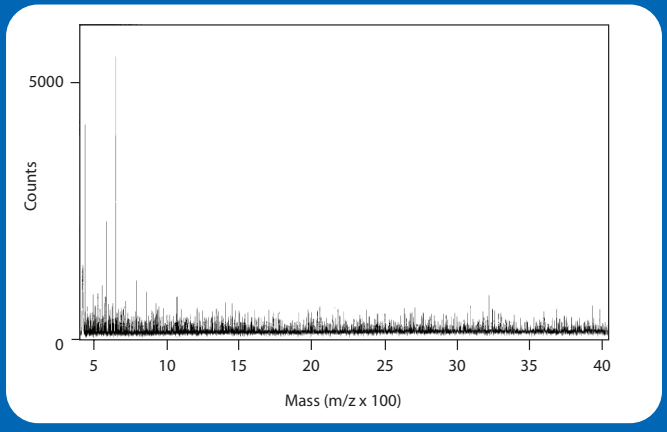
The ZipTip® pipette tip is simple and easy to use

- 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

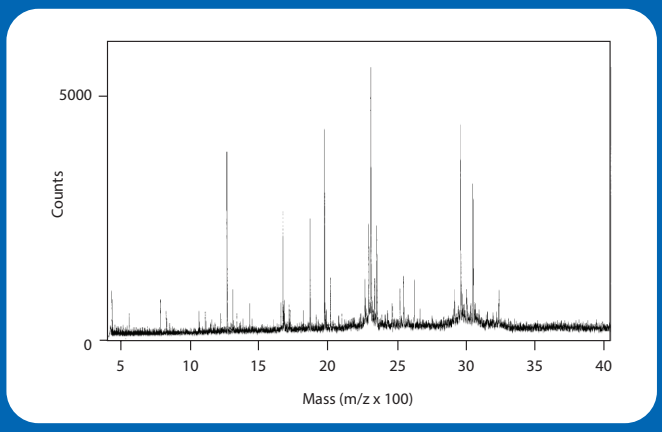
For applications requiring smaller elution volumes (e.g., < 1 µL), a micro-bed format containing 0.2 µL of media is available

Product 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**

A. Direct Spotting



B. After ZipTip® µ-C18



ZipTip® pipette tips 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 tip prior to MALDI-ToF MS analysis.

Millipore®
Preparation, Separation, Filtration & Monitoring Products

MS-Compatible Millex® LCR Syringe Filters

Obtain immaculate, particle-free samples for LC–MS with the confidence 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.

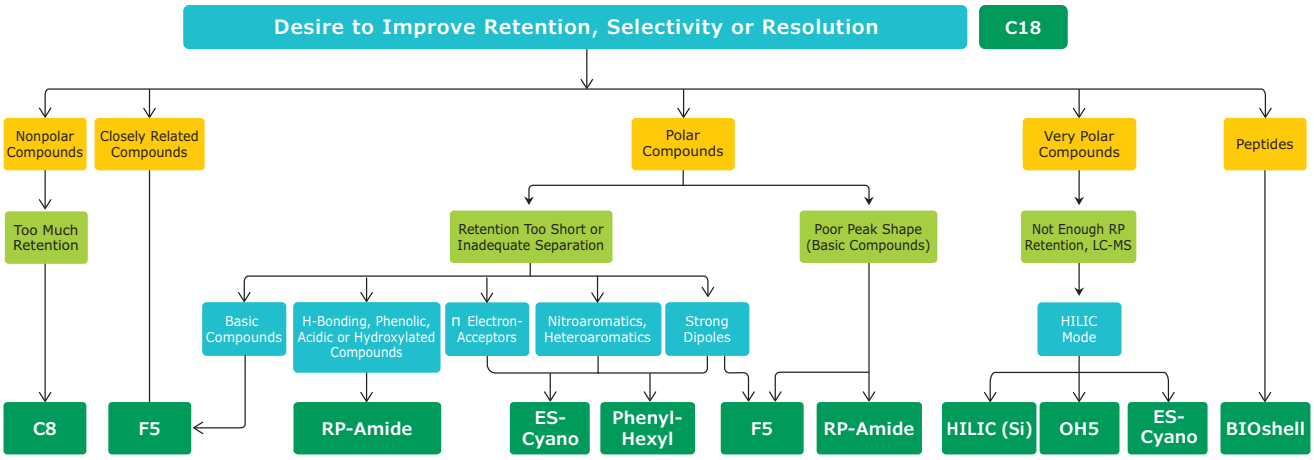
Product Description	Cat. No.
Millex® LCR Filter, 13 mm, Hydrophilic PTFE, 0.45 µm, 100/pk	**SLCR013NL**
Millex® LCR Filter, 13 mm, Hydrophilic PTFE, 0.45 µm, 1,000/pk	**SLCR013NK**
Millex® LCR Filter, 25 mm, Hydrophilic PTFE, 0.45 µm, 250/pk	**SLCR025NB**
Millex® LCR Filter, 25 mm, Hydrophilic PTFE,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

A C18 column is the standard choice when starting a new LC-MS method. You can consider selecting another stationary phase when C18 doesn't provide 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 (A)	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**

Available in a variety of analytical and capillary column dimensions

	Column Length (cm)						
Column I.D	**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**

Supelco®
Analytical Products

LC-MS & (U)HPLC Columns

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

Key Features and Benefits

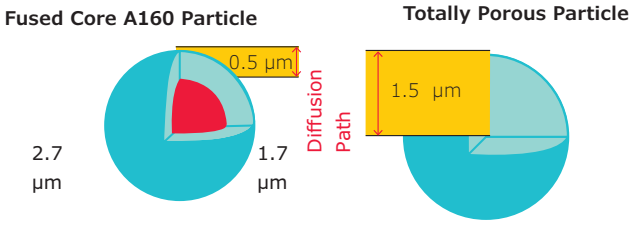
- Maximize speed with sharp peaks even at ultra-high flow rates
- Stable low bleed for LC-MS and LC-UV
- Suitable for any HPLC, UHPLC, or LC-MS instruments
- Achieve UHPLC performance on a traditional HPLC system
- Available in both 2.0, 2.7 and 5 µm particles
- Wide variety of pore sizes, ranging from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

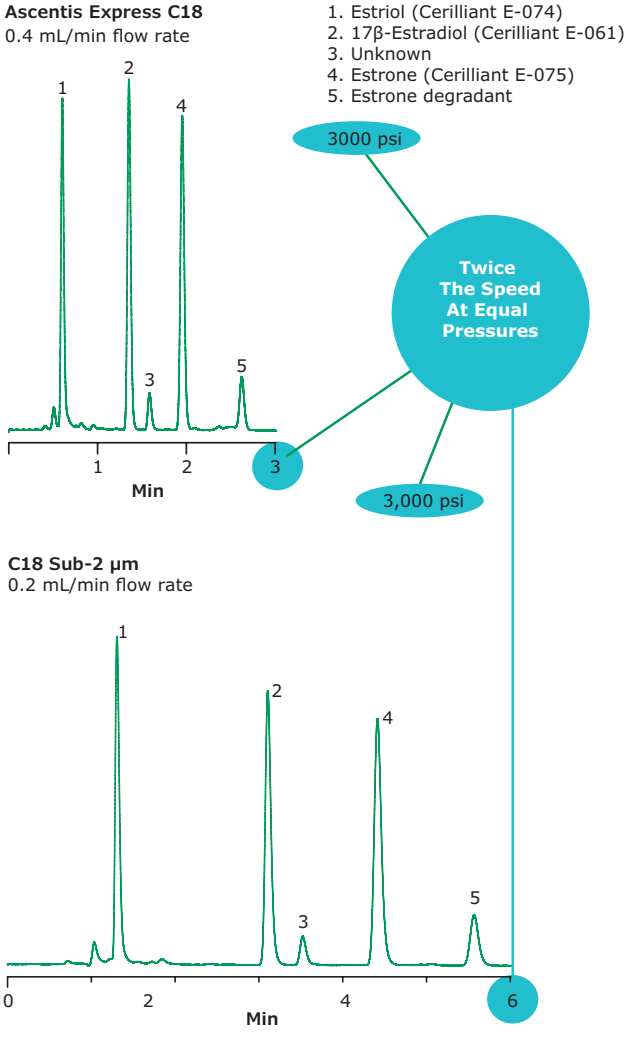
Ascentis® Express Fused-Core® Columns

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 columns 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





Supelco®
Analytical Products

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**

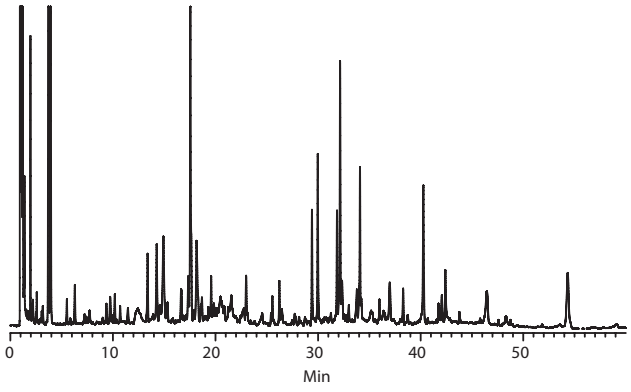
Particle Size	I.D.	Length	C18	C8	OH5
5 µm	3.0 mm	5 cm	**50523-U**	**50377-U**	**50335-U**
5 µm	3.0 mm	7.5 cm	**50525-U**	**50378-U**	**50336-U**
5 µm	4.6 mm	10 cm	**50536-U**	**50391-U**	**50346-U**
5 µm	4.6 mm	15 cm	**50537-U**	**50392-U**	**50347-U**
5 µm	4.6 mm	25 cm	**50538-U**	**50394-U**	**50348-U**
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 Supelco	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

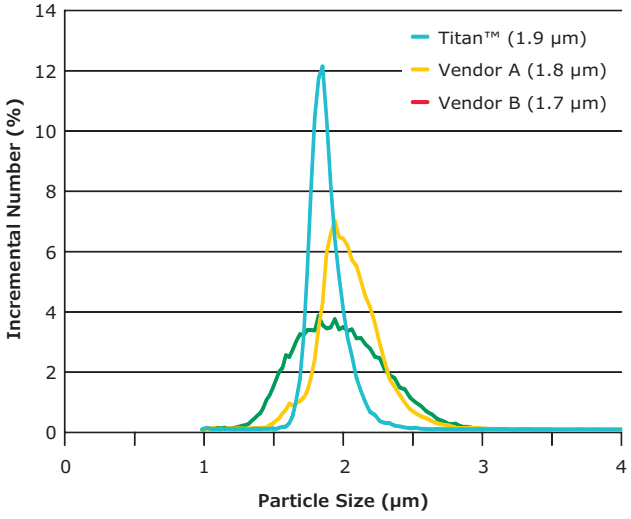
Titan™ C18 is based on a silica particle platform that has the narrowest particle size distribution available of any totally porous particles. This provides performance advantages in the A-term of the van Deemter equation and in the elimination of fines associated with broader particle size distributions. 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 effect on separation impedance or kinetic performance, resulting in more robust and rugged LC-MS columns

Particle Size Distribution Comparison for Different Silica



Supelco®
Analytical Products

SeQuant® ZIC®-HILIC columns

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 straightforward chromatographic technique for separation of many types of polar and hydrophilic compounds. Put simply, HILIC is a normal-phase (NPLC) type of separation that uses reversed-phase (RPLC) type eluents.

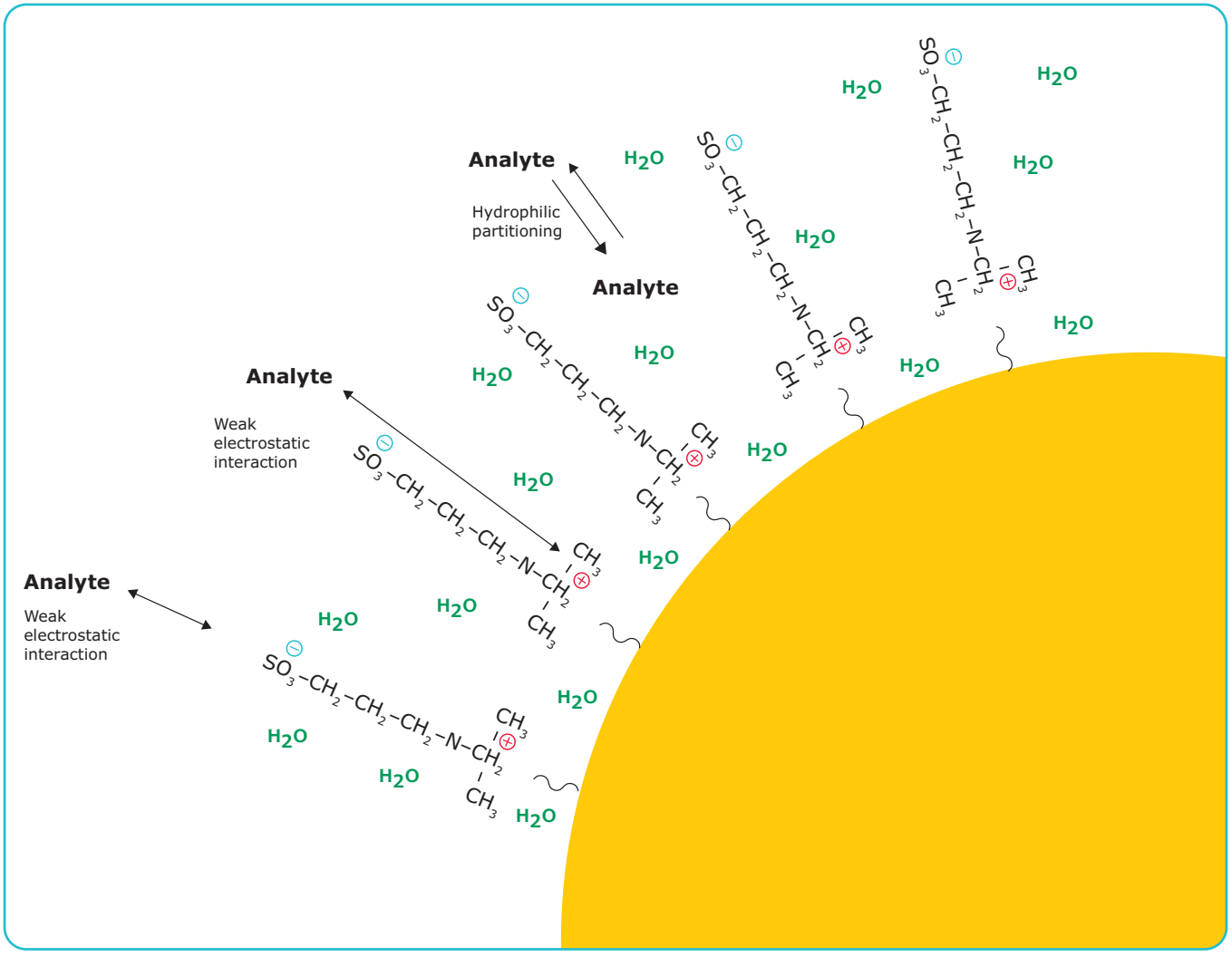
HILIC provides:

- 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 stationary phase being covalently bonded to the silica surface, CHIROBIOTIC® columns have exceptional stability and long column life, even with repeated injections of biological samples.

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**

Astec® CHIROBIOTIC® Columns

Many more dimensions are available. Please visit **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**

Supelco®
Analytical Products

Chemical Derivatization Reagents for LC-MS

Derivatization is used in mass spectrometry to increase ionization efficiency and enhance the sensitivity of the ionization used, resulting in lower analyte detectability.[1] 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"). Precise quantitative analysis to profile comparatively small analyte molecules, particularly in metabolomics, also has a positive effect on derivatization.

References:

1. (a) A Handbook of Derivatives for *Mass Spectrometry, V. Zaikin, J: Halket*, IM Publications LLP, **2009**, Chichester; (b) T. Santa, Drug Discov. Ther. **2013**, 7, 9-17; (c) *T. Santa, Biomed.* Chromatogr. **2011**, 25, 1-10; (d) *T. Santa,* et al., Drug Discov. Ther. **2007**, 1, 108-118.

For more information, visit
SigmaAldrich.com/derivatization

Product 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**
N,N-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**
(*N*-Succinimidyloxycarbonylmethyl) 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**
N-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-(N,N-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**

Product 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 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 learn more, visit
SigmaAldrich.com/derivatization

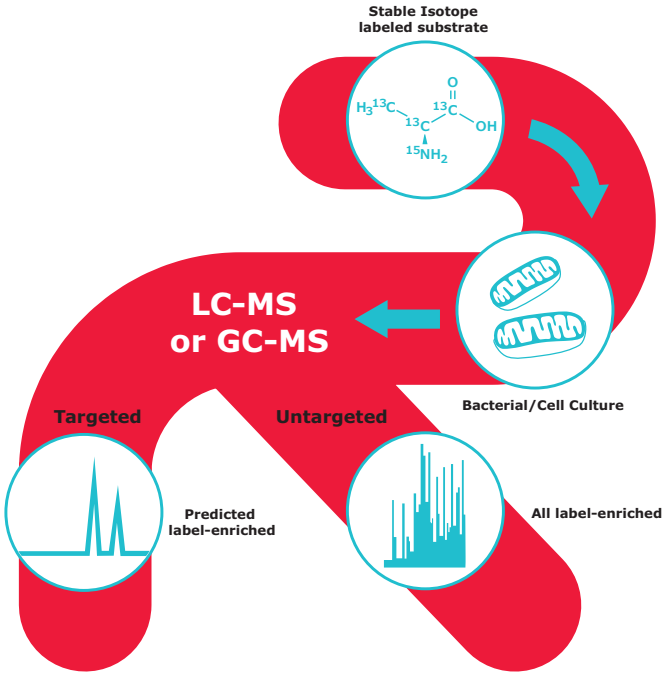
Product Description	Cat. No.
1,1,3,3-Tetramethyl-1,3-diphenyldisilazane	**43340**
4-(Trimethylsiloxy)-3-penten-2-one	**69649**
Bis(dimethylamino)dimethylsilane	**14755**
BSA + TMCS	**15256**
Chlorodimethyl(pentafluorophenyl)silane	**76750**
Chlorotriethylsilane	**90383**
Chlorotrimethylsilane	**89595**
Hexamethyldisilazane	**52619**
Hexamethyldisiloxane	**01565**
N-(Trimethylsilyl)acetamide	**91566**
N,N-Bis(trimethylsilyl)methylamine	**15235**
N,O-Bis(tert-butyldimethylsilyl)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-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',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.
D-Methionine-(*methyl*-^{13}C)	**589780**
L-Methionine-2-d	**589802**
L-Methionine-^{15}N	**609242**
L-Phenylalanine-1-^{13}C	**490091**
L-Phenylalanine-^{15}N	**490105**
L-Phenylalanine-2-^{13}C	**490113**
L-Phenylalanine-3-^{13}C	**490121**
L-Phenylalanine-2,3,3-d_3	**490148**
L-Phenyl-$^{13}C_6$-alanine	**604879**
L-Phenyl-1-^{13}C-alanine	**605042**
L-Phenyl-d_5-alanine	**615870**
L-Phenylalanine-3,3-d_2	**615889**
L-Phenylalanine-$^{13}C_9$	**795844**
L-Phenylalanine-2-d	**589438**
L-Proline-1-^{13}C	**589497**
L-Proline-2,5,5-d_3	**791261**
L-Proline-^{15}N	**608998**
L-Selenomethionine-(*methyl*-^{13}C)	**634093**
L-Serine-1-^{13}C, 99 ATOM % ^{13}C	**490156**
L-Serine-2-^{13}C	**604712**
L-Serine-3-^{13}C	**604720**
L-Serine-2,3-$^{13}C_2$	**605174**
L-Serine-^{15}N	**609005**
L-Threonine-1-^{13}C	**605034**
L-Threonine-$^{13}C_4$	**677604**
L-Threonine-1,2-$^{13}C_2$	**668060**
L-Tryptophan-1-^{13}C	**604836**
L-Tryptophan-(*indole ring*-2-^{13}C)	**604844**
L-Tryptophan-(*indole*-d_5)	**615862**
L-Tyrosine-2,6-d_2	**485829**
L-Tyrosine-(*phenyl*-$^{13}C_6$)	**489794**
L-Tyrosine-(*phenyl*-d_4)	**489808**
L-Tyrosine-(*phenyl*-3,5-d_2)	**489816**
L-Tyrosine-1-^{13}C	**489824**
L-Tyrosine-3-^{13}C	**489859**
L-Tyrosine-(*phenyl*-4-^{13}C)	**605093**
L-Tyrosine-2-^{13}C	**605107**
L-Tyrosine-(4-*hydroxy*-^{18}O)	**609919**
L-Tyrosine-^{15}N	**332151**
L-Tyrosine-3,3-d_2	**489840**
L-Valine-1-^{13}C, 99 ATOM % ^{13}C	**490164**
L-Valine-2-^{13}C	**604917**
L-Valine-^{15}N	**490172**

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_7	**729051**
D-Fructose-1-^{13}C	**415553**

Carbohydrates	Cat. No.
D-Fructose-2-^{13}C	**492140**
D-Fructose-1,6-$^{13}C_2$	**587613**
D-Fructose-$^{13}C_6$	**587621**
D-Fructose-6-^{13}C	**605395**
D-Fructose-6,6-d_2	**488720**
D-Fructose-d_{12}	**723908**
L-Fucose-1-^{13}C	**605425**
D-Galactose-1-^{13}C	**415545**
D-Galactose-2-^{13}C	**454621**
D-Galactose-$^{13}C_6$	**605379**
D-Galactose-1-d	**495077**
D-Glucose-1-^{13}C	**297046**
D-Glucose-4-^{13}C	**668648**
D-Glucose-1,6-$^{13}C_2$	**453196**
D-Glucose-2-^{13}C	**310794**
D-Glucose-1,2-$^{13}C_2$	**453188**
D-Glucose-3-^{13}C	**605409**
D-Glucose-1,2,3-$^{13}C_3$	**720127**
D-Glucose -4,5,6-$^{13}C_3$	**731501**
D-Glucose-4,5-$^{13}C_2$	**605468**
D-Glucose-5-^{13}C	**717355**
D-Glucose -5,6-$^{13}C_2$	**755893**
D-Glucose-$^{13}C_6$	**389374**
D-Glucose-6-^{13}C	**310808**
D-Glucose-1-d	**310816**
D-Glucose-2-d	**310824**
D-Glucose-3-d	**615498**
D-Glucose -6-^{13}C,6,6-d_2	**734403**
D-Glucose-6,6-d_2	**282650**
D-Glucose-d_{12}	**616338**
D-Glucose-1,2,3,4,5,6,6-d_7	**552003**
Inulin-^{13}C	**900388**
D-Mannose-1-^{13}C	**415537**
D-Mannose-2-^{13}C	**605344**
D-Mannose-3-^{13}C	**749419**
D-Mannose-4-^{13}C	**733733**
D-Mannose-5-^{13}C	**749400**
D-Mannose-6-^{13}C	**605387**
D-(+)-Mannose-$^{13}C_6$	**592994**
D-Ribose-1-^{13}C	**605352**
D-Ribose-2-^{13}C	**310840**
D-Ribose-1,2-$^{13}C_2$	**605476**
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-(*glucose*-1-^{13}C)	**705136**
Sucrose-(*glucose*-$^{13}C_6$)	**738786**
D-Xylose-$^{13}C_5$	**666378**
D-Xylose-1-^{13}C	**331104**

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
Glyceryl tri(oleate-1,2,3,7,8-$^{13}C_5$)	772941
Glyceryl-$^{13}C_3$ trioleate	605638
Glyceryl tri(palmitate-d_{31})	616966
Glyceryl tri(octanoate-d_{15})	617121
Glyceryl tri(palmitate-1,2,3,4-$^{13}C_4$)	777862
Glyceryl tri(octanoate-1,2,3,4-$^{13}C_4$)	808563
Glyceryl 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
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
Palmitoleic acid-$^{13}C_{16}$	724173

Fatty Acids and Lipids	Cat. No.
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 to specifically 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

To learn more, visit
SigmaAldrich.com/Solvents-Blends-LCMS

Benefits:

- Time and cost savings
- 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

Product Name	Product 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**

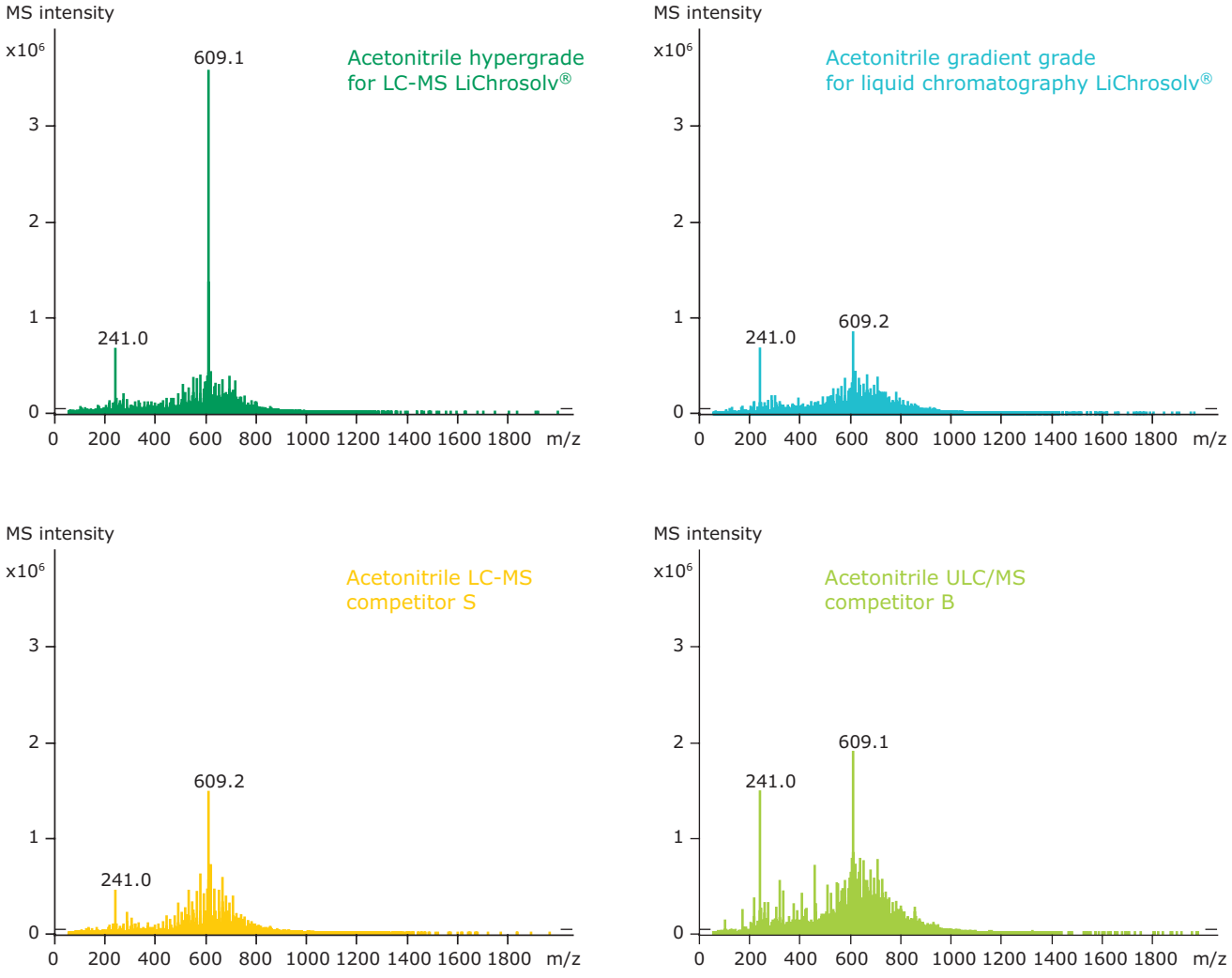
*specially treated amber glass bottle

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 MilliporeSigma and two alternative competitors.

Supelco®
Analytical Products

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, and salts

For more information, visit
SigmaAldrich.com/lcms-reagents

Product Name	Product 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 metabonomics). 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.

Refer to other sections of this publication for 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.

References

1. D. Wishart, Chapter 10, "*Metabolomics in Humans and Other Mammals", in Metabolome Analysis: An Introduction*, S. G., 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–Timeof- 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. Temperature limits for ≤0.25 mm I.D. are -60 °C to 340 °C (isothermal) or 360 °C (programmed).

I.D. (mm)	df (µm)	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	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.

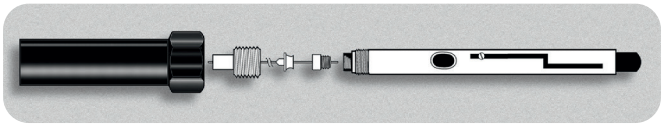
For more information about guard column selection, visit **SigmaAldrich.com/gc-guard**

SPME: A Unique Sample Preparation Technique

Solid phase microextraction (SPME) 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.



Product 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

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

Product 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 to:

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

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

Product 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-butyldimethylsilyl)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**

To learn more, visit **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

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Product Description	Purity	Abbreviation	Proteins	Peptides	Glycans	Oligonucleotides	Polymers	Lipids	Other Analytes	Note	Pack Sizes	Cat. No.
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:ClCCA		•				•	Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS		100 mg	**68914**
4-Aminoquinaldine	≥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**

Product Description	Purity	Abbreviation	Proteins	Peptides	Glycans	Oligonucleotides	Polymers	Lipids	Other Analytes	Pack Sizes	Cat. No.
4-Bromo-α-cyanocinnamic acid – α-Cyano-2,4-difluorocinnamic acid mixture	≥95%	BrCCA:DiFCCA		•				•	Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	**55841**
Caffeic acid	≥99.0%		•	•						1 g 5 g	**60018**
4-Chloro-α-cyanocinnamic acid	≥95%	ClCCA		•				•	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	≥95%	ClCCA:DiFCCA		•				•		100 mg	**39379**
α-Cyano-2, 4-difluorocinnamic acid	≥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	≥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	≥99.0%	CHCA	•	•	•					250 mg 1 g	**70990**
α-Cyano-4-hydroxycinnamic acid	≥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	≥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	≥95%	PentawFCCA		•					Phosphopeptides, phospholipids, chlorinated lipids, drugs, fragile analytes, ionic liquids (quantification), ME-SIMS, CID-MS/MS	100 mg	**38419**
1,5-Diamino naphthalene	≥99.0%			•		•			1,5-DAN In-Source-Decay	250 mg	**56451**
2', 6'-Dihydroxy acetophenone	≥99.5%	2,6-DHAP	•	•	•			•		1 g 5 g	**37468**
2, 5-Dihydroxybenzoic acid	≥99.0%	DHB	•	•	•		•	•	Organic molecules	10 mg 250 mg 1 g	**85707**
2, 5-Dihydroxybenzoic acid	≥99.5%, Ultra pure	DHB	•	•	•		•	•	Organic molecules	10 × 10 mg	**39319**
trans-Ferulic acid	≥99.0%	FA	•	•						1 g 5 g	**46278**
2-(4-Hydroxy phenylazo) benzoic acid	≥99.5%	HABA	•	•	•		•			1 g 5 g	**54793**
3-Hydroxypicolinic acid	≥99.0%	3-HPA				•			Oligosaccharides	250 mg 1 g	**56197**
3-Nitrobenzyl alcohol	≥99.5%									5 g	**73148**
3-Nitrobenzonitrile	≥99.0%	3-NBN							Tissues via MAIV	1 g	**80362**
Salicylamide	≥99.0%					•				1 g	**84228**
Sinapic acid	≥99.0%	SA	•	•					Dendrimers, Fullerenes	1 g 5 g	**85429**
Sinapic acid	≥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	≥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' disease[5] and hypertension,[6] the study of fatty acid oxidation,[7] and the analysis of androgenic steroids in wastewater.[8]

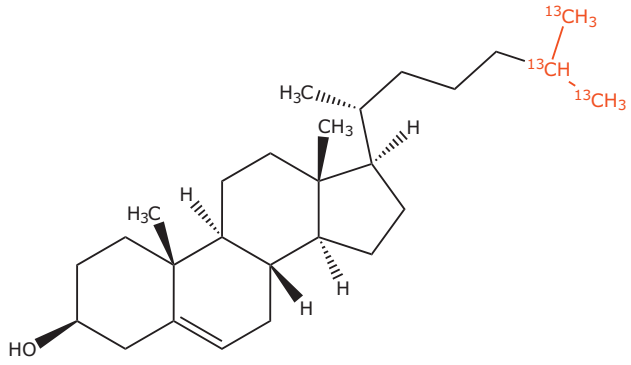
ISOTEC® MS standards have high chemical and isotopic purities with labeling patterns including ^{13}C, ^{15}N, and deuterium. The ^{13}C and ^{15}N labels do not exchange within the mass spectrometer source, providing further advantage.[9]

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

Amino acids

Product 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.



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

To inquire about stable isotope pricing and availability, email us at **isosales@milliporesigma.com**

Fatty acids

Product 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

Product 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**

Steroids and Hormones

Product 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**
Etiocholanolone-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 lipid and fatty acid products, visit **SigmaAldrich.com/lipid**
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Vitamins

Product 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 D3-(26,26,26,27,27,27-d_6)	**803030**
(24*R*), 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-dioxopyrimidine-$^{13}C_4$, $^{15}N_2$	**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_7(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

Product 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 taurolithocholate-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

Product Description	Cat. No.
L-Arbrine-(*methyl*-d_3)	**750913**
Aldicarb-(*N-methyl*-^{13}C,d_3, *carbomoyl*-^{13}C)	**733865**
Aldicarb-(*N-methyl*-^{13}C,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,d_3	**746274**
Yohimbine-(*methyl*-^{13}C,d_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**

BIOshell™ Glycan HPLC Columns

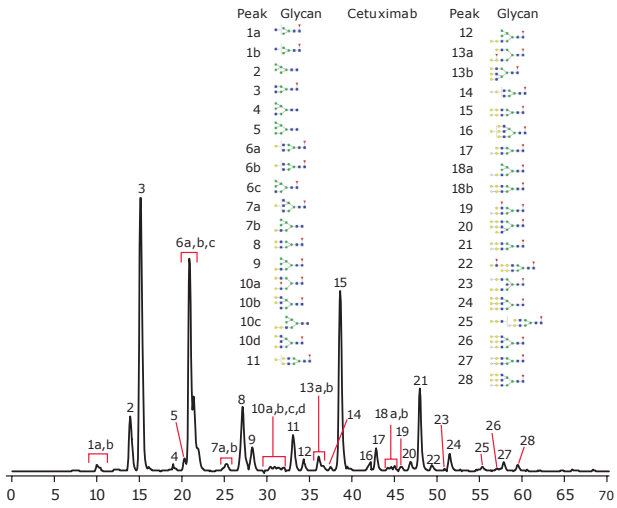
Empowering the Analysis of Glycoproteins with Exceptional Reproducibility

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, due to 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 – We supply reagents and consumables needed for each step in glycoprotein analysis as indicated in Figure 1.

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.

Steps in Glycoprotein Analysis

Glycan Release → **Procainamide Labeling** → **Cleanup** → **LC-MS Analysis**

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

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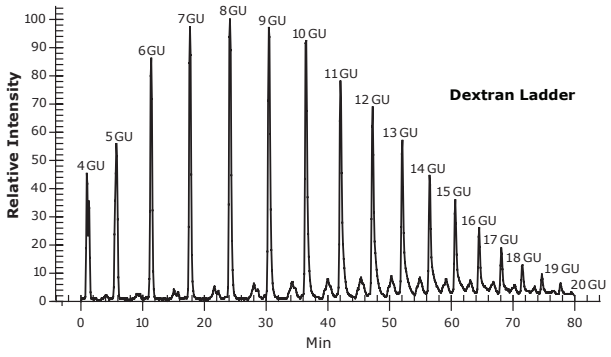
Analytical Products

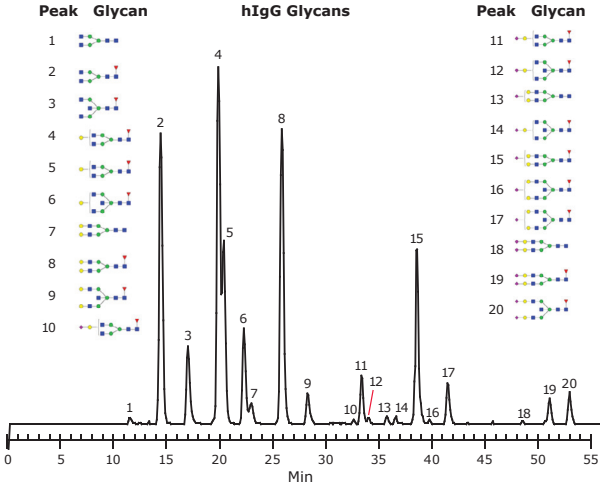
BIOshell™ Glycan Applications

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 integrate 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

Product 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	**A6283**
Dextran hydrolysate	**31417**
Step 3: Cleanup	
Acetonitrile	**34851**
DPA-6S 50 mg cartridges (Supelco)	**52624-U**
Step 4: LC-MS analysis	
BIOshell™ glycan, 15 cm × 2.1 mm I.D., 2.7 µm (Supelco)	**50994-U**
Ammonium formate (Supelco)	**70221**
Formic acid	**F0507**

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 m^2/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**

Supelco®
Analytical Products

Translation to Clinical Applications

Metabolite analysis has been used for centuries in clinical chemistry to diagnose and treat diseases. Our wide range of products support researchers in identifying biomarkers for drug development and clinical diagnostics.

Inborn Errors of Metabolism of Amino Acids

Inborn errors of metabolism are caused by changes in specific enzymatic reactions. Hundreds of different such alterations, which affect about 1 of every 5,000 newborns, have been characterized newborns. 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 through screenings 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.

Characteristic Metabolites for Inborn Errors of Amino Acid Metabolism

Product Description	Cat. No.
N-Acetyl-l-aspartic acid, puriss., ≥99.0% (T)	**00920**
γ-Aminobutyric acid, BioXtra, ≥99%	**A5835**
Argininosuccinic acid disodium salt hydrate, ≥80%	**A5707**
l-Citrulline, ≥98% (TLC)	**C7629**
l-Cystathionine, ~90% (TLC)	**C7505**
Fumaric acid, purum, ≥99.0% (T)	**47910**
Glutaric acid, 99%	**G3407**
dl-Homocysteine, ≥95% (titration)	**H4628**
l-Homocystine, ≥98% (TLC)	**H6010**
Homogentisic acid	**H0751**

Product Description	Cat. No.
3-Hydroxy-3-methylglutaric acid, ≥95%	**H4392**
l-Isoleucine, ≥99.5% (NT)	**58879**
Isovaleric acid, 99%	**129542**
l-Leucine, ≥99.5% (NT)	**61819**
Melanin	**M8631**
Methylmalonic acid, 99%	**M54058**
l-Phenylalanine, ≥99.0% (NT)	**78019**
l-Tyrosine, ≥99.0% (NT)	**93829**
l-Valine, ≥99.5% (NT)	**94619**

For more information, visit
SigmaAldrich.com/Amino-Acid-Metabolism

Genotype-Phenotype Relationships in Inborn Errors of Metabolism

More than a century has passed since Archibald Garrod discovered four genetic disorders (albinism, alkaptonuria, cystinuria and pentosuria) as "inborn errors of metabolism". Since then, research has advanced considerably. Current newborn screening is able to diagnose many metabolic disorders early on so they can be treated accordingly, for example with enzyme replacement therapy (ERT). As further progress is made in chemistry and technology to identify metabolomic pathways in human genetic disorders and their relationship to Mendalian inheritance, gene therapy may revolutionize treatment in the future.

Our company is proud to have been involved in the analysis of inborn errors of metabolism from the early days to the present. We offer an ever-increasing range of metabolites to support research in establishing genotype-phenotype relationships, understanding the complex metabolic mechanisms of lipids and other cellular processes, and the role of epigenetics in inborn errors of metabolism.

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**.

For more information, visit
SigmaAldrich.com/metabolomics

Characteristic Metabolites for Inborn Errors of Lipid Metabolism

Inborn errors of metabolism are rare genetic disorders in which specific enzymes that help metabolize food are defect, leading to a wide range of symptoms, including developmental delays or other medical problems.

Many inherited metabolic diseases are caused by defects in lipid metabolism. Lipid metabolism disorders, such as Fabry disease, Gaucher disease, metachromatic leucodystrophy, Niemann-Pick disease, Refsum disease, Tangier disease, and Tay-Sachs disease,often result from a harmful accumulation of unusual lipids in the blood and tissues of affected patients that can lead to damage in cells. Since many of these conditions are impairing and can be fatal, correct identification of these lipids is vital for proper diagnosis and treatment of these disorders.

Promising therapeutic approaches are being developed with our wide range of metabolites.

Product 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**

For more information, visit
SigmaAldrich.com/Lipid-Metabolism

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