

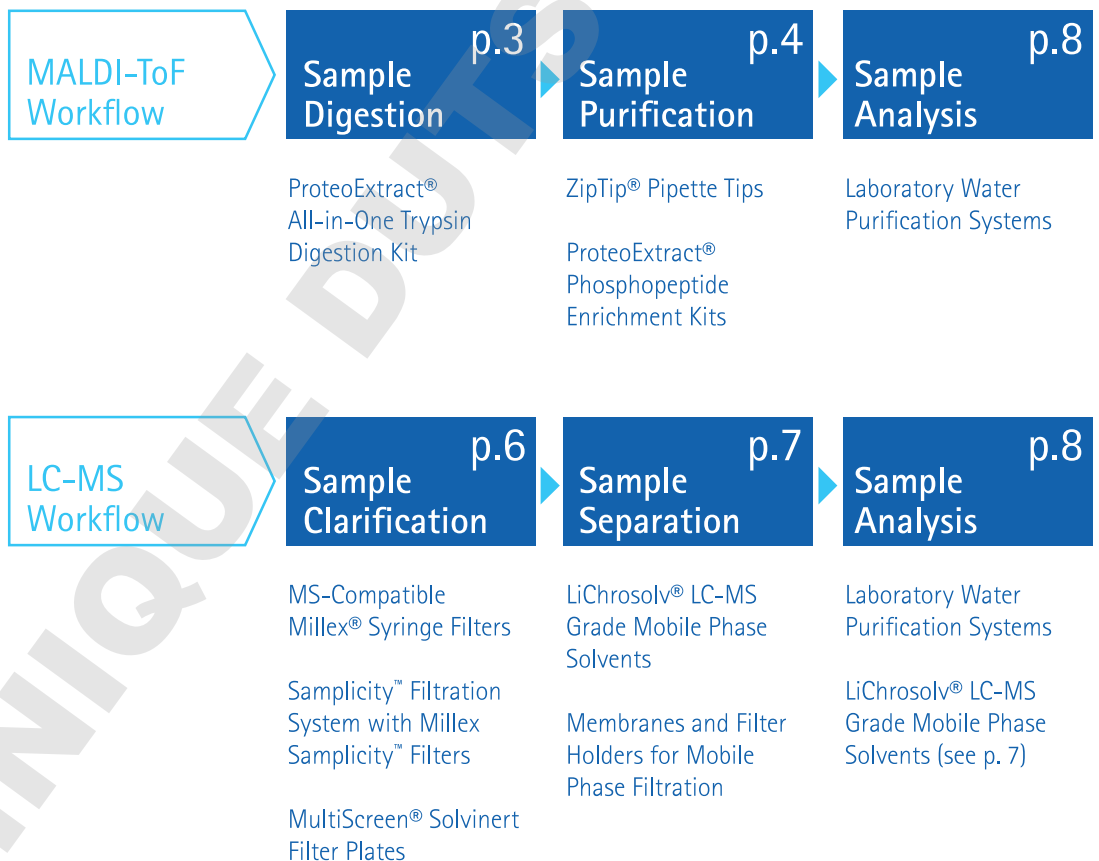
Perfection in preparation  
for better mass spectra.



# Mass Spectrometry Workflow Solutions

Because of its high sensitivity and extreme versatility, mass spectrometry has become a popular technique for identifying and quantifying molecules within complex mixtures, in diverse research areas that range from systems biology and proteomics to environmental analysis.

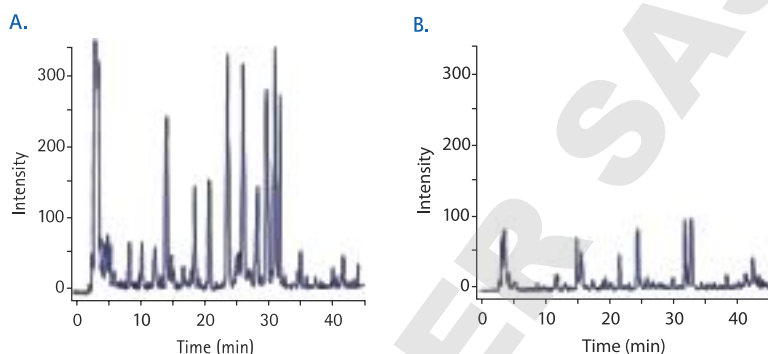
Successful mass spectrometry requires extremely careful sample preparation, in order to avoid contamination and decrease the complexity of the mixtures being analyzed. Merck Millipore supports researchers using mass spectrometry with tools for multiple steps of the workflow, including purification, clarification, and analysis.



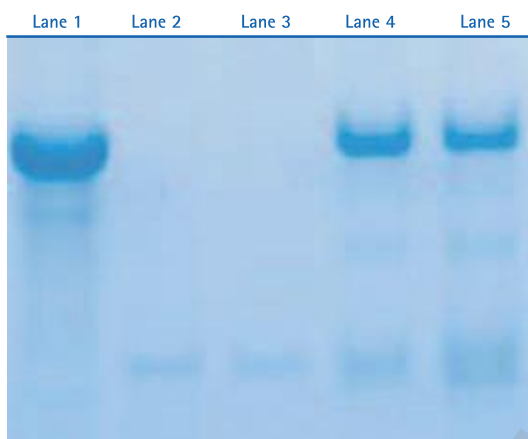
# Sample Digestion

## ProteoExtract® All-in-One Trypsin Digestion Kit

For accurate protein identification by mass spectrometry, you need a fast, efficient and reproducible proteolytic digestion method. This kit enables tryptic digestion of various sample types: polyacrylamide gel spots or bands, liquid protein samples or tissue homogenates. Each protocol is optimized using affinity-purified trypsin, guaranteeing efficient digestion of protein samples and high yield of tryptic peptides, even with hard-to-digest proteins. The results show improved LC-MS peak patterns and sequence coverage.



ProteoExtract® All-in-One Trypsin Digestion Kit enables comprehensive analysis and enhanced detection compared to competitor's kit. Ovalbumin was digested using the ProteoExtract® kit (A) or Supplier Z kit (B) and analyzed by nanoLC-MS.



### Improved digestion of hard-to-digest proteins.

Ovalbumin was analyzed as follows: lane 1: ovalbumin, chicken egg, 43 kDa; lane 2: ovalbumin digest incubated 3 h using ProteoExtract® All-in-One Trypsin Digestion Kit; lane 3: ovalbumin digest incubated 4 h using the same kit; lane 4: ovalbumin digest incubated 3 h using reagent from Supplier I; lane 5: ovalbumin digest incubated 3 h using kit from Supplier II.

Description	Catalogue No.
ProteoExtract® All-in-One Trypsin Digestion Kit, 100 reactions	650212

To place your order or for complete product information visit: [www.merck4biosciences.com](http://www.merck4biosciences.com).

# Sample Purification

## ZipTip® Pipette Tips

The ZipTip® is a 10 µL pipette tip with a 0.6 or 0.2 µL bed of chromatography media fixed at its end with no dead volume. It is ideal for concentrating and purifying samples for sensitive analyses such as MALDI-ToF MS.

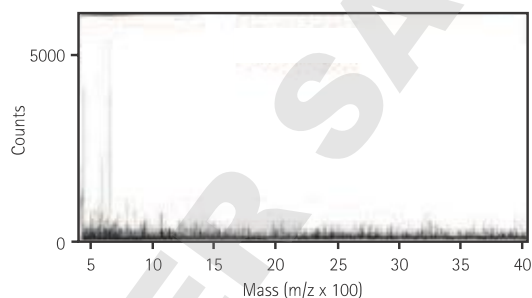
### Advantages:

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

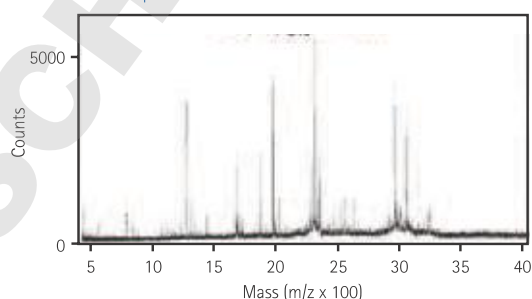
Description	Catalogue No.
ZipTip® <sub>C4</sub> 96/pk	ZTC04S096
ZipTip® <sub>µ-C18</sub> 96/pk	ZTC18M096
ZipTip® <sub>C18</sub> 96/pk	ZTC18S096
ZipTip® <sub>SCX</sub> 96/pk	ZTSCXS096

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### A. Direct Spotting



### B. After ZipTip®<sub>µ-C18</sub>



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

## ProteoExtract® Phosphopeptide Enrichment Kits

Advance your cell signaling research by using mass spectrometry to identify phosphorylated sites. These kits make it easy, enabling you to isolate specifically and quantitatively phosphorylated peptides derived from cleaved or digested protein samples or kinase reactions. Phosphopeptides are captured and highly purified in order for identification through LC-MS or MALDI-ToF MS.

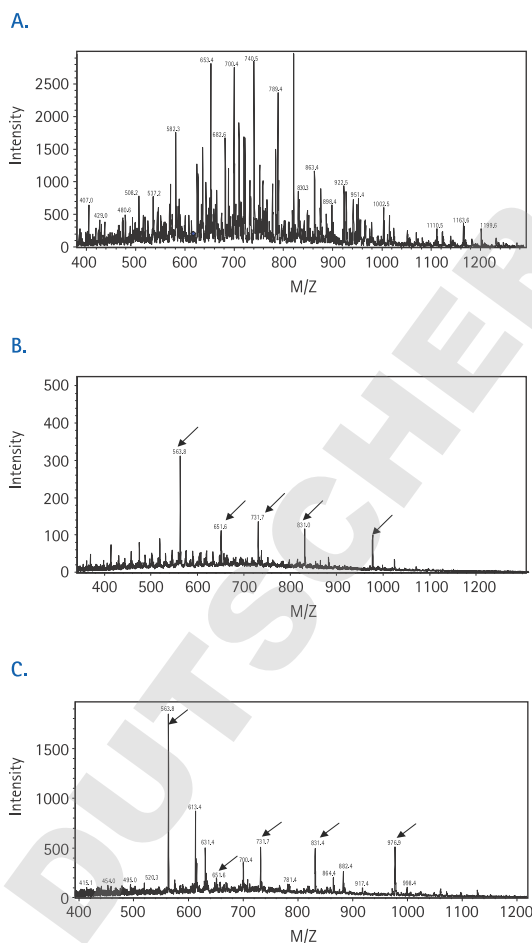
No one method of phosphopeptide capture is sufficient for enrichment of the entire phosphoproteome. The two different ProteoExtract® Phosphopeptide Enrichment Kits enrich for different, partially overlapping segments of the phosphoproteome, which is especially useful when working with complex samples. While the SCIMAC kit enriches phosphopeptides by cation exchange coupled to affinity chromatography, the TiO<sub>2</sub> kit is based on selective enrichment by a titanium dioxide resin. As a result of different binding mechanisms, maximum subsets of phosphopeptides are captured, independent of peptide properties like amino acid sequence, additional posttranslational modifications, and conformational features.

### Advantages:

- Fast – just 30-60 minutes to isolate phosphopeptides
- Specific, high affinity capture
- Scalable to various sample quantities
- Solid phase extraction (SPE) for desalting not required
- Validated, compatible protocols for LC/ESI- and MALDI-ToF mass spectrometry

Description	Catalogue No.
ProteoExtract® Phosphopeptide Enrichment TiO <sub>2</sub> Kit	539722
ProteoExtract® Phosphopeptide Enrichment SCIMAC Kit	539723

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Selective and sensitive enrichment of phosphopeptides from complex mixtures using either the SCIMAC or TiO<sub>2</sub> ProteoExtract® Phosphopeptide Enrichment Kits. A complex peptide mixture derived from a tryptic digest of porcine liver extract was spiked with  $\alpha$ -casein and 2 synthetic phosphopeptides and subsequently processed using the materials and protocols from the SCIMAC or TiO<sub>2</sub> Kits. Mass spectrometry analysis was performed using an ESI-LC/MS instrument operated in positive mode. A. Unprocessed sample, B. Enrichment of phosphopeptides using the SCIMAC Kit, C. Enrichment of phosphopeptides using the TiO<sub>2</sub> Kit. Arrows indicate the predominant phosphopeptide ions.

# Sample Clarification

## MS-Compatible Millex® LCR Syringe Filters

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

Description	Catalogue No.
Millex®-LCR Filter, 13 mm, Hydrophilic PTFE, 0.45 µm, 100/pk	SLCR013NL
Millex®-LCR Filter, 13 mm, Hydrophilic PTFE, 0.45 µm, 1000/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, 1000/pk	SLCR025NK

To place your order or for complete product information visit: [www.millipore.com](http://www.millipore.com)

Millex® filters provide the best reproducibility combined with the lowest level of extractables.

	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).



## Smplicity™ Filtration System

The first vacuum-driven system with the flexibility to filter 1 to 8 samples directly into standard 12 x 32 mm sample vials. Just attach a vacuum pump, load your samples, and flip the lever to recover your particulate-free samples in seconds.

Built upon decades of our membrane filtration expertise, the system's Millex Smplicity™ filters are chemically compatible with a broad range of solvents and buffers and are extremely low in extractables with low analyte binding. The performance of the Millex Smplicity™ hydrophilic PTFE membranes make them ideal for sample clarification prior to LC/MS.

## Smplicity™ Systems

Description	Catalogue No.
Smplicity™ Filtration System, Glossy Green	SAMPSYSGR
Smplicity™ Filtration System, Bold Blue	SAMPSYSBL

## Millex Smplicity™ Filters

Description	Catalogue No.
Millex Smplicity™ Filters, 0.20 µm Hydrophilic PTFE, 96/pack	SAMPLG001
Millex Smplicity™ Filters, 0.45 µm Hydrophilic PTFE, 96/pack	SAMPLCR01

To place your order or for complete product information visit: [www.millipore.com](http://www.millipore.com)

**MultiScreen® Solvintert Filter Plates** are the perfect choice for automated sample clarification. To accommodate use with aqueous and non-aqueous samples, MultiScreen® Solvintert plates – in deep well and standard well volumes – are available with a choice of either chemically resistant hydrophobic or hydrophilic PTFE membranes. For product and order information visit: [www.millipore.com/96MSprep](http://www.millipore.com/96MSprep)

# Sample Separation

## LiChrosolv® LC-MS Grade Mobile Phase Solvents: Ideal for MS Sample Separation and Analysis

To avoid artifactual peaks in mass spectra, use LC-MS grade solvents free of metal ions (particularly sodium and potassium) and other contaminants. Highly distilled and purified, LiChrosolv® solvents must pass the most rigorous specification testing. All LiChrosolv® LC-MS Grade Solvents pass metal ion tests and are also tested by both ESI(+) and ESI(-) mass spectrometry to guarantee absence of signals greater than 50 ppb reserpine or 50 ppb p-nitrophenol.

All LiChrosolv® solvents list lot-specific, complete testing results on every label so you know you are getting the best solvent every time.

Description (available in 1L and 4L sizes)	Catalogue No.
Acetonitrile LiChrosolv® Hypergrade LC-MS	1.00029
Methanol LiChrosolv® Hypergrade LC-MS	1.06035
LiChrosolv® Water	1.15333

To place your order or for complete product information visit: [www.merck4biosciences.com](http://www.merck4biosciences.com)

## Membranes, Filter Holders, and Pumps for Mobile Phase Filtration

Membrane filtration prior to separation via liquid chromatography removes contaminating particles from solvents and mobile phases, increasing column life, preventing system failure, and ensuring pure samples for downstream mass spectrometric analysis. Merck Millipore's membrane disc filters, combined with our filter holders and pumps, provide an easy, low-extractable system for generating LC-ready solvents and mobile phases.

### Membrane Filter Discs

Description	Catalogue No.
0.2 µm Durapore® PVDF Membrane Filter, 47 mm	GVWP04700
0.2 µm Durapore® PVDF Membrane Filter, 90 mm	GVWP09050
0.2 µm Millipore Express® PLUS PES Membrane Filter, 47 mm	GPWP04700
0.2 µm Millipore Express® PLUS PES Membrane Filter, 90 mm	GPWP09050
0.2 µm Omnipore® PTFE Membrane Filter, 47 mm	JGWP04700
0.2 µm Omnipore® PTFE Membrane Filter, 90 mm	JGWP09025
0.22 µm Fluoropore™ Membrane Filter, 47 mm	FGLP04700
0.2 µm Nylon Membrane Filter, 47 mm	GNWP04700

### Filter Holders

Description	Catalogue No.
47 mm All Glass Filter Holder with 300 mL Funnel	XX1504700
90 mm Glass Filter Holder with Stainless Steel Screen and 1 L Funnel	XX1009020
Filter forceps, blunt-tipped, sterilizable	XX6200006P

### Vacuum Pumps

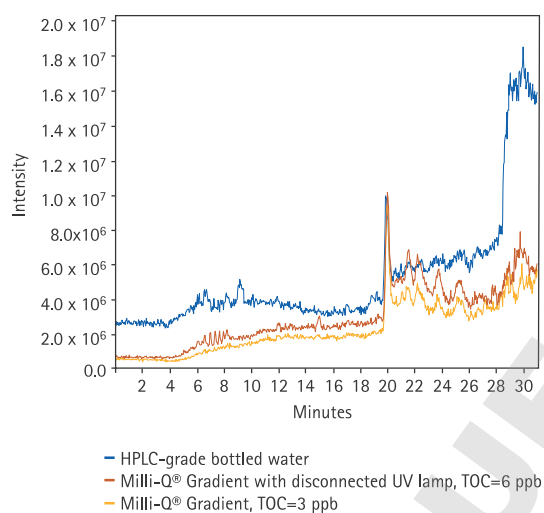
Description	Catalogue No.
Millivac® Mini Vacuum Pump, 115 V	XX5411560
Millivac® Mini Vacuum Pump, 230 V	XF5423050
Millivac® Maxi Vacuum Pump, 230 V	SD1P014M04

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# Sample Analysis

## High Quality Ultrapure Water Can Improve Mass Spectrometry Results

As shown in figure to the right, water contaminants, such as those leached into bottled or stored water, may impact the quality of mass chromatograms and mass spectra. Merck Millipore has developed a range of solutions adapted to the needs of scientists performing mass spectrometry. Use our LiChrosolv® LC-MS Grade Bottled Water (p. 7) or our Milli-Q® ultrapure water purification systems to ensure that your samples and mobile phases are free of organic contaminants, for the best, most reproducible mass spectrometry results. Especially when fitted with a 0.2 µm final filter, Milli-Q® systems are the ideal water source for MALDI-ToF, LC-MS, and other ultrasensitive analyses.



Ultrapure water, freshly delivered from a lab water purification system, eliminates the high background peaks in mass chromatograms of bottled water, especially when the purification system is equipped with a UV lamp. HPLC-grade bottled water and freshly delivered ultrapure water (with and without UV lamp) were subjected to trace enrichment and analyzed by LC-MS using reverse-phase LC and electrospray ionization in positive mode.



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Description	Catalogue No.
Milli-Q® Integral 15 Pure (15 L/hour) and Ultrapure Water Production Unit with built-in resistivity and TOC meter	ZRXQ015T0*
Milli-Q® Advantage A10 Ultrapure Water Purification System	Z00Q0V0WW*
LC-Pak™ point-of-use polisher for the production of at least 500 L of ultrapure water for organic trace analysis.	LCPAK0001*

\*Contact your local Merck Millipore sales representative for a country-specific part number.

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Italy: 848 845 645  
Spain: 901 516 645 Option 1  
Switzerland: 0848 645 645  
United Kingdom: 0870 900 46 45

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+44 (0) 115 943 0840

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