Thermo Scientific
Pierce Controls and Standards
for Mass Spectrometry

calibration tools

for mass spectrometry

Ensure confidence in instrument performance with
Thermo Scientific Pierce Calibration Solutions and Standards.

Thermo
SCIENTIFIC

optimal performance

Calibration solutions
for mass spectrometers

Thermo Scientific™ Pierce™ Calibration Solutions for mass spectrometry are ready-to-use liquid formulations that can quickly calibrate Thermo Scientific™ LC-MS Instrumentation.

In addition to calibration solutions, we offer standards for sensitivity assessment or determination of digestion efficiency, or as a control for complex sample analysis.

Selection Guide for Thermo Scientific™ Calibration Solutions and Standards

Thermo Scientific Instrument	Pierce LTQ ESI Positive Ion Calibration Solution	Pierce LTQ Velos ESI Positive Ion Calibration Solution	Pierce ESI Negative Ion Calibration Solution	Pierce Triple Quad Calibration Solution	Pierce Peptide Retention Time Calibration Mixture	Pierce Reserpine Standard for LC-MS	Pierce Digestion Indicator for Mass Spec	Pierce HeLa Protein Digest Standard
Product #	88322 p. 3	88323 p. 4	88324 p. 5	88325 p. 6	88320, 88321 p. 7	88326 p. 8	84841 p. 9	88328, 88329 p. 10
LXQ	+++	NR	+++	NR	+++	++	+++	+++
LCQ Fleet	+++	NR	+++	NR	+++	++	+++	+++
LTQ XL ETD	+++	NR	+++	NR	+++	++	+++	+++
LTQ Velos	NR	+++	+++	NR	+++	+++	+++	+++
LTQ Velos Pro	NR	+++	+++	NR	+++	++	+++	+++
LTQ Orbitrap Discovery	+++	NR	+++	NR	+++	++	+++	+++
LTQ Orbitrap XL	+++	NR	+++	NR	+++	++	+++	+++
LTQ Orbitrap XL ETD	+++	NR	+++	NR	+++	++	+++	+++
LTQ Orbitrap Velos	NR	+++	+++	NR	+++	++	+++	+++
LTQ Orbitrap Velos Pro	NR	+++	+++	NR	+++	++	+++	+++
MALDI LTQ XL	NR	NR	NR	NR	+++	NR	+++	+++
MALDI LTQ Orbitrap XL	NR	NR	NR	NR	+++	NR	+++	+++
Orbitrap ELITE	NR	+++	+++	NR	+++	++	+++	+++
Orbitrap Fusion Tribrid	NR	+++	+++	NR	+++	+++	+++	+++
Exactive	+++	NR	+++	NR	+++	+	+++	+++
Exactive Plus	NR	+++	+++	NR	+++	+	+++	+++
Q Exactive/Q Exactive Plus	NR	+++	+++	NR	+++	+	+++	+++
LTQ FT Ultra	+++	NR	+++	NR	+++	++	+++	+++
TSQ Access Max	NR	NR	NR	+++	+++	+++	+++	+++
TSQ Quantum Ultra	NR	NR	NR	+++	+++	+++	+++	+++
TSQ Vantage	NR	NR	NR	+++	+++	+++	+++	+++
TSQ Endura	NR	NR	NR	+++	+++	+++	+++	+++
TSQ Quantiva	NR	NR	NR	+++	+++	+++	+++	+++

+++ = Highly recommended
++ = Recommended
+ = Can be used, but not recommended
NR = Not recommended

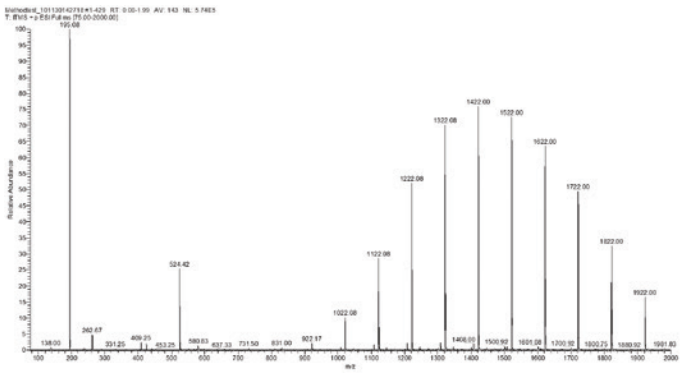
calibration solutions

Thermo Scientific Pierce LTQ ESI Positive Ion Calibration Solution

Use to calibrate Thermo Scientific™ LTQ Series, the LTQ Orbitrap™ Series, the LXQ, LCQ FLEET™ and the Exactive (classic) Mass Spectrometer instruments.

The Thermo Scientific™ Pierce™ LTQ ESI Positive Ion Calibration Solution is a mixture of highly purified ionizable molecules specifically designed for positive mode calibration of Thermo Scientific™ Ion Trap and Orbitrap instruments.

The Pierce LTQ ESI Positive Ion Calibration Solution is a ready-to-use liquid formulation ideal for quickly performing the routine calibration required to maintain the robust performance of Thermo Scientific™ Mass Spectrometers. The LTQ ESI Positive Ion Calibration Solution is manufactured at an ISO 9001 facility and each lot is quality controlled with strict specifications. The stable solution is provided in a leak-proof, high-purity PTFE bottle.



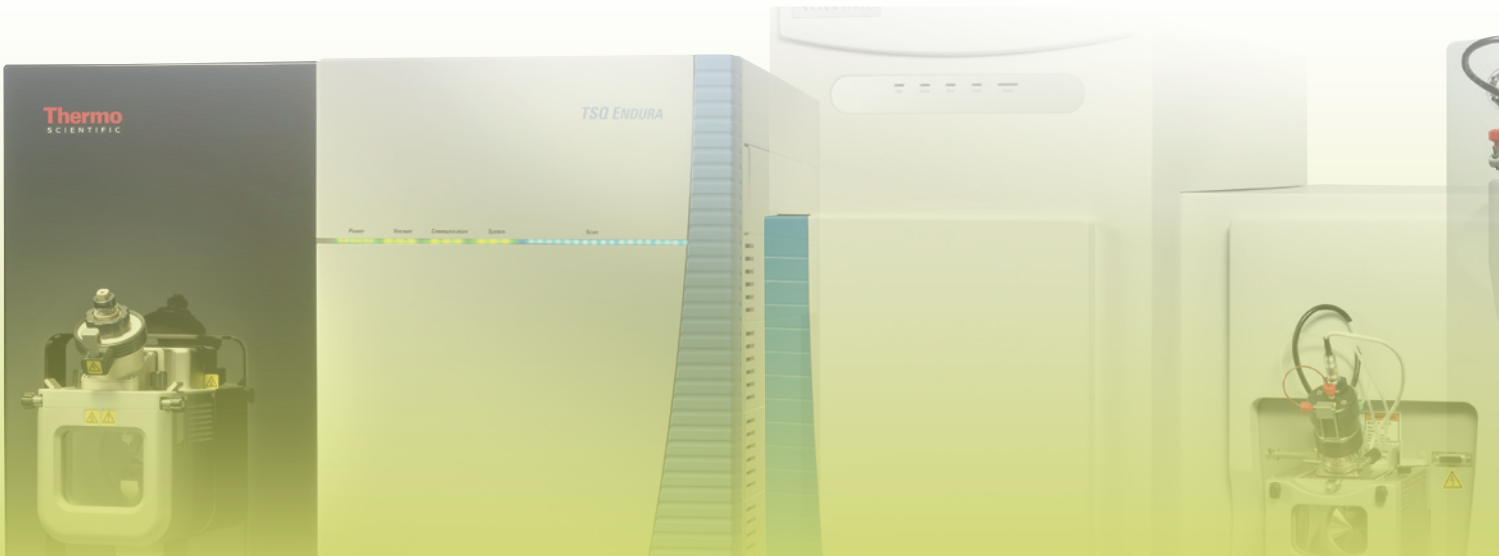
Thermo Scientific Pierce LTQ ESI Positive Ion Calibration Solution spectra. Formulation: Caffeine (20µg/mL), MRFA (1µg/mL) and Ultramark 1621 (0.001%) in an aqueous solution of acetonitrile (50%), methanol (25%) and acetic acid (1%).

Highlights:

- **Strong peaks** – mixture of caffeine, MRFA and Ultramark 1621 in an acetonitrile/methanol/acetic solution
- **Ready to use** – load the mass reference standard into a syringe and inject into the instrument
- **High purity** – mass spectrometry-grade reagents in a non-leachable container
- **Stable** – store at room temperature for more than one year

Ordering Information

Product #	Description	Pkg. Size
88322	Pierce LTQ ESI Positive Ion Calibration Solution *Sufficient for 10 to 20 calibrations*	10mL

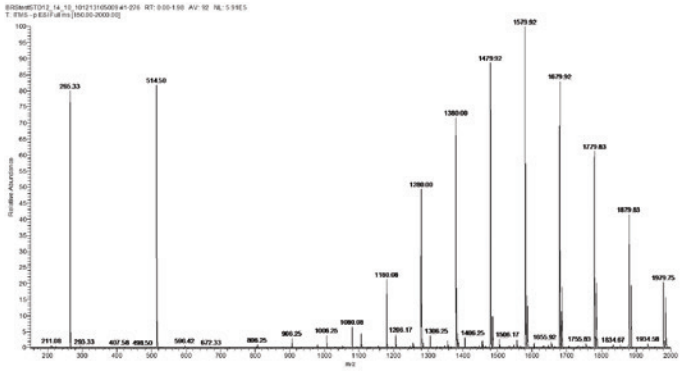


Thermo Scientific Pierce LTQ Velos ESI Positive Ion Calibration Solution

Use to calibrate the Thermo Scientific™ LTQ Velos™ Series and LTQ Orbitrap™ Velos™, Q Exactive Series and Exactive Plus Mass Spectrometer instruments.

The Thermo Scientific™ Pierce™ LTQ Velos ESI Positive Ion Calibration Solution is a mixture of highly purified ionizable molecules designed for positive mode calibration of Thermo Scientific LTQ Velos Series Mass Spectrometer instruments.

The Pierce LTQ Velos ESI Positive Ion Calibration Solution is a ready-to-use liquid formulation ideal for quickly performing the routine calibration required to maintain the robust performance of Thermo Scientific Mass Spectrometers. The LTQ Velos ESI Positive Ion Calibration Solution is manufactured at an ISO 9001 facility and each lot is quality controlled with strict specifications. The stable solution is provided in a leak-proof, high-purity PTFE bottle.



Thermo Scientific Pierce LTQ ESI Positive Ion Calibration Solution spectra. Formulation: Caffeine (20µg/mL), MRFA (1µg/mL) and Ultramark 1621 (0.001%) in an aqueous solution of acetonitrile (50%), methanol (25%) and acetic acid (1%).

Highlights:

- **Strong peaks** – mixture of caffeine, MRFA, Ultramark 1621 and n-butylamine in an acetonitrile/methanol/acetic solution
- **Ready to use** – load the mass reference standard into a syringe and inject into the instrument
- **High purity** – mass spectrometry-grade reagents in a non-leachable container
- **Stable** – store at room temperature for more than one year

Ordering Information

Product #	Description	Pkg. Size
88323	Pierce LTQ Velos ESI Positive Ion Calibration Solution *Sufficient for 10 to 20 calibrations*	10mL

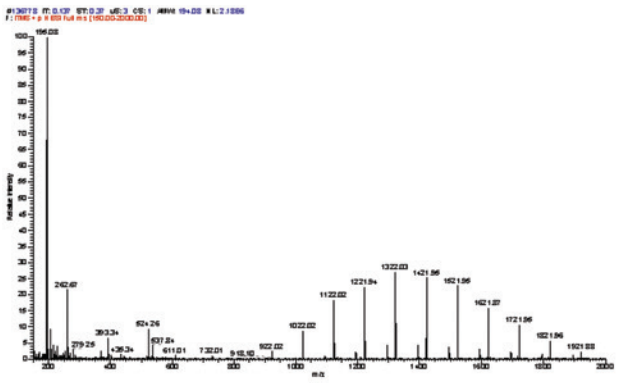
calibration solutions

Thermo Scientific Pierce ESI Negative Ion Calibration Solution

Use to calibrate Thermo Scientific LTQ Series, LTQ Velos Series, the LTQ Orbitrap Series and Exactive Mass Spectrometer instruments.

The Thermo Scientific™ Pierce™ ESI Negative Ion Calibration Solution is a mixture of highly purified ionizable molecules designed for negative mode calibration of Thermo Scientific LTQ Series Mass Spectrometer instruments.

The Pierce ESI Negative Ion Calibration Solution is a ready-to-use liquid formulation ideal for quickly performing the routine calibration required to maintain the robust performance of Thermo Scientific Mass Spectrometers. The ESI Negative Ion Calibration Solution is manufactured at an ISO 9001 facility and each lot is quality controlled with strict specifications. The stable solution is provided in a leak-proof, high-purity PTFE bottle.



Thermo Scientific Pierce ESI Negative Calibration Solution spectra. Formulation: sodium dodecyl sulfate (2.9µg/mL),sodium taurocholate (5.4µg/mL) and Ultramark 1621 (0.001%) in an aqueous solution of acetonitrile (50%), methanol (25%) and acetic acid (1%).

Highlights:

- **Strong peaks** – mixture of SDS, sodium taurocholate and Ultramark 1621 in an acetonitrile/methanol/acetic solution
- **Ready to use** – load the mass reference standard into a syringe and inject into the instrument
- **High purity** – mass spectrometry-grade reagents in a non-leachable container
- **Stable** – store at room temperature for more than one year

Ordering Information

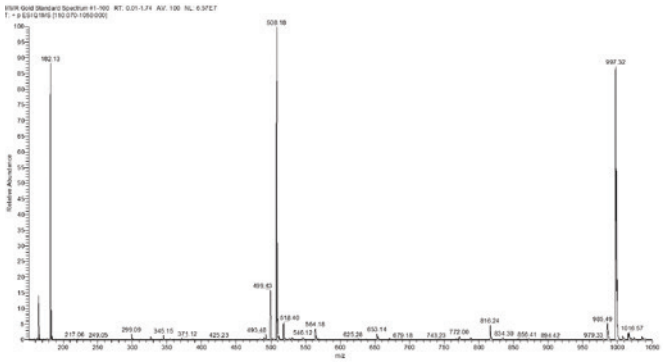
Product #	Description	Pkg. Size
88324	Pierce ESI Negative Ion Calibration Solution *Sufficient for 10 to 20 calibrations*	10mL

Thermo Scientific Pierce Triple Quadrupole Calibration Solution

Use to calibrate Thermo Scientific™ TSQ Quantum™, TSQ Discovery™, TSQ Quantum Ultra™, TSQ Quantum Access™, TSQ Vantage, TSQ Endura and TSQ Quantiva Series Mass Spectrometer instruments.

The Thermo Scientific™ Pierce™ Triple Quadrupole Calibration Solution is a mixture of high purity, ionizable components specifically designed for positive mode calibration of Thermo Scientific™ Triple Stage Quadrupole instruments.

The Pierce Triple Quadrupole Calibration Solution is a ready-to-use liquid formulation ideal for quickly performing the required routine calibration to maintain the robust performance of Thermo Scientific Mass Spectrometers. The Triple Quadrupole Calibration Solution is manufactured at an ISO 9001 facility and each lot is quality controlled with strict specifications. The stable solution is provided in a leak-proof, high-purity PTFE bottle.



Thermo Scientific Pierce Triple Quadrupole Calibration Solution. Formulation: 25µM Tyr_1, 25µM Tyr_3 and 25µM Tyr_8, in an aqueous of methanol (50%) and formic acid (0.1%).

Highlights:

- **Strong peaks** – mixture of three tyrosine polymers in methanol/formic acid solution
- **Ready to use** – load the reference standard into a syringe and inject into the instrument
- **High purity** – mass spectrometry-grade reagents in a non-leachable container
- **Stable** – store at 2 to 8°C for more than one year

Ordering Information

Product #	Description	Pkg. Size
88325	**Pierce Triple Quadrupole Calibration Solution** *Sufficient for 10 to 20 calibrations*	10mL

Thermo Scientific Pierce Peptide Retention Time Calibration Mixture

The prediction of peptide retention time is a tool to assess chromatographic performance and to assist in the development of multiplexed, high-throughput mass spectrometric assays. Thermo Scientific™ Pierce™ Peptide Retention Time Calibration Mixture and Thermo Scientific™ Pinpoint™ Software can be used to predict peptide retention time from sequence alone or to streamline the transition from qualitative protein discovery results to the development of targeted mass spectrometry (MS) assays on Thermo Scientific™ Triple Quadrupole, Orbitrap™, Exactive™ and Ion Trap Mass Spectrometers.

The Pierce Peptide Retention Time Calibration Mixture can be used for optimization and regular assessment of chromatographic performance and for rapid development of multiplexed, scheduled targeted MS assays for the quantification of dozens to hundreds of peptide targets per run.

Applications:

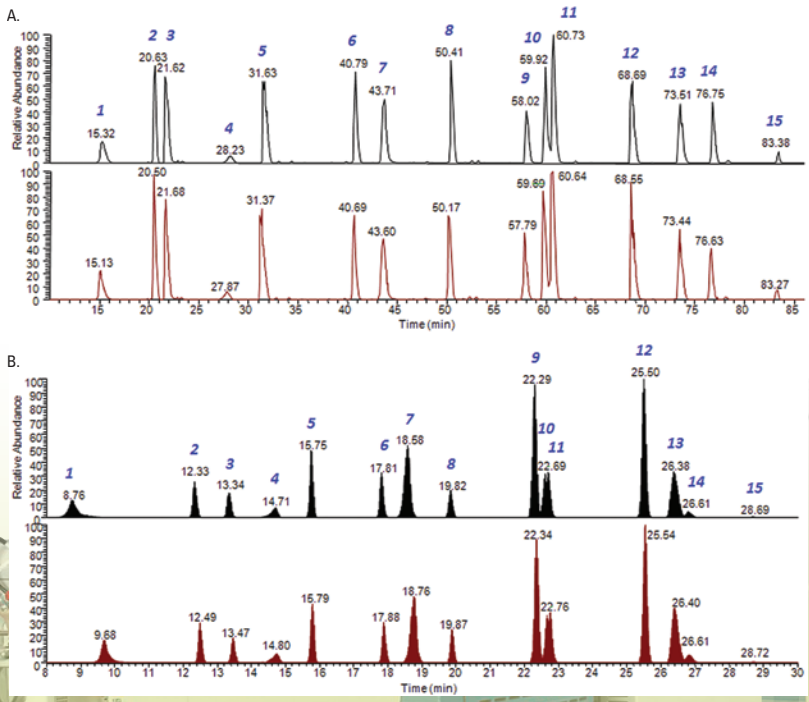
- Assessment of chromatography and MS instrument performance
- Prediction of peptide retention across multiple instrument platforms
- Prediction of peptide retention time from sequence using calculated hydrophobicity factor
- Optimization of scheduled MS acquisition windows for improved quantification and increased multiplexing
- Internal standard to normalize for variation in retention times and peak intensities between runs

The Pierce Peptide Retention Time Calibration Mixture contains 15 synthetic heavy peptides mixed at an equimolar ratio that elute across the chromatographic gradient. The peptide sequences and chromatographic results are used to assess LC performance. In addition, the observed retention times and hydrophobicity factors (HF) for these calibrants are fit to a linear equation to determine the slope of the retention time/HF relationship. This equation and the HF of uncharacterized peptides are then used to predict retention time.

Thermo Scientific Pierce Peptide Retention Time Calibration mixture components and properties.

The peptide sequences, peptide masses and chromatographic behavior of each component of the Pierce Peptide Retention Time Calibration Mixture are given below. The position and identity of the heavy isotope-labeled amino acid in each sequence is indicated in bold.

	Peptide Sequence	Mass	Hydrophobicity Factor (HF)
1	SSAAPPPPP**R**	985.5220	7.56
2	GISNEGQNASI**K**	1224.6189	15.50
3	HVLTSIGE**K**	990.5589	15.52
4	DIPVPKP**K**	900.5524	17.65
5	IGDYAGI**K**	843.4582	19.15
6	TASEFDSAIAQD**K**	1389.6503	25.88
7	SAAGAFGPELS**R**	1171.5861	25.24
8	ELGQSGVDTYLQT**K**	1545.7766	28.37
9	GLILVGGYGT**R**	1114.6374	32.18
10	GILFVGSGVSGGEEGA**R**	1600.8084	34.50
11	SFANQPLEVVYS**K**	1488.7704	34.96
12	LTILEEL**R**	995.5890	37.30
13	NGFILDGFP**R**	1144.5905	40.42
14	ELASGLSFPVGF**K**	1358.7326	41.18
15	LSSEAPALFQFDL**K**	1572.8279	46.66



Chromatographic analysis of the Thermo Scientific Pierce Peptide Retention Time Calibration Mixture. A. The Pierce Peptide Retention Time Calibration Mixture (250fmoles) was analyzed in duplicate on a Thermo Scientific LTQ XL Orbitrap Mass Spectrometer using a self-packed column (75µm x 20cm) containing Magic™ C18 (Michrom Bioresources) and using a 0.25% per minute gradient of Buffer A (0.1% formic acid) and Buffer B (0.1% formic acid/99.9 % acetonitrile) at 300nL per minute. **B.** The Pierce Retention Time Calibration Mixture was also analyzed on a Thermo Scientific TSQ Vantage Mass Spectrometer using a Thermo Scientific™ Hypersil™ GOLD C18 column (1.0 x 150mm, Product # 25005-150165) with a 1.0% per minute gradient at 120µL per minute. Numbered peaks correspond to the calibrant peptides described above.

Ordering Information

Product #	Description	Pkg. Size
88320	Pierce Peptide Retention Time Calibration Mixture, 0.5pmol/µL	50µL
88321	Pierce Peptide Retention Time Calibration Mixture, 5pmol/µL	200µL

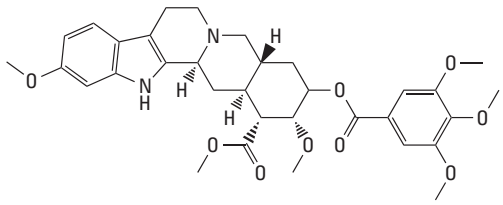
Thermo Scientific Pierce Reserpine Standard for LC-MS

Thermo Scientific™ Pierce™ Reserpine Standard for LC-MS is a precise concentration of reserpine specifically designed for performance evaluation of mass spectrometers, including the Thermo Scientific Ion Trap and TSQ Series of instruments.

The Pierce Reserpine Standard for LC-MS is a pre-diluted liquid formulation that is ideal for performing installation tests of Thermo Scientific and other manufacturers' mass spectrometers. The standard is provided at a concentration of 100pg/µL in 50% isopropyl alcohol and requires minimal additional dilutions. The product is provided as a pack of 5 x 1mL glass amber vials with PTFE-lined screw caps. The Pierce Reserpine Standard for LC-MS is manufactured at an ISO 9001 facility and each lot is quality controlled with strict specifications.

Highlights:

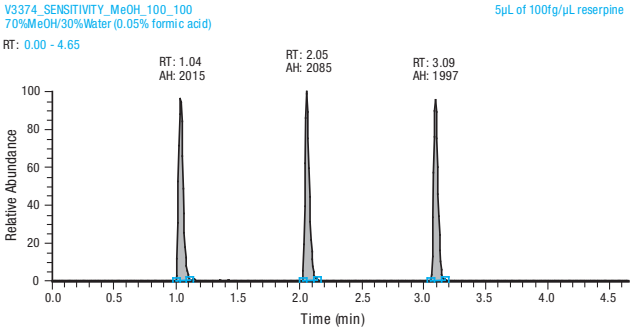
- **Convenient** – provided at a concentration of 100pg/µL in 50% isopropyl alcohol, requiring minimal additional dilutions to reach target concentration for injection
- **Safe handling** – unlike glass ampules, cap can be easily removed and replaced when withdrawing solution
- **High purity** – mass spectrometry-grade reagent in non-leachable screw-cap vials
- **Stable** – store at 4°C for up to one year

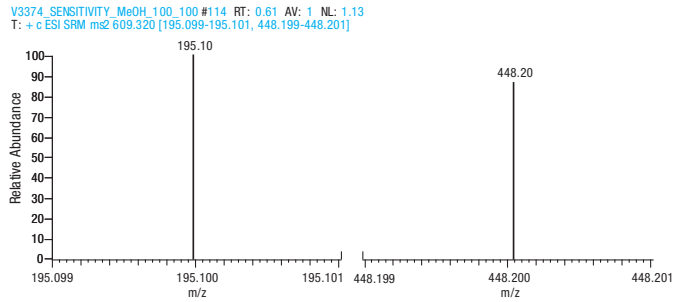


Reserpine

MW 608.68
Exact Mass: 608.27

Chemical structure of reserpine. The Pierce Reserpine Standard for LC-MS consists of high-purity reserpine at 100pg/µL in 50% isopropyl alcohol.





Example selected reaction monitoring (SRM) of 500fg reserpine on a Thermo Scientific™ Vantage™ triple quadrupole mass spectrometer. Chromatogram of three 5µL loop injections of 100fg/µL Pierce Reserpine on a Hypersil GOLD aQ 2.1x20mm Javelin column with isocratic 300µL/min flow of 70% methanol: 30% water: 0.05% formic acid (upper panel).The SRM transitions monitored were 609.3-195.1 and 609.3-448.2 m/z with a 0.2 FWHM Q1 peak width (lower panel).

Ordering Information

Product #	Description	Pkg. Size
88326	Pierce Reserpine Standard for LC-MS *Sufficient for 5 to 500 injections*	5 x 1mL

Thermo Scientific Pierce Digestion Indicator

Thermo Scientific™ Pierce™ Digestion Indicator is a unique, non-mammalian protein (26kDa) that can be spiked into cell lysates and carried through the sample preparation procedure, resulting in five distinct peptides that can be quantified. The Digestion Indicator is provided as a frozen liquid (10µg) and an aliquot of 0.5µg is recommended per 100µg sample of lysate. The Pierce Digestion Indicator is also provided as a component of the Thermo Scientific™ Pierce™ Mass Spec Sample Prep Kit for Cultured Cells (Product # 84840).

Highlights:

- **Non-mammalian** – Pierce Digestion Indicator peptides can be easily distinguished from endogenous mammalian peptides
- **Ready to use** – just thaw and spike into lysate
- **Validated** – contains 5 distinct peptides that can be quantitated to assess digestion efficiency

The Pierce Digestion Indicator serves as an internal digestion control standard protein to assure protocol performance and to quantify sample preparation processing and digestion efficiency across samples. The properties of the signature peptides following digestion are indicated in Table 1.

To test the reproducibility of the Pierce Mass Spec Sample Prep Kit for Cultured Cells (Product # 84840), triplicate samples of a HeLa cell culture were processed and analyzed using the Pierce Digestion Indicator protocol by spiking the Digestion Indicator into each lysate after the initial lysis step. The samples were analyzed by LC-MS/MS on a Thermo Scientific Velos Pro Ion Trap Mass Spectrometer. Digestion indicator peptides were quantified with Thermo Scientific Pinpoint 1.2 software, which is pre-programmed to quantify the Pierce Digestion Indicator peptides and MS^2 transitions. The coefficients of variation (CV) for replicates of the five peptides were 6-16% (Table 2).

Table 1. Properties of the five Thermo Scientific Pierce Digestion Indicator peptide sequences.

Digestion Indicator Peptide Sequence	Observed Mass/Charge	Observed Charge	Hydrophobicity Factor
ITGTLNGVEFELVGGGEGTPEQGR	**1209.1007**	**+2**	**40.59**
VMGTGFPEDSVIFTDK	871.9189	+2	40.24
DGGYYSSVVDSHMHFK	610.2701	+3	27.24
SAIHPSILQNGGPMFAFR	648.3367	+3	42.42
VEEDHSNTELGIVEYQHAFK	587.0315	+4	35.13

Table 2. Digestion indicator peptides and example assessment of reproducibility. Sequences of the five peptides that result from the Thermo Scientific Pierce Digestion Indicator, and coefficients of variation (CV) for triplicate samples processed using the product protocol.

Digestion Indicator Peptide Sequence	Observed Mass/Charge	Coefficients of Variation (CV)
ITGTLNGVEFELVGGGEGTPEQGR	**1209.1010**	**16**
VMGTGFPEDSVIFTDK	871.9189	13
DGGYYSSVVDSHMHFK	610.2701	6
SAIHPSILQNGGPMFAFR	648.3367	13
VEEDHSNTELGIVEYQHAFK	587.0315	13

Ordering Information

Product #	Description	Pkg. Size
84841	**Pierce Digestion Indicator for Mass Spectrometry** *Sufficient for production of five signature peptides upon digestion for mass spectrometry*	10µg

Thermo Scientific Pierce HeLa Protein Digest Standard

Superior-quality complex mammalian protein digest standard.

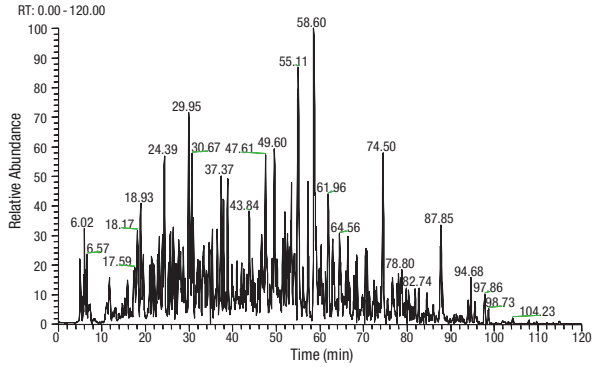
The Thermo Scientific™ Pierce™ HeLa Protein Digest Standard is a highly validated mammalian protein digest that may be used as a quality control sample for MS analysis of complex proteomic samples.

Highlights:

- **Positive control sample** – complex mammalian proteome sample protein digest (> 15,000 proteins)
- **High digestion efficiency** – less than 10% missed cleavages using trypsin and LysC
- **Superior peptide quality** – less than 10% methionine oxidation and less than 10% lysine carbamylation
- **Rigorously tested** – high-quality, efficient protein digest with lot-to-lot digest uniformity
- **Stable** – provided in a stable, lyophilized format

The Pierce HeLa Protein Digest Standard is a lyophilized tryptic peptide mixture that can be used as a quality control standard for liquid chromatography (LC) separation, MS method development and MS performance benchmarking. The digest is specifically formulated for LC/MS experiments and does not contain salts or detergents. Using the digest standard routinely before analysis of complex samples makes it possible to monitor and normalize LC/MS performance between samples and over time.

The protein digest is derived from a well-established adenocarcinoma (HeLa) reference cell line, which expresses over 15,000 proteins with relevant post-translational modifications making it an ideal standard for complex proteome MS applications. The protein lysate has been digested with both LysC and trypsin to reduce tryptic missed cleavages and improve protein sequence coverage. Moreover, unlike other commercially available protein digests for MS, the Pierce HeLa Protein Digest Standard must meet stringent quality testing specifications including peptide quality, digestion efficiency and lot-to-lot digest uniformity.



Thermo Scientific Pierce HeLa Digest Standard base peak chromatogram. Chromatogram of 200ng Pierce HeLa Protein Digest Standard separated using a Thermo Scientific™ Acclaim™ PepMap™100 3µm x 75µm x 15cm column (Product # 160321) with a 2-35% gradient (A: 0.1% FA in water, B: 0.1% FA in 100% acetonitrile) at 300nL/min for 120 minutes and detected on a Thermo Scientific LTQ Orbitrap XL Mass Spectrometer.

Thermo Scientific Pierce HeLa Protein Digest Standard quality testing specifications.

Analysis	Specification
UV Absorbance	A_{280} = 1.0 -/+ 0.1
LC/MS Chromatogram	LC/MS chromatogram conforms to reference
Reference Peptide Area	Ratio of peptide area to reference = 0.75-1.25
***Peptide Missed Cleavage**	Tryptic peptide missed cleavage ≤ 10%
***Peptide Alkylation**	Cysteine carbamidomethyl modification ≥ 98%
***Peptide Oxidation**	Methionine oxidation ≤ 10%
***Other Peptide Modification**	Carbamylation < 10%

** Peptide missed cleavage, alkylation, oxidation and modification determined by Preview™ Software (Protein Metrics)™ using a human protein Swiss-Prot database.*

Ordering Information

Product #	Description	Pkg. Size
88328	Pierce HeLa Protein Digest Standard	20µg
88329	Pierce HeLa Protein Digest Standard	5 x 20µg

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Email: perbio.euromarketing@thermofisher.com
thermoscientific.com/pierce

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1602867 01/15 Printed in the U.S.

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