

Thermo Scientific Q Exactive
Orbitrap LC-MS/MS System

Unmatched Confidence for Quan/Qual Analyses

Identify • Quantify • Confirm

Thermo
SCIENTIFIC

Quantification

\,kwän-fər-'mā-shän\ n

1 : the ability to confidently identify, quantify, and confirm using a single

mass spectrometer : *syn* **Q EXACTIVE
MASS SPECTROMETER**

The unsurpassed performance of Orbitrap™ technology has revolutionized mass spectrometry. The Thermo Scientific Q Exactive benchtop LC-MS/MS is the next step in that revolution, combining high-performance quadrupole precursor selection with high-resolution, accurate-mass (HR/AM) Orbitrap detection for outstanding performance and tremendous versatility.

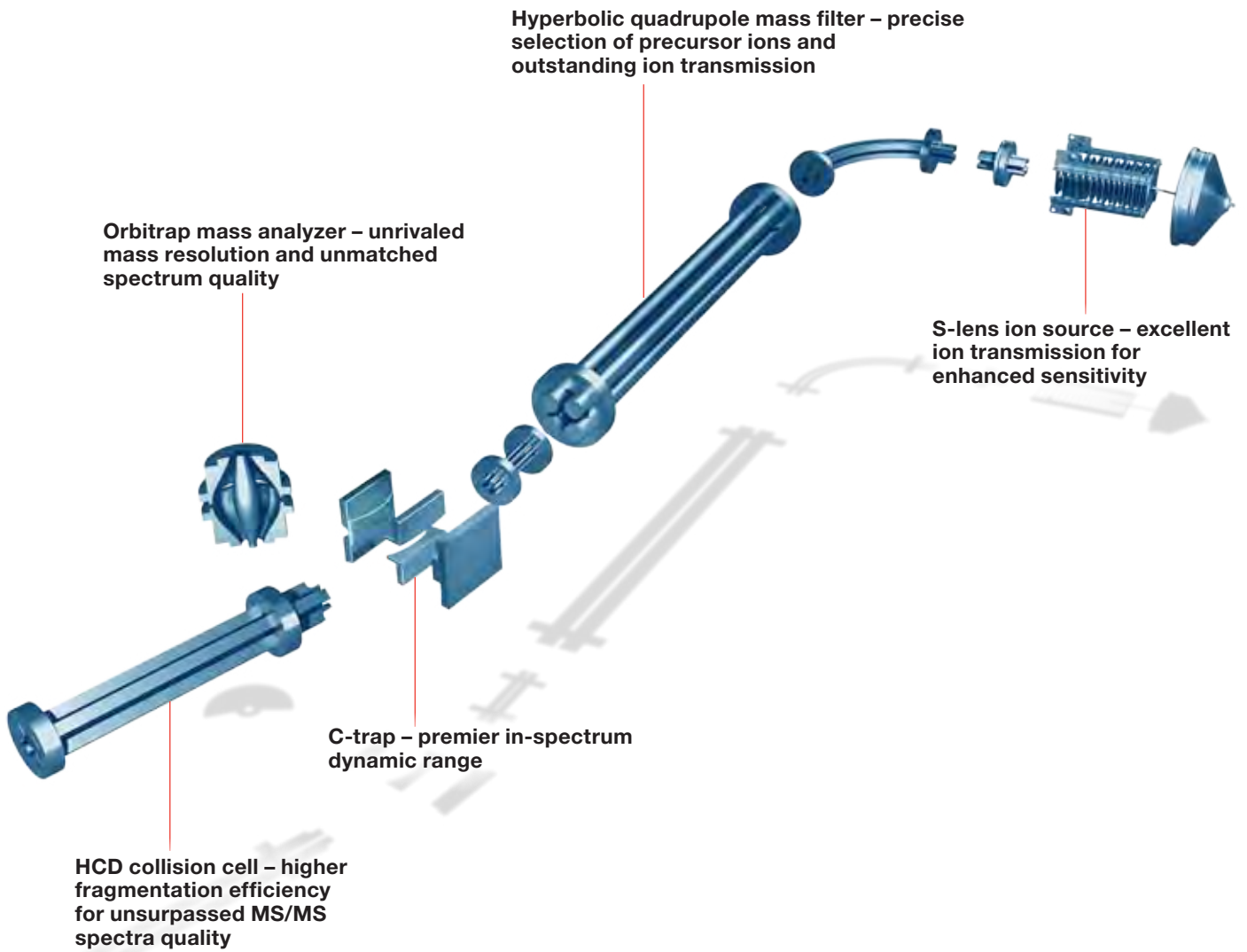
The Q Exactive™ mass spectrometer is superbly suited to untargeted or targeted screening with high-confidence confirmation, but is equally capable of a broad range of qualitative and quantitative applications.

The superior quality of Q Exactive data enables identification and quantitation of more compounds with greater confidence.

With the Q Exactive LC-MS/MS:

- Proven S-lens ion source provides the enhanced sensitivity needed to find more analytes
- 140,000 resolution at m/z 200 and <1 ppm mass accuracy provide outstanding ID confidence
- Spectrum multiplexing and advanced signal processing ensure UHPLC-compatible data acquisition speed for increased throughput
- Fast scan-to-scan polarity switching in both MS and MS/MS reveals more compounds in a single run

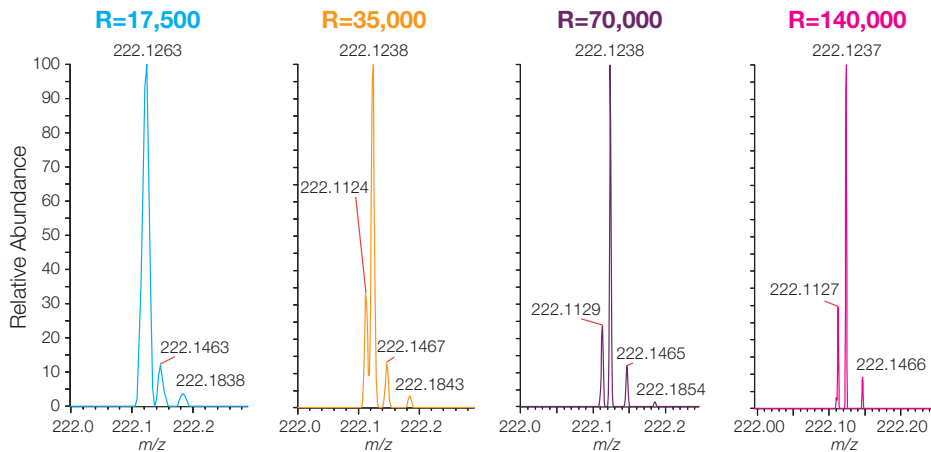




Carbofuran
Formetanate

$C_{12}H_{15}NO_3$
 $C_{11}H_{15}N_3O_2$

$M+H^+ = 222.1125$
 $M+H^+ = 222.1237$



Nominally isobaric pesticides carbofuran and formetanate are unresolved or only poorly resolved at the highest resolutions available in Q-TOF instruments. The higher resolutions easily achieved by the Q Exactive instrument clearly resolve analytes from complex matrix interferences without sacrificing sensitivity.

Metabolic Analyses in Drug Discovery

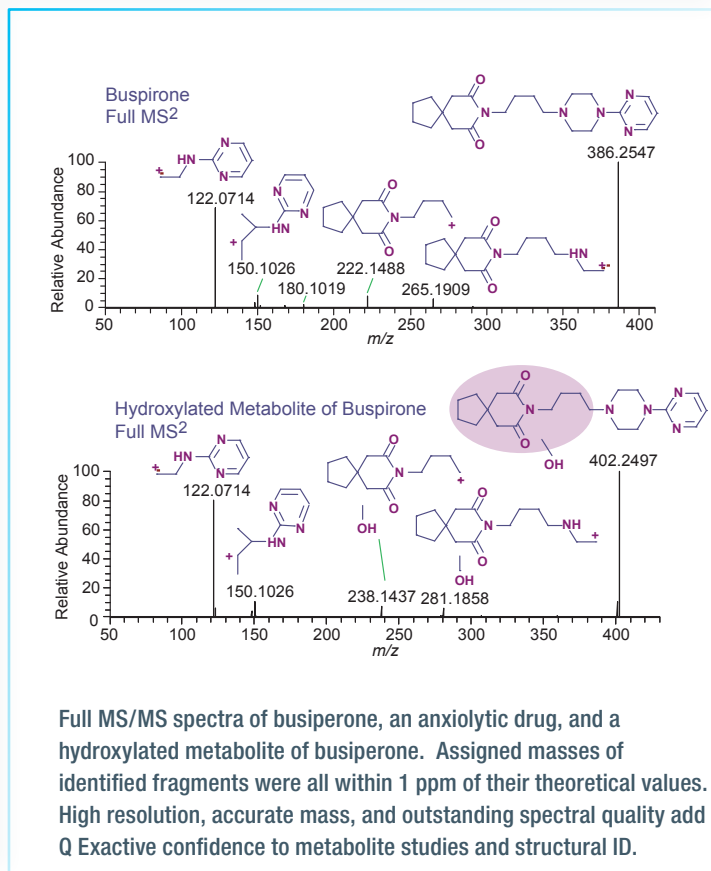
The flexible quantification capabilities of the Q Exactive instrument make it a versatile solution for drug discovery and metabolism research.

Greater throughput for drug discovery studies

For DMPK quan/qual screening studies, the Q Exactive instrument provides triple quadrupole-equivalent ability to quantify parent compounds and metabolites, and identity confirmation with MS/MS sensitivity and selectivity superior to Q-TOFs. Thermo Scientific MetQuest software enables laboratories to quantify metabolic stability and confirm putative metabolites from a single injection for better throughput.

Confident metabolite structural identification

For structural identification of metabolites, the Q Exactive mass spectrometer leverages the accuracy and confidence of Orbitrap technology to eliminate interferences. The Q Exactive instrument provides superior MS/MS sensitivity and greater confidence in structural identification. Thermo Scientific Networks metabolite identification software and Mass Frontier spectral interpretation software assist with fast, confident structural elucidation.



From acquisition to reporting, MetQuest software automates processing of metabolic stability screening data from the Q Exactive LC-MS/MS.

Faster reactive-metabolite screening

Metabolites from the same parent compound can have a large variance in ionization efficiency between ionization polarities. With fast scan-to-scan polarity switching in both MS and MS/MS, the Q Exactive instrument maximizes metabolite detection and identification from a single chromatographic run.

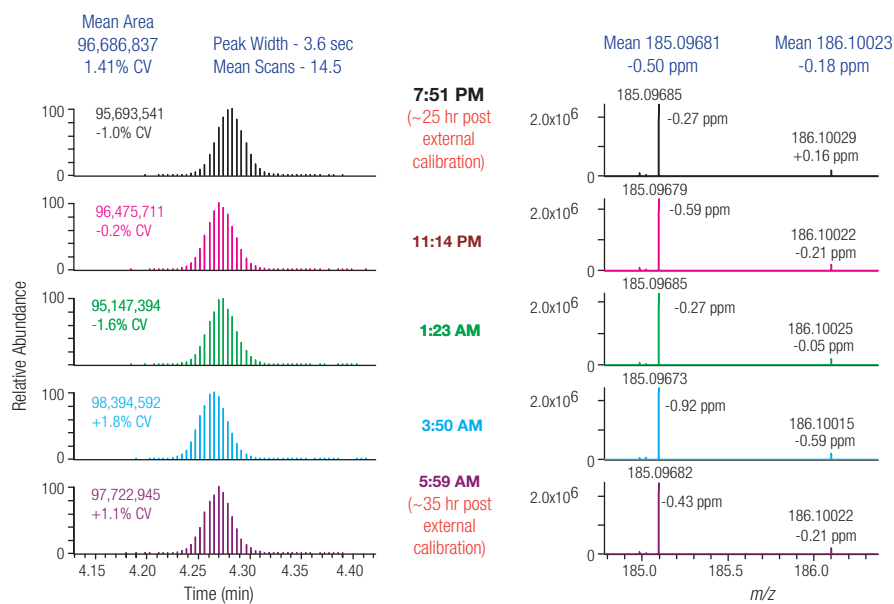
High-confidence drug impurity analysis

Whether you are screening to find the toughest impurities, genotoxic compounds, or leachables and extractables, the quantification capabilities of the Q Exactive mass spectrometer provide a greater measure of confidence.

Powerful Engine

for Large-Scale Metabolomic Profiling

With the high mass resolution to differentiate analytes from interferences, the scan speed to keep up with UHPLC, and fast polarity switching to find more endogenous metabolites, the Q Exactive mass spectrometer is the platform of choice for the large-scale profiling of complex metabolomics samples. The component elucidator algorithm in Thermo Scientific SIEVE software removes chemical background signals and groups related adducts, dimers and isotopes, dramatically improving confidence, reducing the false discovery rate, and accelerating biomarker discovery.



A 12-hour continuous UHPLC-MS analysis of d5 hippuric acid (m/z 185.0969) from rat plasma demonstrates the Q Exactive mass spectrometer's robust ion statistics and highly stable mass accuracy.

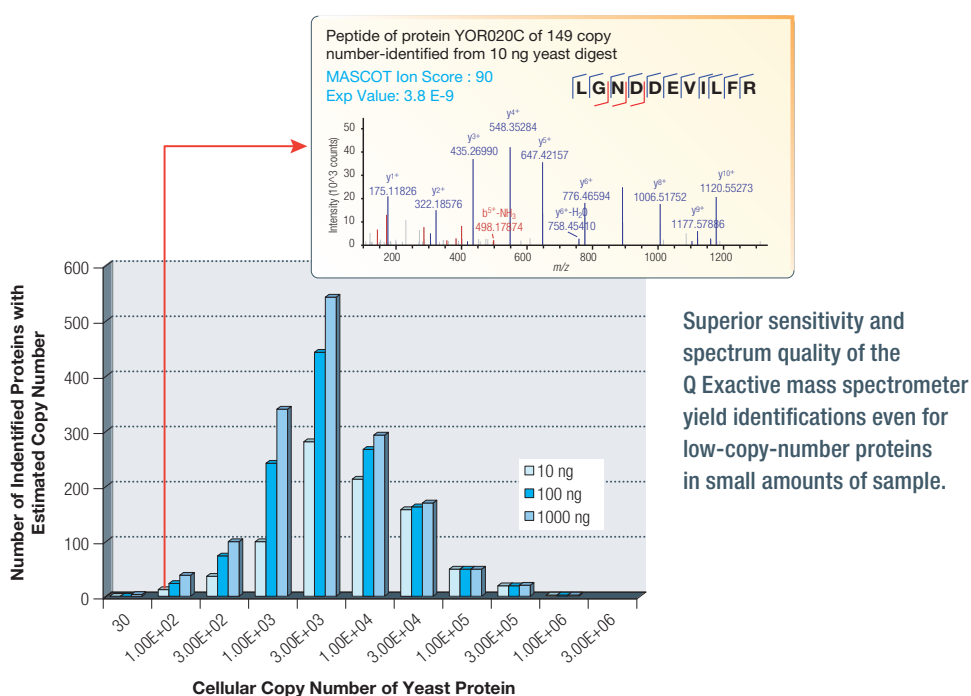
Profiling

All Classes of Lipids

The Q Exactive mass spectrometer is also well-suited for lipid profiling. Its outstanding resolution helps unravel complex samples. The Q Exactive LC-MS/MS is an excellent solution for analysis of fragile labile lipids and can perform qualitative and quantitative analyses of all classes of lipids.

Making High-Resolution, Accurate-Mass Quan/Qual More Accessible for Proteomics Research

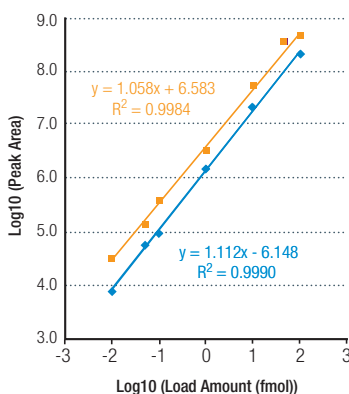
Proteomics, more than any other field, has benefited from Orbitrap technology. The Q Exactive mass spectrometer provides robust, easy-to-use high-resolution, accurate-mass (HR/AM) capabilities for quantitative and qualitative proteomics applications. It is ideally suited for proteomics labs already benefiting from Orbitrap technology that need to expand their analytical capacity. And it makes HR/AM confidence available to labs relying on unit resolution instruments for high-throughput quantitation.



- Higher-energy collisional dissociation (HCD) often yields superior fragmentation and higher-quality MS/MS spectra compared CID.
- Superior spectral quality and a wide dynamic range make it possible to explore deeper in the proteome, identifying more proteins and quantifying proteins other instruments cannot find.
- Unlike Q-TOF technology, Orbitrap technology requires no tradeoff between high sensitivity and mass resolution.
- The quan/qual capabilities of the Q Exactive instrument make it easier than ever to transition from proteomic discovery experiments to targeted protein quantitation and confirmation.

Timed SIM MS quantitative analysis of two peptides in a 1- μ g yeast digest demonstrates both outstanding LOD (10 attomoles) and excellent linearity.

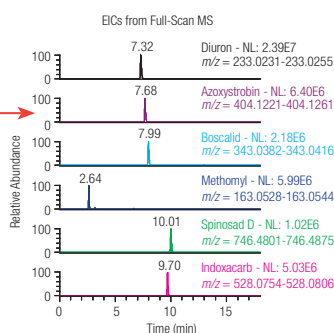
■ GLILVGGYGTR*
 ◆ NGFILDGFPR*



Supporting the Q Exactive LC-MS/MS for proteomics research is a range of software including Thermo Scientific Proteome Discoverer software for protein identification, SIEVE software for differential expression analysis, and Pinpoint software for quantitation and verification.

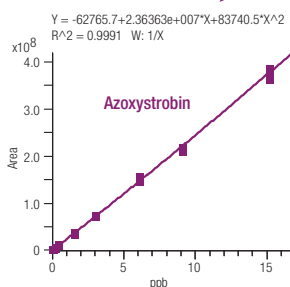
Screening and Quantifying Environmental and Food Samples with Greater Confidence

The Q Exactive LC-MS/MS is the ideal quan/qual screening platform, with specificity that far exceeds triple quadrupole, Q-TOF, or Q-Trap levels. Whether screening and quantifying antibiotics, pesticides or hormones, its data-dependent™, full-scan MS/MS capabilities, superior 140,000 resolution and mass accuracy ensure the highest possible confidence in every ID. Thermo Scientific ExactFinder software simplifies every step from method development through data processing and reporting. Even with challenging experiments like multi-residue analyses involving hundreds of compounds in multiple classes, the Q Exactive MS and ExactFinder™ software provide results that stand up to the closest scrutiny.

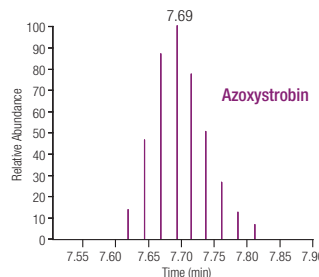


Quantification capabilities of the Q Exactive system provide simultaneous quan/qual analysis of a 60-pesticide mixture. Fast scanning ensures high-quality MS/MS data from narrow UHPLC peaks.

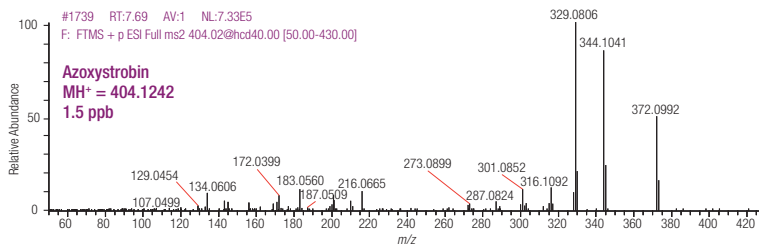
Quantitation



Multiple MS/MS Scans Across Each Peak



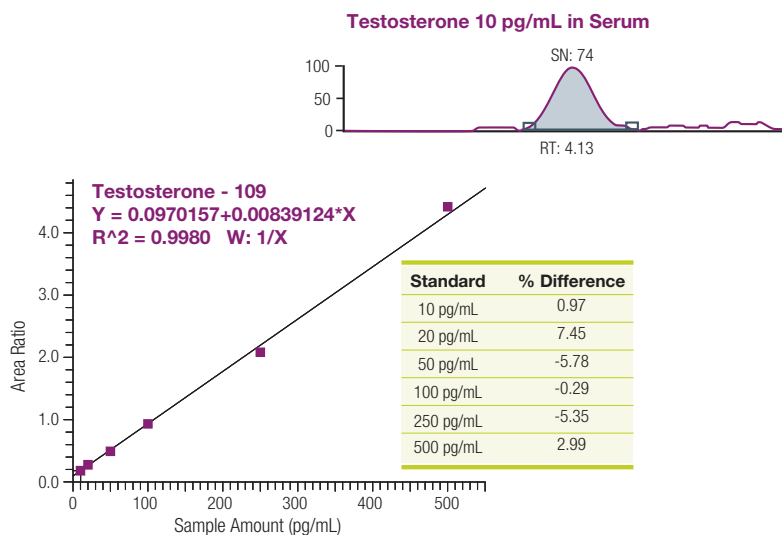
Confirmation



Mass [m/z]	Retention Time (min)	Abundance	Identification
17	210.11249		
18	222.11249		
19	224.09176		
20	255.13390		
21	202.08542		
22	202.0862		
23	320.108		
24	404.01		
25	336.1		
26	355.1		
27	297.1		
28	301.11776	Positive	6.35
29	233.02432	Positive	6.47
30	301.11776	Positive	6.48
31	260.02398	Positive	6.48
33	404.12412	Positive	6.72
34	312.11653	Positive	6.81
35	226.08910	Positive	6.90
36	388.13104	Positive	6.90
37	200.11825	Positive	6.92
38	249.01923	Positive	6.97
39	312.11653	Positive	8.81
40	233.02432	Positive	8.90
41	301.11776	Positive	8.90
42	260.02398	Positive	8.92
43	312.11653	Positive	8.97
44	233.02432	Positive	9.03
45	301.11776	Positive	9.07
46	260.02398	Positive	9.15

Moving Quantitation Confidence to Another Level in Clinical Research and Forensic Toxicology

SRM is the standard approach to quantitative analysis in clinical research, toxicology, and doping control. The Q Exactive LC-MS/MS takes quantitative analyses to another level, providing the strength of SRM with a level of confidence only possible with high-resolution, accurate-mass Orbitrap technology. The superior Q Exactive quantification capabilities make it possible to identify, quantify, and confirm endogenous steroids, drugs of abuse, and pain-management therapeutics with equal ease.



Sample	Fragment m/z 97		Fragment m/z 109	
	ng/dL (Calibrators in water)	ng/dL (Calibrators in plasma)	ng/dL (Calibrators in water)	ng/dL (Calibrators in plasma)
T1	15	15	13	14
T2	17	17	19	20
T3	156	156	156	152
T4	34	34	37	36
T5	8	8	8	7

Analysis of testosterone in water and in charcoal-stripped serum demonstrates the excellent sensitivity and ion-ratio stability of the Q Exactive LC-MS/MS.



www.thermoscientific.com/qexactive

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