



Thermo Scientific
EQvan MAX Plus Systems

Automated, high-throughput LC-MS solutions for water and beverage analysis

Pesticides • Pharmaceuticals • Personal care products
Endocrine disruptors • Perfluorinated compounds

Thermo
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Ensure water and beverage safety

Thermo Scientific™ EQuan MAX Plus™ systems provide turn-key liquid chromatography/mass spectrometry (LC/MS) solutions for the analysis of trace contaminants in environmental water, drinking water, and beverage samples.

Exposure to pesticides, pharmaceuticals, personal care products, endocrine disruptors, and perfluorinated compounds in water is a significant health concern. As our understanding of their hazards increases, lower limits of detection (LODs) become critical. With the emergence of potential new contaminants, laboratories performing water and beverage analysis will be challenged to detect and quantify both targeted and nontargeted contaminants, and to do so faster than ever before.

LC/MS is the technique of choice for screening, identification, and quantitation of these contaminants. However, traditional LC/MS methods require time-consuming and expensive sample preparation and method development prior to sample analysis.

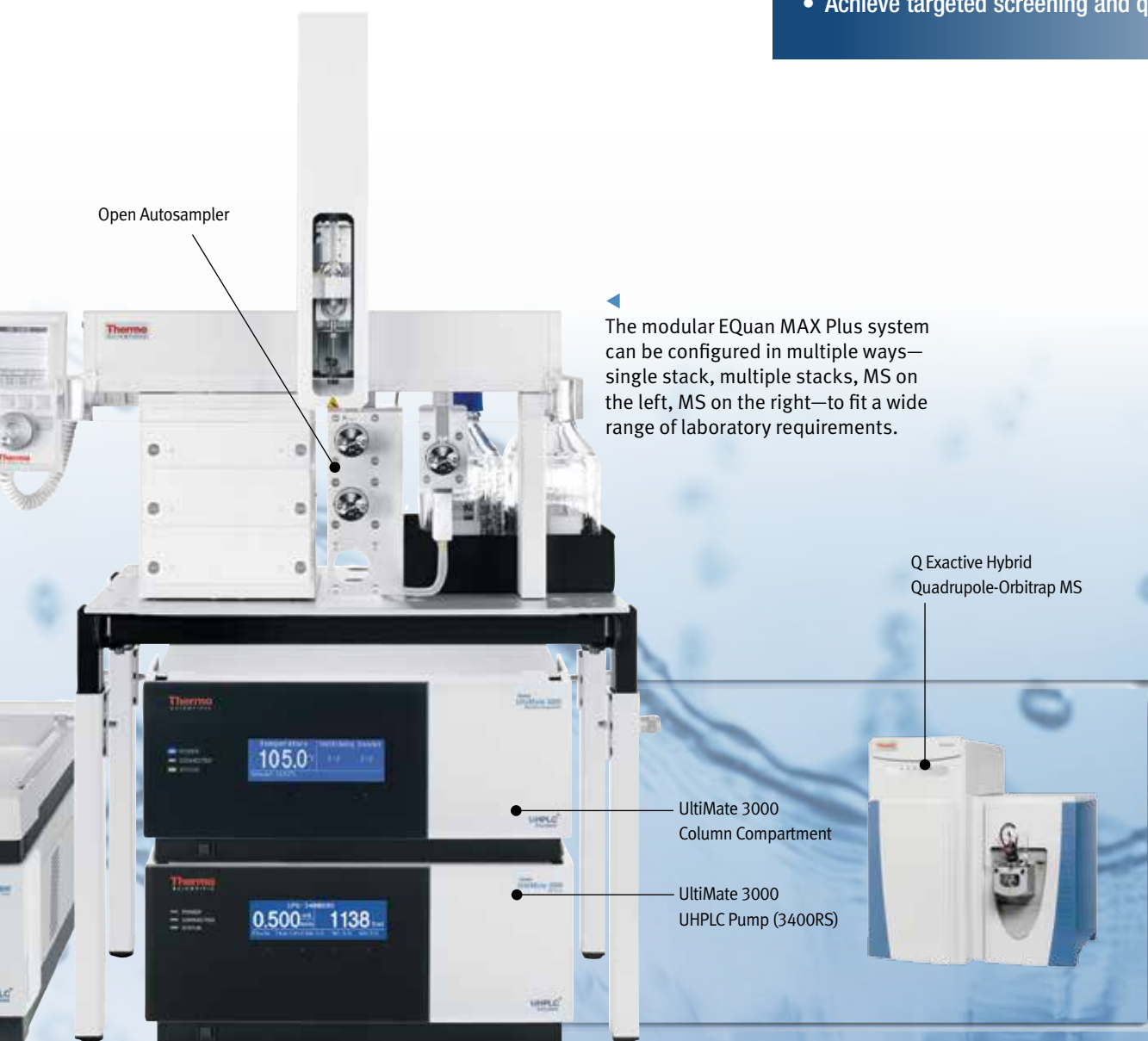
EQuan MAX Plus liquid chromatograph-mass spectrometer (LC-MS) systems automate many of the sample preparation steps, reducing preparation time and the possibility of human error. When combined with Thermo Scientific TraceFinder™ software, analytical methods and report formats can be selected from an extensive list of preconfigured options, making data acquisition, analysis, and reporting remarkably simple.



An EQuan MAX Plus system can be equipped with a TSQ Series triple stage quadrupole mass spectrometer, Exactive Plus benchtop Orbitrap mass spectrometer or Q Exactive hybrid quadrupole-Orbitrap mass spectrometer depending on your analytical requirements.

“With the EQuan MAX system we are able to inject and enrich samples followed straightaway by LC-MS/MS analysis, significantly reducing analysis times and improving LODs.”—
Dr. Sébastien Sauvé, Associate Professor, Environmental Chemistry, Université de Montréal

- Improve productivity
- Simplify assay development
- Perform nontargeted screening and quantitation
- Achieve targeted screening and quantitation



Improve laboratory productivity



To increase laboratory productivity, EQuan MAX Plus LC-MS systems employ an innovative online sample preparation method. It uses column switching to automate sample preconcentration and analysis. Samples as large as 1–20 mL, or as low as 1 μ L, can be directly injected, saving valuable time.

Rather than spending days on offline sample preparation, samples are loaded onto an EQuan MAX Plus LC-MS system, concentrated, and analyzed, yielding results in a fraction of the time. In addition, online sample preparation reduces loss of sample, and analytical variability due to human error.

EQuan MAX Plus LC-MS systems offer the flexibility of switching between conventional HPLC and very large injection volumes

without the need to replumb between experiments. Switching of injection volumes can be automated for unattended or overnight operation, increasing system flexibility and productivity.

The Thermo Scientific Dionex™ UltiMate™ 3000 ultrahigh pressure liquid chromatograph (UHPLC) pump enables fast separations of complex mixtures over an expansive range of flow rates and pressures.

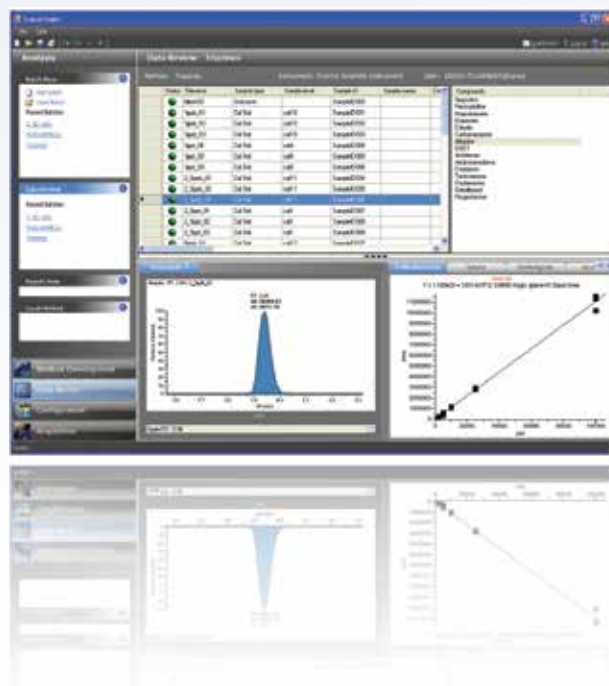
Catalog Number	Column
25012-022130	20 x 2.1 mm, 12 μ m Hypersil GOLD C18-like column for a wide variety of compounds
25205-022130	20 x 2.1 mm, 5 μ m Hypersil GOLD C8 Offers similar selectivity to Hypersil GOLD, but with less retention
25312-022130	20 x 2.1 mm, 12 μ m Hypersil GOLD aQ Retention of polar compounds in highly aqueous samples
25412-022130	20 x 2.1 mm, 12 μ m Hypersil GOLD PFP Can offer alternative selectivity in reverse-phase applications
25905-022130	20 x 2.1 mm, 5 μ m Hypersil GOLD Phenyl Alternative selectivity for aromatic and moderately polar analytes
35007-022130	20 x 2.1 mm, 7 μ m Hypercarb Exceptional retention of very polar compounds
73105-022130	20 x 2.1 mm, 5 μ m BioBasic AX Weak anion exchange column
73205-022130	20 x 2.1 mm, 5 μ m BioBasic SCX Strong cation exchange column

Simplify assay development

EQuan MAX Plus LC-MS systems offer exceptional flexibility. Based on the demands of the analyses, a system can be equipped with one of the Thermo Scientific TSQ™ Series triple stage quadrupole mass spectrometers, an Orbitrap™-based high-resolution, accurate-mass Thermo Scientific Exactive™ Plus mass spectrometer, or a Thermo Scientific Q Exactive™ hybrid quadrupole-Orbitrap mass spectrometer. Regardless of the solution chosen, assay development is simple and fast.



▶ Data review is simplified with TraceFinder software. Inspect sample and reference mass spectra, evaluate peak integration, review different curve fits, and observe ion ratio values easily and interactively.



TSQ Series Mass Spectrometers

TSQ Series triple stage quadrupole mass spectrometers provide the proven specificity and sensitivity of selected-reaction monitoring (SRM). EQuan MAX systems with TSQ Series mass spectrometers can be enhanced with TraceFinder software. The software allows the analyst to quickly and accurately develop high-throughput targeted screening and quantitative assays. TraceFinder software

includes built-in methods for commonly found contaminants, and an exhaustive list of SRM transitions and their associated parameters. In addition, TraceFinder software provides preconfigured report formats.

Exactive Plus Mass Spectrometer

With the Exactive Plus instrument, high-resolution accurate-mass (HR/AM) screening and quantitation methods are easy to set up because compound-dependent parameter optimization is unnecessary.

With the ability to collect mass spectral data at resolutions from 17,500 to 140,000, you can easily discern matrix artifacts from analytes of interest. False positives and false negatives are significantly reduced.

Q Exactive Mass Spectrometer

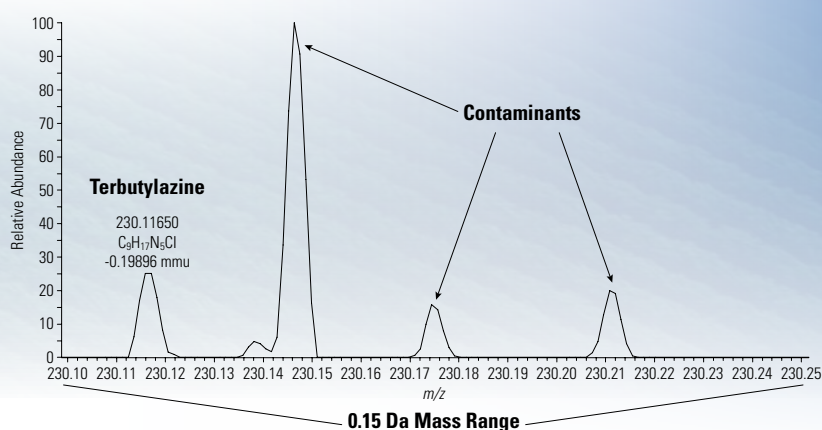
The Q Exactive mass spectrometer combines the benefits of triple quadrupole and Orbitrap instruments for ultimate screening flexibility. Equally adept at targeted or untargeted screening and quantitation, its full-scan MS/MS capabilities, superior resolution, and mass accuracy ensure the highest possible confidence in every ID. TraceFinder software facilitates development and execution of Q Exactive-based methods. The exhaustive list of commonly found contaminants and their characteristic SRM transitions greatly simplifies the setup of targeted assays.

◀ Selection of loading and analytical columns available with EQuan MAX Plus LC-MS systems

EQuan MAX Plus system with Exactive Plus LC-MS

Nontargeted screening and quantitation

Without HR/AM, the three contaminant peaks shown here would not have been resolved from the analyte terbutylazine – leading to a false negative or false positive depending on the intensity of the contaminants.



The high-resolution, accurate-mass capabilities of the Exactive Plus mass spectrometer make it ideally suited for nontargeted screening and quantitative experiments. The system provides full-scan data with mass resolution of up to 140,000 for structural confirmation, and mass accuracy to <1 ppm with internal calibration. Its high resolving power and mass accuracy enable accurate confirmation of all compounds, including isobaric pesticides.

With the full-scan data from the Exactive Plus mass spectrometer, every scan collects all ions present in the sample. The data can be analyzed retrospectively for contaminants that may not have been included on an initial target list, without the need to rerun the samples.

HR/AM facilitates both screening and quantitation of isobaric compounds that differ by only a few milli-mass units. Accurate mass measurements help eliminate false positives that result from interfering matrix components at masses close to those of the analytes of interest. HR/AM ensures positive identification of contaminants, increasing confidence in results. The instrument also provides excellent linearity over several orders of magnitude.

EQuan MAX Method

Online Sample Preparation

LC/MS

Preconcentrate

Analyze, Detect, Confirm

~30 MINUTES

Time
(Hours)

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30

Conventional Method

Offline Sample Preparation

Filter

Condition

Extract

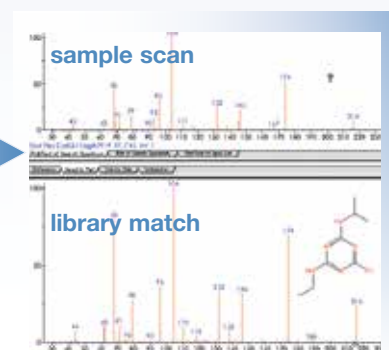
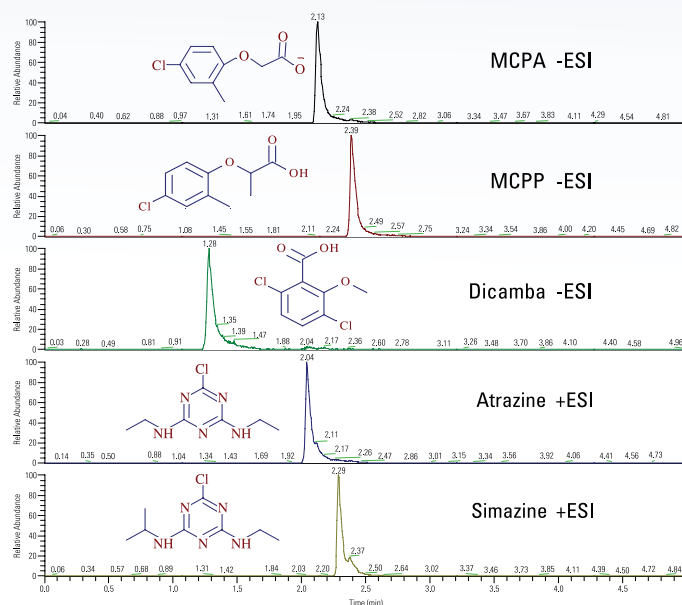
Wash

Dry

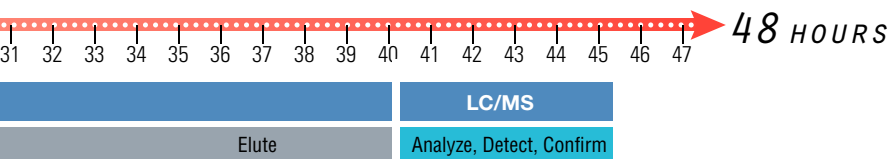
EQuan MAX Plus system with TSQ Series LC-MS/MS

Targeted screening and quantitation

EQuan MAX Plus systems with TSQ Series triple stage quadrupole mass spectrometers provide the proven specificity and sensitivity of selected-reaction monitoring (SRM) for targeted screening and quantitative experiments. The TSQ Series mass spectrometers offer exclusive technology benefits such as high-resolution selected-reaction monitoring (H-SRM) and quantitation-enhanced data-dependent MS/MS (QED-MS/MS). Using the H-SRM scanning mode for sample analyses provides excellent analyte specificity and improved limits of quantitation (LOQs). Using QED-MS/MS, quantitation followed by simultaneous structural confirmation becomes routine, facilitating multi-residue screening of beverage and water samples. The TSQ Series triple stage quadrupole mass spectrometers also offer fast scan speeds and positive/negative polarity switching for enhanced productivity.



- 1) H-SRM followed by QED-MS/MS in the same chromatographic run provides simultaneous quantitation and structural confirmation in multi-residue screens.
- 2) Sample scan (top) and library match (bottom) showing confirmation of atrazine.



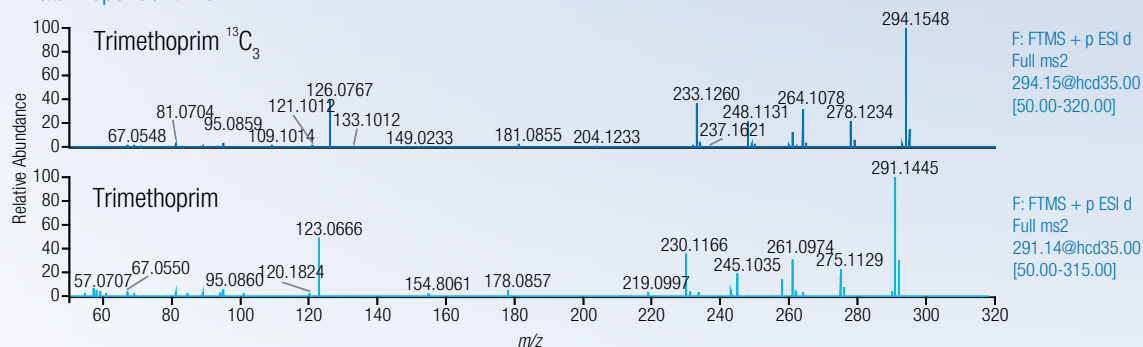
EQuan MAX Plus systems can reduce analysis times from hours to minutes.

EQuan MAX Plus System with Q Exactive MS

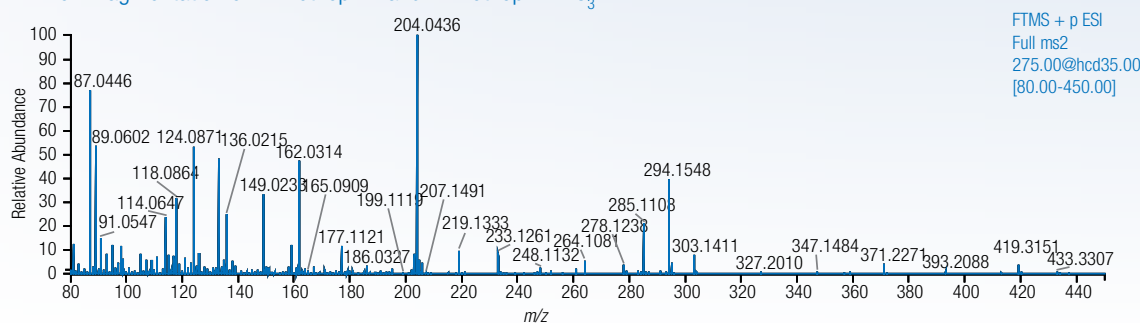
Targeted or nontargeted screening, quantitation, and confirmation

An EQuan MAX Plus system equipped with the Q Exactive hybrid quadrupole-Orbitrap mass spectrometer brings together the strengths of triple quadrupole and Orbitrap mass analyzers, providing simultaneous quantitative measurement and qualitative confirmation. High-resolution, accurate-mass MS data minimizes interference of isobaric matrix components for more accurate quantitation. At the same time, full-scan HR/AM MS/MS data ensures the highest possible confidence in every ID.

A. Data-Dependent MS²



B. All-Ion Fragmentation of Trimethoprim and Trimethoprim ¹³C₃



High-resolution data-dependent MS² on the Q Exactive MS easily distinguished a compound and its heavy-isotope-labeled internal standard (A) that could not be distinguished by all-ion fragmentation (B).

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