

EQuan

Environmental Quantitation
Using LC-MS/MS



Automated solution for environmental and drinking water analysis

EQuan is a turnkey system for the analysis of pesticides, herbicides, antimicrobials, antibiotics and other pharmaceuticals in environmental and drinking water samples. EQuan's unique on-line sample enrichment technique significantly reduces analysis time—from days to minutes. Its high injection volume (1–5 mL) improves detection limits over conventional LC-MS/MS analysis.

- On-line clean-up of environmental samples results in improved throughput, sensitivity and RSDs
- Significant time savings over off-line sample cleanup and enrichment
- Enhanced resolution (H-SRM) for analyte specificity
- Simultaneous quantitation and structural confirmation with QED-MS/MS

Challenges

Exposure to pesticides, antibiotics, and veterinary residues in drinking water is a significant health concern. As these chemicals become more potent, lower limits of detection (LODs) become critical. The emerging technique of choice in the environmental industry for the identification and quantitation of these residues is LC-MS/MS. However, this methodology typically requires extensive sample preparation prior to analysis, which tends to be time consuming and expensive.



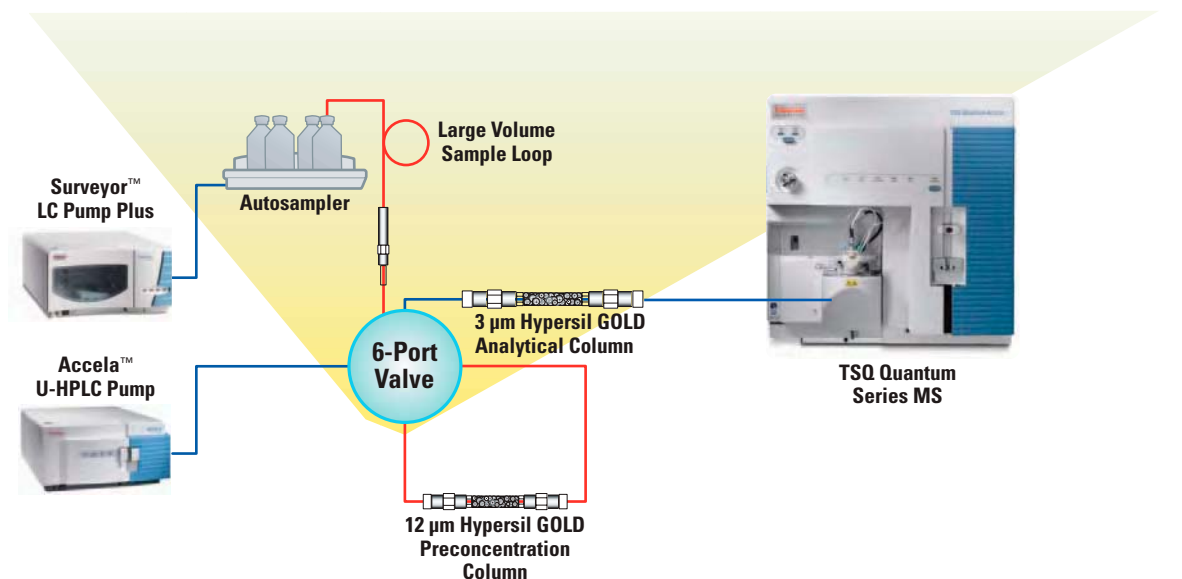
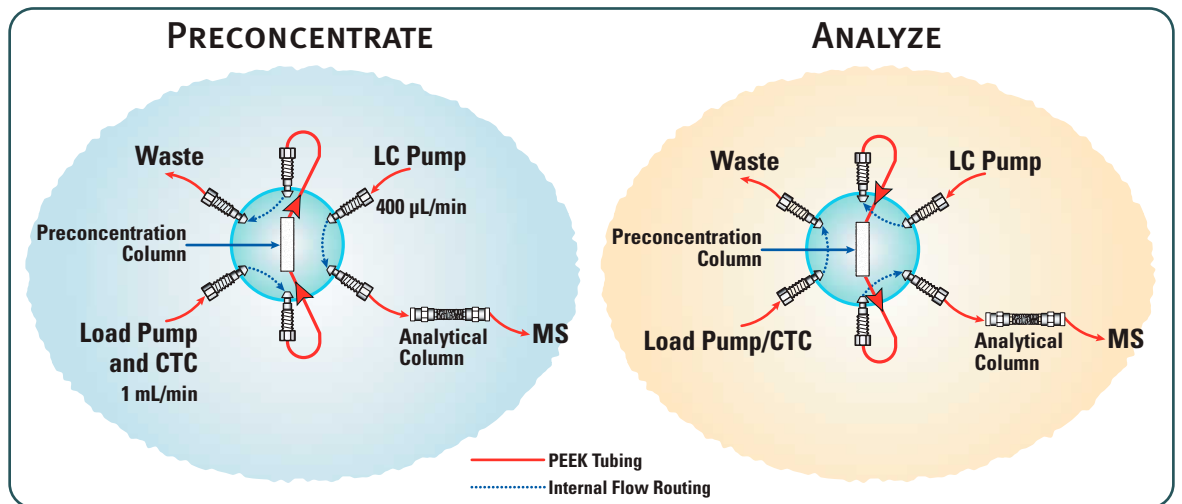
The Thermo Scientific Solution

With EQuan, environmental samples are directly injected for LC-MS/MS analysis, eliminating the need for off-line sample preconcentration, saving valuable time. Detection limits are improved by up to 100 times and limits of quantitation (LOQs) by up to 50 times, when compared to conventional LC-MS/MS detection using a triple quadrupole mass spectrometer.

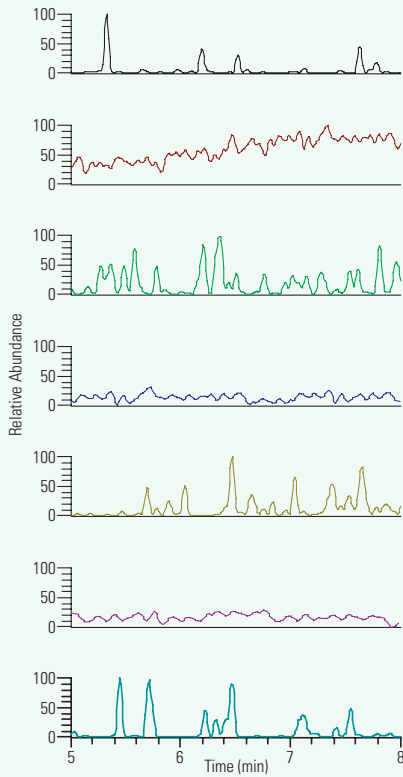
The basis of this technology is an on-line extraction method involving column switching. The EQuan system consists of two HPLC pumps with a preconcentration column (Hypersil GOLD™ 12 µm, 20 × 2.1 mm), an analytical column (Hypersil GOLD 3 µm, 50 × 2.1 mm), a CTC PAL autosampler, and a TSQ Quantum™ triple quadrupole mass spectrometer.

Using this setup, direct injection of 100–5000 µL of neat samples for on-line LC-MS/MS reduces sample preparation time from days to minutes, and minimizes ion suppression due to the matrix effects from environ-

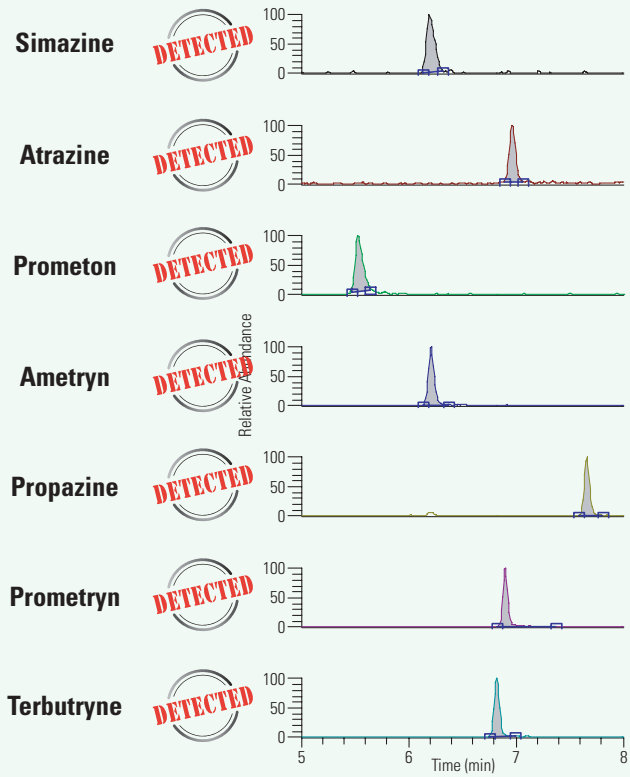
mental samples. In addition, the on-line sample preparation method reduces human error and consequent loss of sample. EQuan includes exclusive technology benefits such as Enhanced Resolution capability (H-SRM) and Quantitation-Enhanced Data-Dependent™ MS/MS (QED-MS/MS), available only on the TSQ Quantum series. Analysis of samples using the unique H-SRM scanning mode allows unmatched analyte specificity and improved LOQs. Using QED-MS/MS, quantitation followed by simultaneous structural confirmation becomes routine, facilitating multi-residue screening of environmental samples.



(a) Conventional Injection



(b) EQuan 100x Improvement in Detection Limits



Triazine Pesticide Mix at 10 ppt, showing a comparison between conventional LC-MS/MS and EQuan.

(a) shows the detection limits achieved with conventional methodology. No components were detected.

(b) shows the same samples analyzed by EQuan. EQuan detected all components, improving detection limits by 100 times.

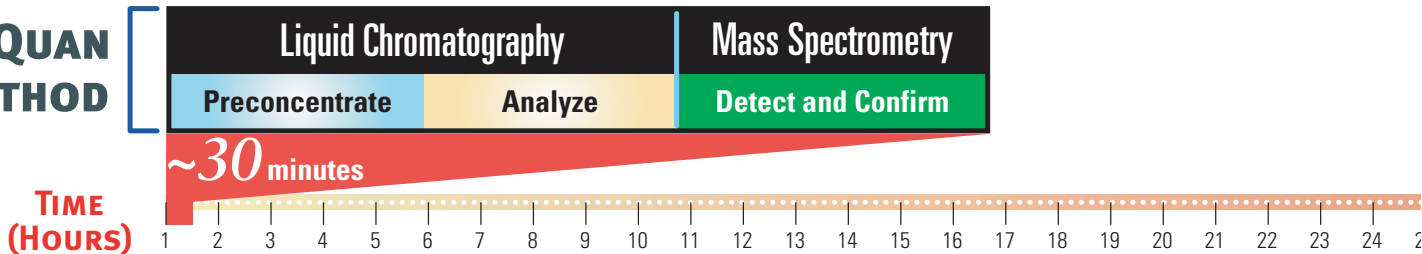
EQuan Accessory Kit

- 12 µm Hypersil GOLD Preconcentration Columns
- 3 µm Hypersil GOLD Analytical Column
- 5 µm Hypersil GOLD Analytical Column
- PEEK® tubing, fittings, cutter and sample loops

Component Name	SRM Transition	LOQ < 10 PPT	
		Conventional	EQuan
Prometon	226.17 > 184.00	Not Detected	Detected
Simazine	202.09 > 132.00	Not Detected	Detected
Ametryn	228.12 > 186.00	Not Detected	Detected
Prometryn	242.16 > 200.00	Not Detected	Detected
Atrazine	216.10 > 174.00	Not Detected	Detected
Propazine	230.12 > 188.00	Not Detected	Detected
Methyl Parathion	262.03 > 138.00	Not Detected	Detected
Thidiazuron	221.04 > 102.00	Not Detected	Detected
Diuron	233.01 > 72.00	Not Detected	Detected
Imidacloprid	256.04 > 209.00	Not Detected	Detected

Limits of quantitation of Triazine pesticide mix in drinking water assayed by conventional methods vs. EQuan.

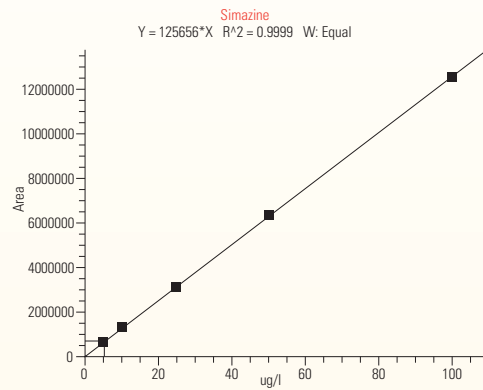
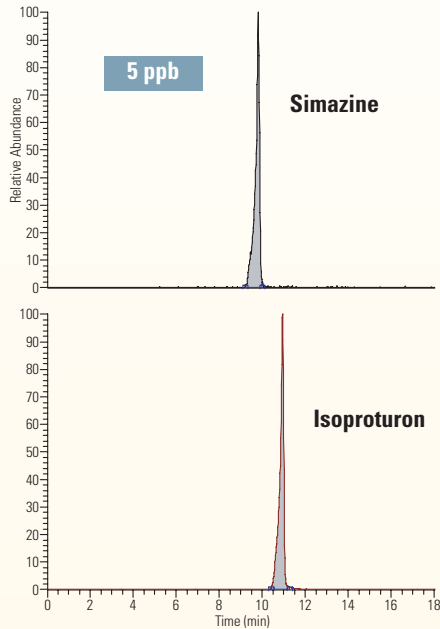
EQUAN METHOD



Conventional Method

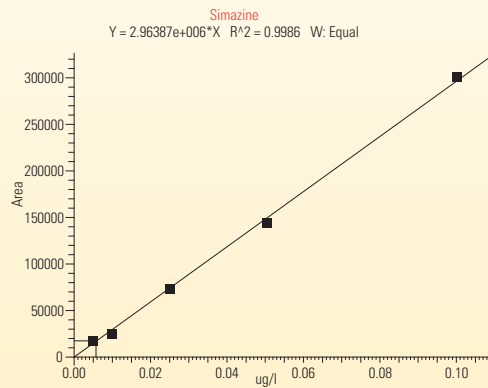
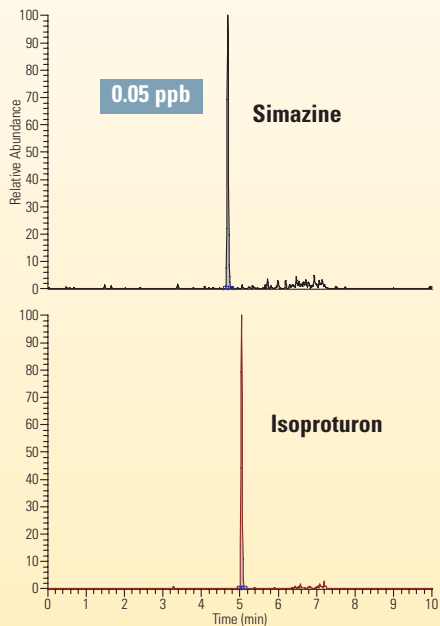


Conventional Method

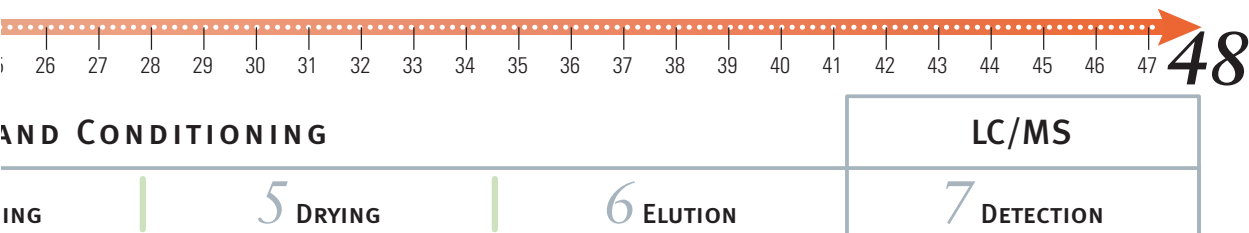


Conventional injection of six pesticides in 18 minutes. Chromatograms on the left show Simazine and Isoproturon at 5 ppb. Calibration curve for Simazine (right) shows linearity from 5 to 100 ppb ($R^2 > 0.99$).

EQuan Method



EQuan analysis of the same six pesticides in 18 minutes. Chromatograms on the left show Simazine and Isoproturon at 0.005 ppb (a 100X improvement over conventional injection). Calibration curve for Simazine (right) shows linearity from 0.005 to 0.1 ppb ($R^2 > 0.99$).



TSQ Quantum™ Triple Quadrupole Mass Spectrometers

Any of the TSQ Quantum series mass spectrometers can be used in the EQuan solution.

TSQ Quantum Access™

Unsurpassed Price to Performance

The TSQ Quantum Access offers versatility with its best in class mass range (m/z 30–3000), QED-MS/MS structural quantitation scan mode, and H-SRM capability. With the ability to scan for more than 300 analytes in a single experiment and with fast positive/negative mode switching, the TSQ Quantum Access enables routine multi-residue screening. The common ion path and ion source shared by the TSQ Quantum product line allows for easy method transfer between the different platforms, a significant advantage in today's business environment.



TSQ Quantum Discovery MAX™

Round-the-clock Productivity

The TSQ Quantum Discovery MAX is ideally suited for the rigorous demands of high-throughput analyses. With the Ion Max source, the TSQ Quantum Discovery MAX addresses the need of laboratories for more rugged and dependable LC-MS/MS to enable round-the-clock productivity. The combination of our patented HyperQuad™ quadrupole mass analyzer system, high-efficiency ion transfer optics, and outstanding ion source robustness provides precise, accurate quantitation – even at the lowest levels.



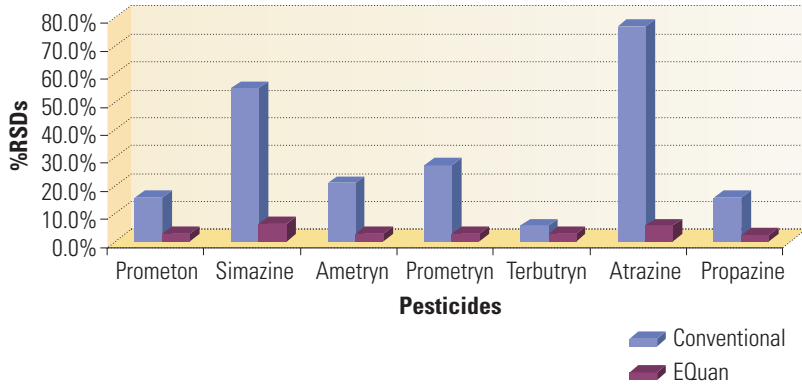
TSQ Quantum Ultra™ with FAIMS

Ultimate Sensitivity for Bioanalysis and Residue Analysis

The TSQ Quantum Ultra with FAIMS assures the best available technology for residue analysis to obtain the most sensitive quantitative LC-MS/MS data. Breakthrough innovations such as FAIMS and H-SRM facilitate the development of robust quantitative methods and provide significant immunity against matrix interferences. Faster method development at the highest possible sensitivity is routinely achievable with these two highly desirable features. The TSQ Quantum Ultra with FAIMS, H-SRM, LCQUAN™, and Watson LIMS™ provides a complete solution for both pharmaceutical and residue analysis from a single vendor.



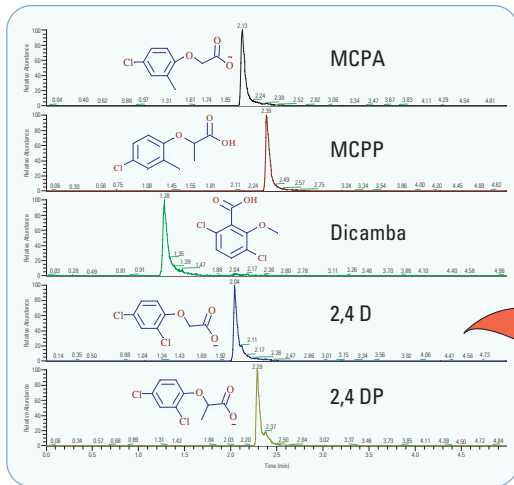
%RSDs for Conventional vs. EQuan Analyses



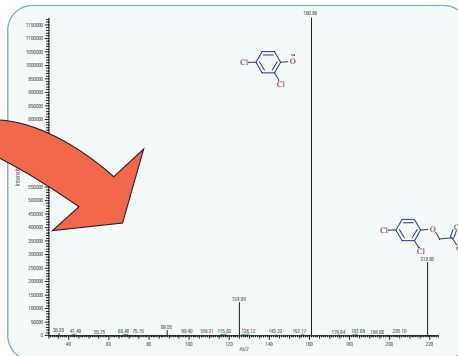
Comparison of Assay Precision for Conventional vs. EQuan Methodologies.
The low %RSDs indicate better precision with EQuan.

QED-MS/MS – Quantitation-Enhanced Data-Dependent MS/MS

This innovative scanning mode, introduced on the TSQ Quantum Access, provides simultaneous quantitation and qualification (Quan/Qual) capability for structural confirmation and quantitation, a feature with significant benefit for multi-residue screening experiments. With the ability to perform H-SRM, the MS/MS data is cleaner and less complex, making it easily searchable against an internal library for added confirmation during screening assays.



SRM Quantitation (Scan Event 1)



MS/MS Confirmation (Scan Event 2)

QED-MS/MS of an Herbicide Mix

QED-MS/MS provides simultaneous “Quan/Qual” for structural confirmation and quantitation in metabolite identification or multi-residue screens.

In addition to these offices, Thermo Fisher Scientific maintains a network of representative organizations throughout the world.

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