

## Thermo Scientific ExactFinder Software



### *Workflow software for routine targeted and general unknown screening*

Unifies qualitative and quantitative high-resolution accurate mass workflows in a single software package

Ensures high confidence in screening results with multiple forms of verification

Advanced algorithms increase throughput in Food Safety, Environmental Safety, and Forensic Toxicology laboratories

## Attain highest productivity and confidence in screening applications – with remarkable ease.

Laboratories performing routine targeted and general unknown screening in a range of applications, from food and environmental safety to forensic toxicology, face increasing pressure to improve productivity and simplify workflows, without compromising the quality of results. This pressure is driven by many trends, including increasing concern for contamination in our food and environment, as well as research in personalized medicine.

As mass spectrometry becomes the preferred technology for routine targeted and general unknown screening of trace compounds, more demands are placed on lab technicians to embrace this technology and produce results. At a time when mass spectrometers are generating increasing amounts of high resolution accurate mass raw data, there is a clear need for simplified data processing and interpretation.

The list of contaminants, drugs, and metabolites for which laboratories must screen and quantitate continues to grow. Laboratories are challenged to streamline time-consuming method development processes, and to respond promptly to new testing requirements.

### Confident identification and easy quantitation

Thermo Scientific ExactFinder software used with any Orbitrap™ or Exactive™ series high-performance liquid chromatography/mass spectrometry system addresses these challenges. ExactFinder™ software offers a single streamlined data-processing, review and reporting workflow for both targeted and general unknown screening applications, in a single easy-to-use software package.

With minimal manual intervention, ExactFinder software readily addresses applications where hundreds of compounds are screened, identified, confirmed, and ultimately quantified with a calibration curve. The software's simplified, intuitive workflows are for operators who process and review data, as well as experts who create processing methods and manage user access.

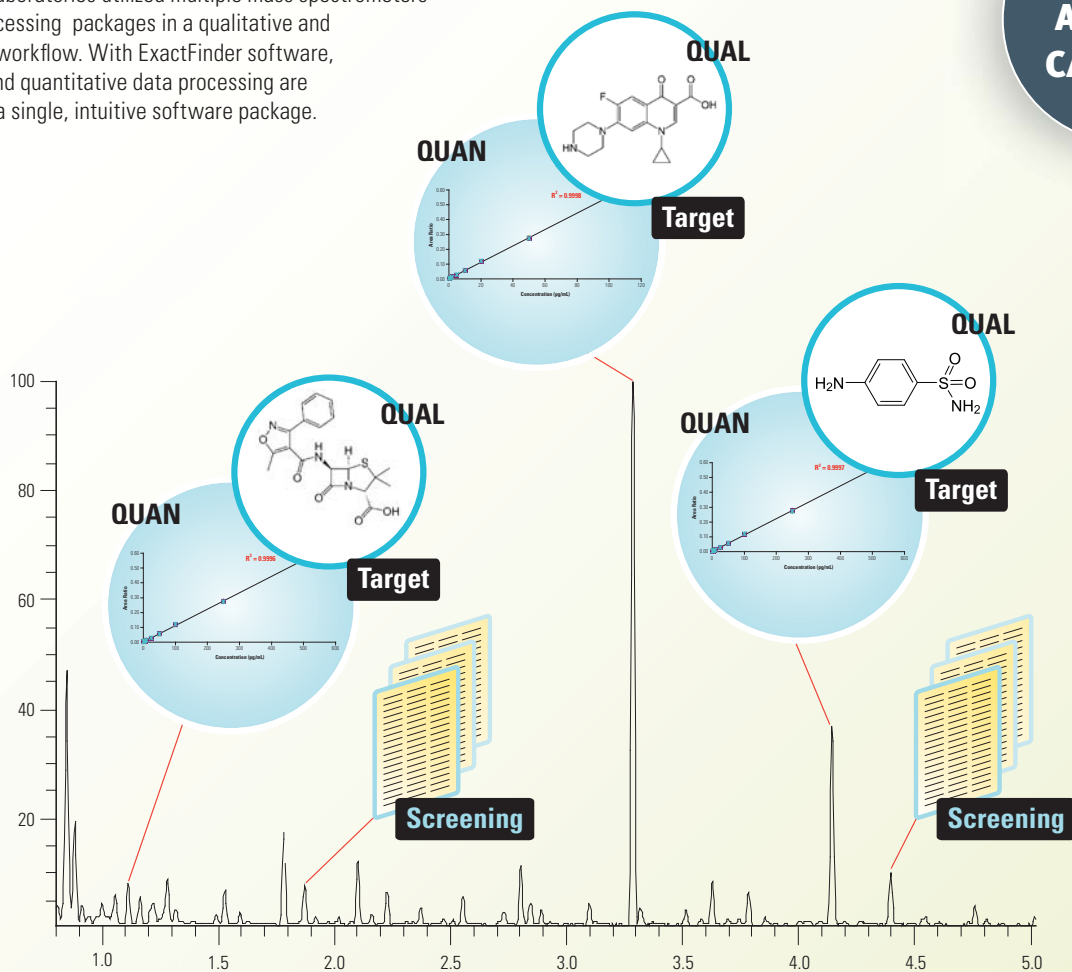


ExactFinder software can be used with any of the Thermo Scientific Orbitrap systems to take advantage of high-resolution, accurate mass (HR/AM) full-scan mass spectral data. ExactFinder software can process data collected using Thermo Scientific Xcalibur or LCQuan™ software.

## Qualitative and quantitative data processing in a single software package

Until today, laboratories utilized multiple mass spectrometers and data processing packages in a qualitative and quantitative workflow. With ExactFinder software, qualitative and quantitative data processing are combined in a single, intuitive software package.

**FULL SCAN,  
ALL IONS  
CAPTURED**



## Superior high-resolution accurate mass capabilities

The Thermo Scientific Orbitrap and Exactive series high-performance LC-MS systems have high-resolution, accurate mass (HR/AM) capabilities ideally suited for the qualitative and quantitative workflow. The systems

provide full-scan mass spectral data with mass resolution up to 100,000 FWHM, and mass accuracy within 2 ppm. The superior resolving power and mass accuracy enable accurate mass confirmation of compounds including isobaric species that differ only by a few milli-mass units.

### BENEFITS OF ORBITRAP TECHNOLOGY:

- Minimal MS method optimization
- Wide in-scan dynamic range of over three orders of magnitude for trace-level detection
- All ions all the time supports retrospective data analysis
- Fast scan speeds, rapid polarity switching, U-HPLC compatibility

HR/AM data helps eliminate analytical false positives and false negatives due to interfering matrix components at masses close to the analytes of interest, increasing confidence in results. The systems also offer complete sample coverage and retrospective data analysis, making it possible to screen previously acquired data for new target compounds.

# Maximize laboratory throughput with unprecedented ease of use

With simplified method setup and data review, plus automated data processing and reporting, ExactFinder software substantially increases laboratory productivity and offers unprecedented ease-of-integration into laboratory workflows.

## Easy setup of targeted and general unknown screening data-processing methods

Whether you are screening or quantifying, method setup is surprisingly easy and fast. Methods are set up in three simple steps: select screening type, select or import the target compound database, and then choose the identification and confirmation settings. Compound databases provide targeted searching based on mass-to-charge, retention time and fragment ions. Compound databases are provided with the software, and user-generated databases can be imported.

When screening for unknowns, identifications can be made via HR/AM spectral library search, elemental composition and Internet search of chemical databases such as ChemSpider. For targeted screening methods with quantitation, parameters can be set for calibration, QC levels, and flagging criteria for data review.

ExactFinder software allows users to cut and paste within the compound grid and automatically calculates molecular weights and mass-to-charge values to speed processing method setup. Because parameter-less peak detection (PPD) automatically and reliably finds peaks, definition of peak integration parameters is unnecessary.

## Fast, information-rich data review

The ExactFinder software provides information-rich data review. Flagging and color-coding of results allows for fast sorting of results.

Review of general unknown results is sample-centric, providing easy access to the compounds and parameters that provided the best match. Click to view integrated chromatograms and corresponding mass spectra, and to compare the expected isotopic pattern, to compare library spectra, or compare actual spectra to actual spectra for



Regardless of your application, method development, laboratory productivity. Create your processing method

rich

Provides fast,  
capabilities.  
options enable

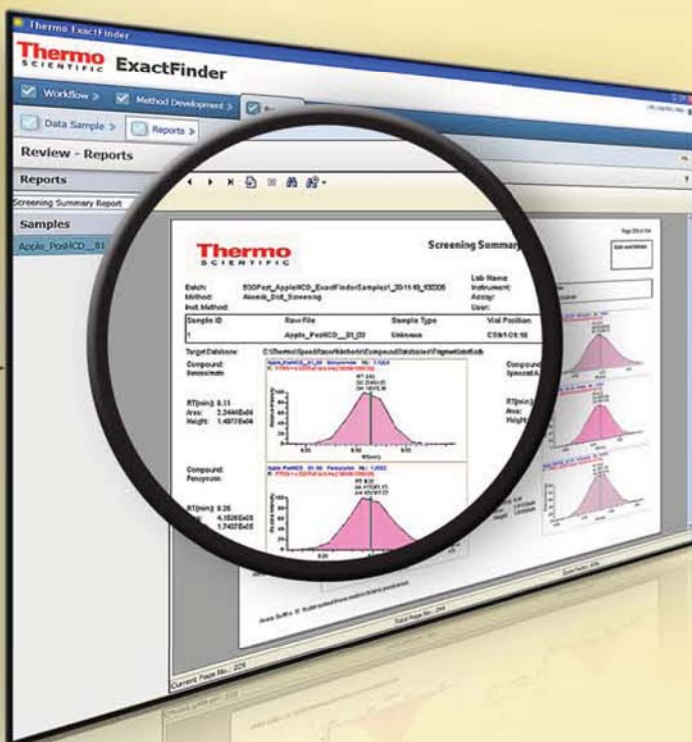
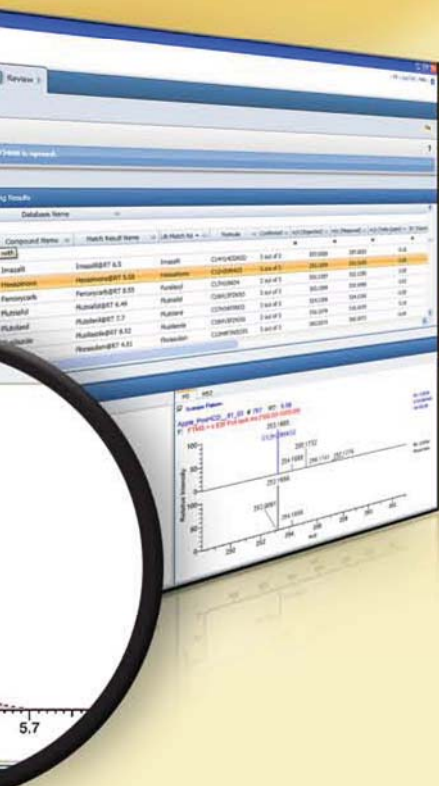
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Review of targeted screening results is compound-centric, providing rapid access to the detailed results for each compound in each sample. Scroll through compound and sample lists, and then click on samples to view in one window the integrated chromatographic peaks, the calibration curve or the mass spectrum and its isotopic pattern.

Parameter-less peak detection (PPD) automates peak detection and integration, yielding high quality data and calibration curves, and improved reproducibility. PPD eliminates manual errors, and increases the consistency and reproducibility of results. The integrated chromatographic peak is overlaid on the peak detected by PPD (shaded in pink). To match your workflow and processes, PPD can be used, or peaks can be manually integrated if desired.

## Simplified reporting

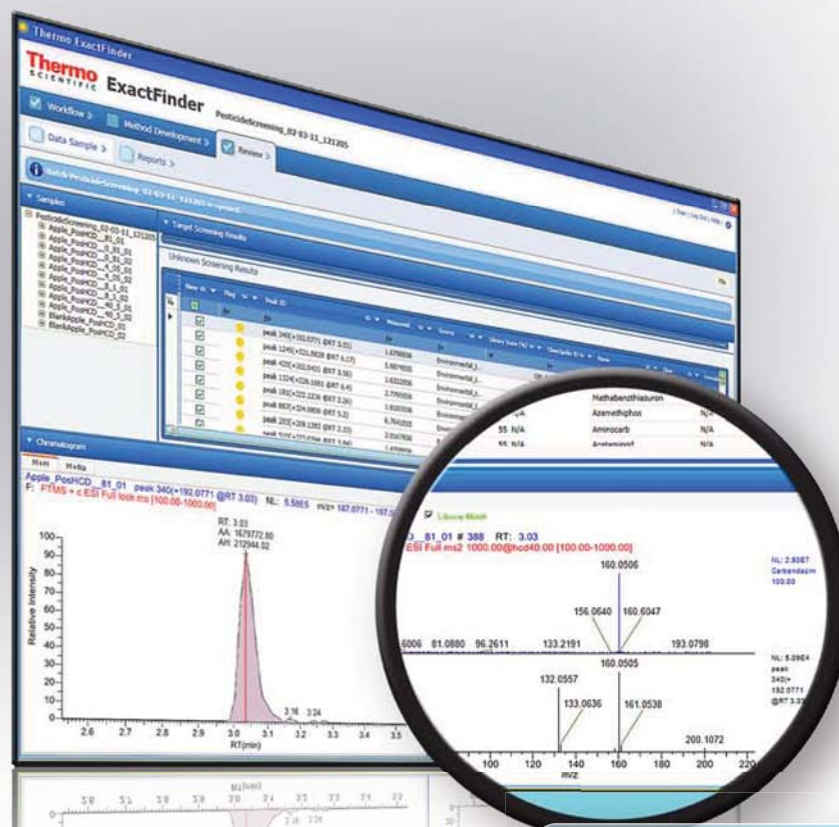
To simplify and speed reporting, the ExactFinder software includes several preconfigured report templates. Report setup is fully integrated with method setup. Simply choose the report type, the results to include and the flagging options. Reports can be saved in several common formats including PDF, and can be exported in XML format.



data review and reporting are simplified for maximum  
d, review your data, and print your report.

## Achieve highest confidence in screening results with multiple forms of compound identification and verification—in one software package

For unprecedented confidence in screening results, ExactFinder software integrates multiple forms of compound identification and verification, including its unique HR/AM spectral library and library search, isotopic pattern matching and ChemSpider database queries.



When screening for unknowns, identifications can be made via HR/AM spectral library search, elemental composition, and Internet search of chemical databases such as ChemSpider – one of the richest sources of structure-based compound information.

### High-confidence HR/AM library matching

For highest confidence in results, the ExactFinder software includes a novel LC/MS/MS HR/AM library of over 5000 mass spectra from over 1000 compounds including pesticides, veterinary pharmaceuticals, PPCPs, common drugs of abuse, and compounds of interest in forensic toxicology. All spectra were acquired with a Thermo Scientific LTQ Orbitrap Velos mass spectrometer under a range of mass spectrometer conditions similar to those used in routine targeted

and general unknown screening experiments: in positive and negative ionization modes, in multiple dissociation modes (HCD and CID) and with multiple collision energies. Laboratories can add mass spectra applicable to their work into the ExactFinder library.

To enhance confidence in library matches when analyzing complex samples, the ExactFinder software employs a reverse library search. In a reverse search, the

experimental spectra are queried for a match with the ten most significant ions in clean library spectra. To help you evaluate match quality, scoring shows how many of the ions had hits and how close they are in mass to the experimental data.

## State-of-the-art isotopic pattern matching

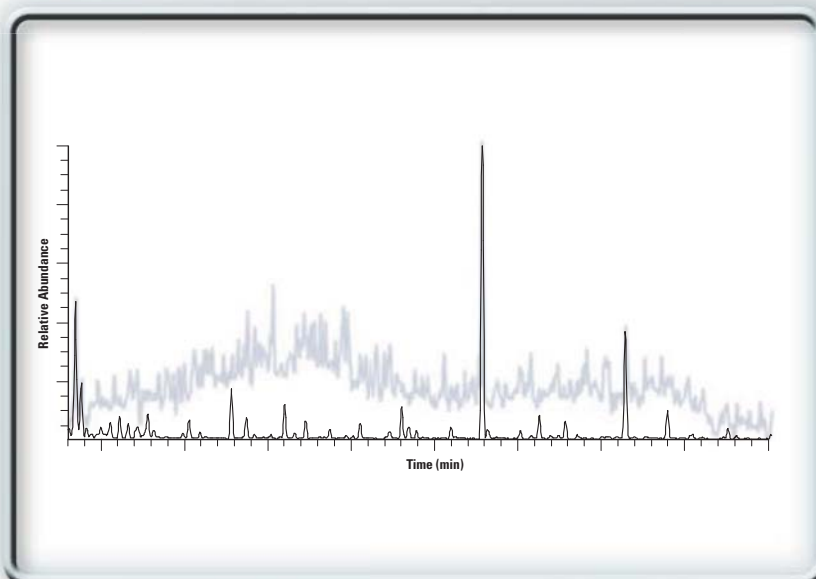
The isotopic pattern matching algorithm with intelligent elemental composition calculation provides a dependable yet sophisticated means of compound verification and identification. In targeted screening experiments, the algorithm matches the expected isotopic pattern (based on the molecular formula) to that found in the experimental data. In general unknown screening experiments, it reliably suggests an elemental composition and provides a fit ranking.



By comparing the expected isotopic pattern with the experimental data, the isotopic pattern matching algorithm strengthens confidence in screening results. Comparisons of the expected versus experimental isotopic patterns are easy to view when reviewing batches.

## Automated component detection

Automated component detection provides rapid and effective peak detection. It detects very low-level components in complex sample matrices by substantially reducing data complexity. Automated component detection reviews raw data to determine which masses are due to chromatographic events and which are due to background. Background masses are then excluded from the processed file leaving only chromatographically significant information for further processing and review. The algorithm groups adducts, multiply charged ions and dimers into one compound, further reducing the number of peaks to be identified. Raw data is retained, if needed, for later review.



Automated component detection excludes background masses to provide superior peak detection and signal-to-noise.

# Increase productivity in your laboratory and your application

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

## Forensic Toxicology

Forensic toxicology laboratories can use ExactFinder software to perform quantitation, targeted screening and general unknown screening. For laboratories performing pain management and drugs of abuse testing, the software substantially increases the productivity of targeted screening and quantitative analyses. The results can be automatically printed in real-time or viewed on the screen and then printed. The color coded flags make review extremely easy. Setting up data processing methods, interpreting results and running reports is simplified. The compound database and spectral library include approximately 1200 drugs of abuse for forensic toxicology screening.

- **Benzodiazepines**
- **Opiates**
- **Synthetic Opioids**
- **Alcohol metabolites EtG/EtS**
- **Other medical drugs of abuse**

## Environmental Testing

For environmental testing laboratories, the ExactFinder software can significantly increase throughput in quantitative and qualitative workflows. Laboratories no longer need to perform extensive method development such as compound-dependent MRM parameter optimization. Routine targeted and unknown screening can be performed with minimal user intervention and training.

- **Pharmaceuticals and personal care products (PPCPs) as per EPA method 1694**
- **Pesticides and herbicides**
- **Perfluorocarbons (PFCs)**

## Food Safety

As new compounds are found in food, beverages, and drinking water, the demand for reliable, targeted and general unknown screening methods is increasing rapidly. The ExactFinder software offers multiple search capabilities enabling laboratories to confidently identify compounds in complex food matrices.

- **Compounds banned or limited by world-wide regulatory agencies**
- **Veterinary pharmaceuticals**
- **Pesticides, herbicides and fungicides**
- **Chemical contaminants such as melamine and acrylamide**
- **Antibiotics and hormones**

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