screening confirmation quantitation



TraceFinder Routine Quantitation and Targeted Screening Software

data collection

Fast, flexible, easy-to-use Mass Spectrometry Software

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Achieve unprecedented simplicity and

The challenge

The constant pressure to increase productivity challenges laboratory staff at every level, from the technician to management. Streamlined, workflow-driven software solutions are needed to address these challenges. At the same time, the growing list of compounds that laboratories must quantify and screen, combined with increasingly complex regulatory requirements, necessitate flexible method development and powerful reporting tools.

TraceFinder software is the solution

Thermo Scientific TraceFinder software makes routine quantitation and targeted screening simple, fast and productive. It is the only software that can be used to develop methods, acquire and process data, and generate reports with the full portfolio of Thermo Scientific quantitative mass spectrometers. The software integrates the full range of popular front end chromatography systems, providing laboratories with the suite of features needed for their particular analyses. Now the technician and method developer need only use one software solution.



Online Sample Preparation & Multiplexing

My Company

MS Analysis

Data Review & Smart Reporting

speed

Simplified everyday use

From data acquisition to data processing, review and reporting, TraceFinder[™] software simplifies every step of routine mass spectrometry (MS) quantitation and targeted screening workflows. Once a method is defined, automated data acquisition and processing is easy to initiate and can be monitored in real time. Subsequent reporting can also be fully automated. Flags make data review fast and informative. When needed, it's easy to manually edit results, and any edits are automatically reflected in the final report.

Powerful method development

TraceFinder software provides powerful tools for method developers, including:

- Preconfigured methods
- Compound data stores (CDS) for selected reaction monitoring (SRM) and high-resolution, accurate mass (HRAM) workflows
- Over 50 report templates
- User-defined flags for nearly every parameter
- Automated retention time and ion ratio adjustment
- The ability to associate a method with any previously saved calibration

These features allow method development to be streamlined, yet retain the flexibility to meet the needs of advanced users demanding regulatory requirements and laboratory protocols.



Single Software

To provide a laboratory-wide solution, TraceFinder software is designed for use with the full range of industry-leading Thermo Scientific MS platforms.

Secure

To protect the integrity of analytical data, the software includes a rights-based secure user login system and dual method hierarchy that limits access to methods and data.

Experience extraordinary power and f

TraceFinder software offers powerful capabilities that significantly streamline method development while addressing regulatory requirements and laboratory protocols in a broad range of applications from environmental and food safety testing to clinical research and forensic toxicology.

Dual method hierarchy

TraceFinder software features a dual method hierarchy: local method and master method. The local method enables the technician to leverage their in-depth knowledge with samples to make minor changes in data processing to improve the quality of analytical results. To save time, changes in the local method can be saved to the master method. To ensure security, the core attributes of the master method—compound names, detection parameters, calibration levels and QC level—cannot be changed in the local method.

Flexible method development

TraceFinder software offers a choice of method-development approaches, enabling laboratories to choose the best approach to streamline their workflows.

- Use Method Forge to upload a raw data file and detect peaks via a library search.
- Import all method parameters from an existing Xcalibur Processing Method.
- Manually detect peaks through association, using a selected raw data file.
- Add analytes to a new method using the CDS.

Time-saving Compound Data Stores

The CDS retains all MS parameters, including parameters for SRM and HRAM workflows, allowing the method developer to select compounds and develop methods rapidly. New analytes and all corresponding MS parameters can be readily added to the CDS. Further, the CDS can be saved in a .csv file format, appended to any pre-existing libraries and imported back into TraceFinder software.

Compound data store with SRM, XIC, HRAM and SIM parameters.

exibility with streamlined method development

Potent method creation

Ion ratio criteria and reporting is streamlined with automated ion ratio set up for SRM-based quantitation and HRAM fragment ion confirmation. Ion ratios are automatically reported in preconfigured report templates. Depending on laboratory requirements, the software offers several flexible alternatives for calculating ion ratios.

TraceFinder software provides user-defined flags for almost every parameter imaginable, and the flags chosen are reflected in data review and reports.



User can apply more than 100 flags to quantitation results.

Simplified targeted screening

Targeted screening capabilities draw from proven Thermo Scientific ToxID software, an easy-to-use tool that substantially simplifies MS/MS targeted screening workflows. The software supports SRM, HRAM, MS/MS and MS²/MS³ workflows, and uses the widely accepted NIST spectra library software for compound identification.

To reduce time spent manually reintegrating peaks when retention times shift, the software provides automatic retention time adjustment. Simply enter an absolute value, select a relative percentage or associate an acquired raw file.

TraceFinder software makes it easy to add a quantitative or qualitative peak to a method. Just right-click on a mass in the spectrum; there is no need to manually enter masses.



Several ion ratio calculation choices offer flexibility in meeting laboratory and regulatory requirements.

Realize easy, workflow-driven analys maximizing laboratory

With simplified data acquisition, review and reporting, TraceFinder software speeds each step of routine MS quantification and targeted screening workflows. Once a method is defined, data acquisition is an easy four-click process that can be monitored in real time. Data review is fast with tools—comprehensive flagging and the ability to associate a batch with a previous calibration—that support the technician's work. When needed, the software makes it easy to edit results, and the edits are dynamically reflected in the final report through Active View Reporting.

Four-click data acquisition

Submitting sample batches and initiating analyses is performed in four simple steps:

- 1. Select appropriate batch template.
- 2. Review selected batch template.
- If needed, choose a system start-up and shut-down method or extend the calibration curve.
- 4. Submit the samples.

Fast access to system status

The Real Time Viewer provides immediate access to data acquisition, instrument status, device status and queues, at any time in the workflow. Useful information, like real time chromatograms, is displayed, enabling users to assess the progress of their batch rapidly and easily.



Submitting sample batches and initiating analyses is straightforward. The Real Time Viewer offers immediate access to system status and queues.

is – throughput

Simple, full-featured data review

TraceFinder software offers simple, yet exceptionally feature-rich data review capabilities. The intuitive, workflow-driven arrangement of the software windows simplify the technician's role in reviewing data. The technician can quickly and easily observe the data processing status, view compound-related flags to locate compounds which need attention, and take appropriate steps to correct any problems.

If the problem is with a particular compound, only the results for that compound are rejected – not the entire sample. To address compound-related difficulties, it's easy to perform compound-specific edits such as manual peak rejection and integration, and to change peak-detection parameters. Feedback is immediate, as data is reprocessed and presented in the same software screen and in the final report automatically.

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Comprehensive flagging facilitates the technician's role in reviewing data.

Powerful, automated reporting

To enhance laboratory productivity, the TraceFinder software offers powerful, automated reporting and numerous report templates. Active View Reporting dynamically links data review and reporting, thus enabling users to toggle between the two for fast feedback.

Fifty preconfigured report templates to meet a variety of requirements, including:

- Environmental Testing
- Food Safety
- Clinical Research
- Forensic Toxicology

A variety of lon Ratio Pass/Fail Reports available.

> If desired, save time and paper by pounds above the LOD, LOQ or LOR.



www.thermoscientific.com/TraceFinder

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N63421_E 09/11S

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