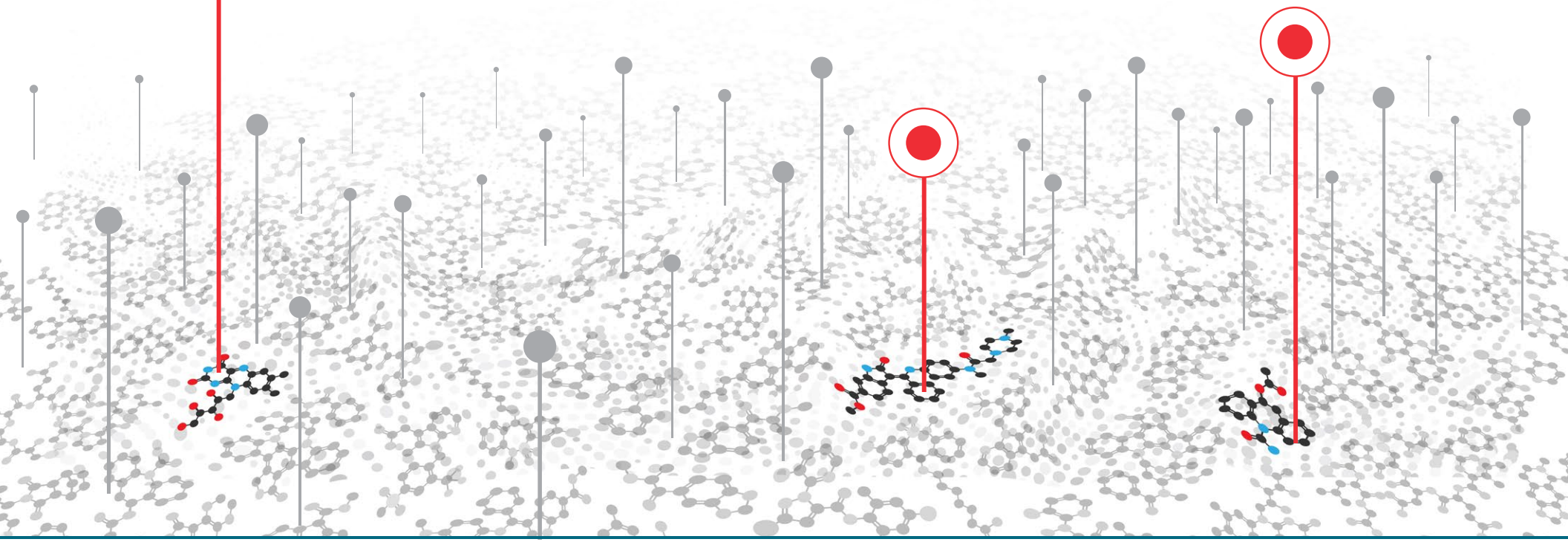
thermo scientific

Maximum productivity. Trusted results.

Thermo Scientific TraceFinder Software

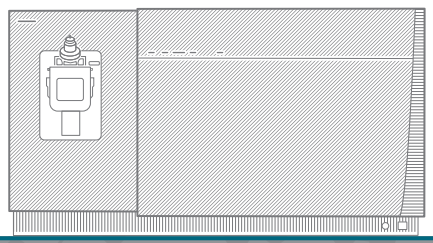


ThermoFisher SCIENTIFIC

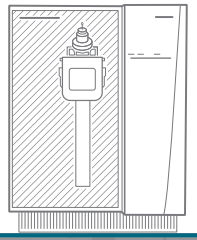
Maximum productivity. Trusted results.

Designed for fast and flexible compound screening and quantitation, Thermo Scientific™ TraceFinder™ software provides unique features and capabilities to support a wide range of applications and analytical laboratories.

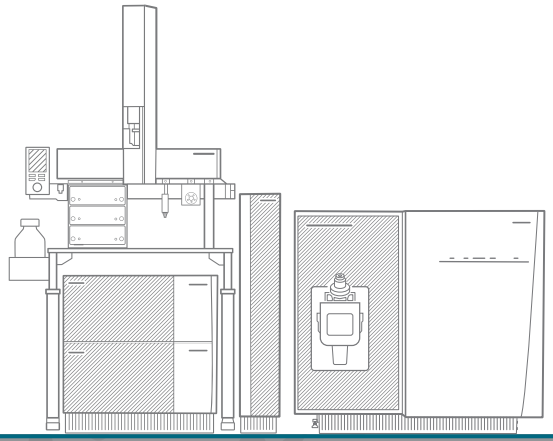
Built with a customizable user interface, flexible method templates, comprehensive compound database, and access to extensive spectral fragmentation libraries, TraceFinder software allows operators of all experience levels to confidently drive laboratory productivity.



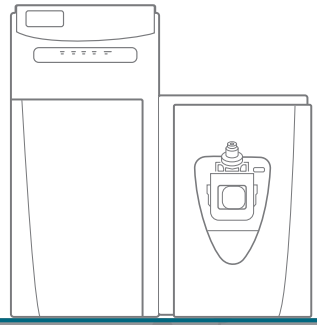
Thermo Scientific™ Orbitrap Tribrid™ mass spectrometer



Thermo Scientific™ Orbitrap Exploris™ mass spectrometer series

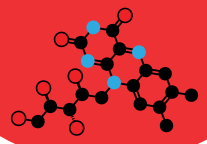


Thermo Scientific™ TriPlus™ RSH autosampler with Thermo Scientific™ TSQ™ Triple Quadrupole mass spectrometer series



Thermo Scientific™ Q Exactive™ HF hybrid quadrupole-Orbitrap™ mass spectrometer series

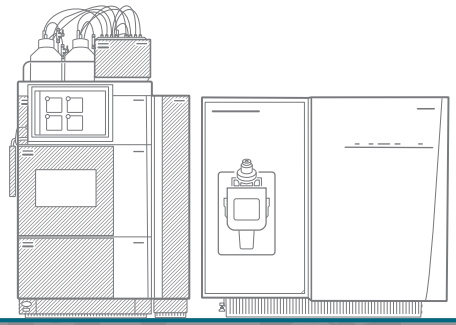
Harmonize your lab productivity



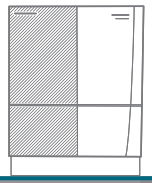
Direct control for a wide range of systems

- Multi-channel LC
- Single Quad MS
- Triple Quad MS
- High-Resolution LC-MS
- Ion chromatography
- Gas chromatography
- High-Resolution GC-MS

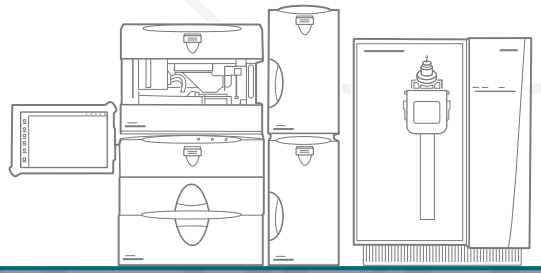
Operating procedures and training can be streamlined and standardized, minimizing training requirements and simplifying lab operations.



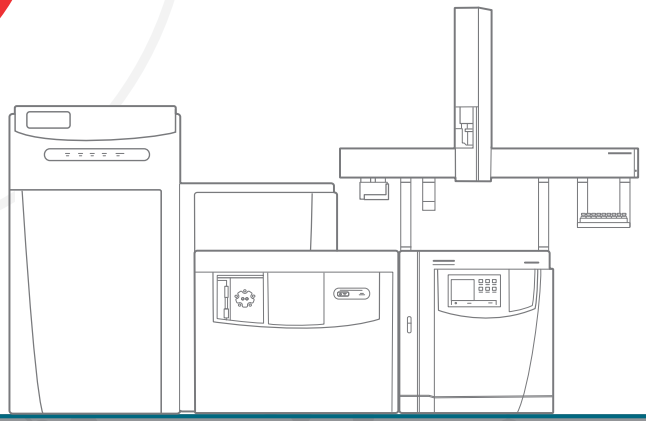
Thermo Scientific™ Vanquish™ Core HPLC system with Thermo Scientific™ TSQ Fortis™ Triple-Stage Quadrupole mass spectrometer



Thermo Scientific™ ISQ™ EC/EM Single Quadrupole mass spectrometer



Thermo Scientific™ Dionex™ ICS-6000 HPIC system with Tablet Interface and Core with Thermo Scientific™ Orbitrap Exploris™ 120 mass spectrometer



Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system with Thermo Scientific™ TRACE™ 1300 Series GC injectors

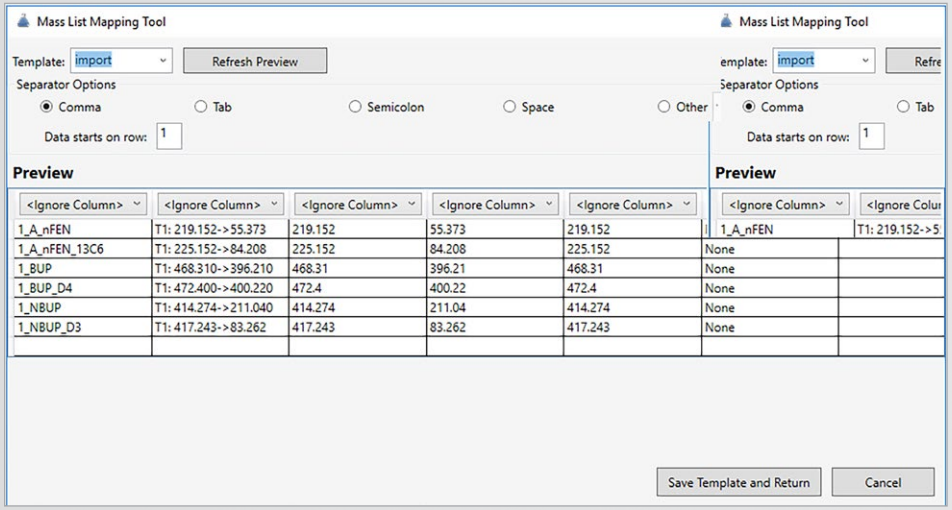
Improve data quality and increase confidence for any screening assay

Your targeted screening list may be long—but method setup doesn't have to be

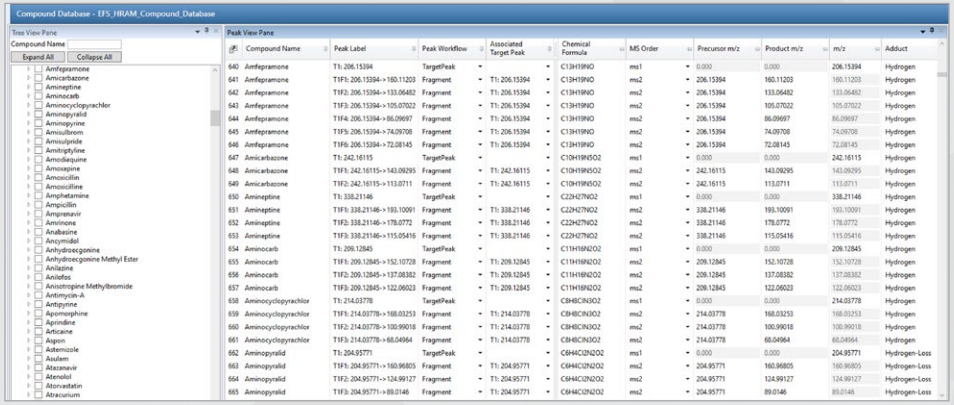
Large lists of target compounds can be easily and accurately managed with the use of TraceFinder customizable compound databases. Target compounds can be added, removed, or edited within the database and subsequently included a new or existing processing method. Compound databases within TraceFinder software are designed to include all the information necessary to accurately define your target compounds and can be easily populated manually as well as through file import.

Formatted text files as well as instrument method export lists can be readily imported to populate a compound database, while non-formatted text files can easily be imported via the built-in mapping tool; eliminating the need for file modification or reformatting prior to import.

Database mapping/import tool → **Database view example**



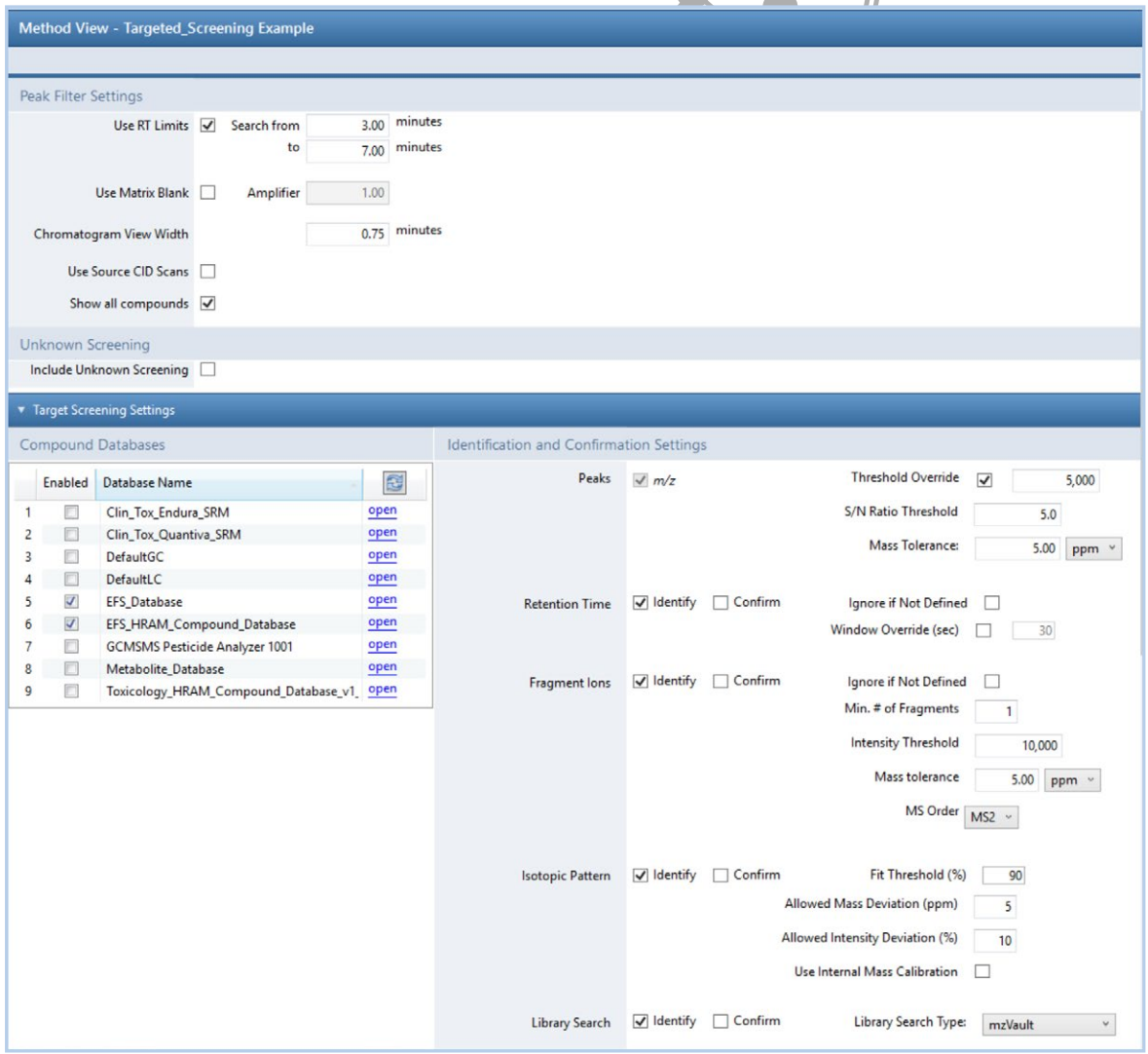
Importing target lists from a range of sources is simplified through the use of TraceFinder's Mass List Mapping Tool.



An example of the Compound Database, showing the range of information stored for each compound such as transitions, precursor and product ion targets, and adducts. Additional information can be applied to aid filtering and reporting, such as compound type and compound grouping.

- **Build**—Targeted screening methods can be built from multiple compound databases to easily include hundreds of compounds
- **Optimize**—TraceFinder target screening methods focus around four main search features, *m/z*, retention time, fragment ions, and isotopic pattern
- **Analyze**—Each search feature within the method can be easily viewed and modified to provide the right level of search requirements for any assay

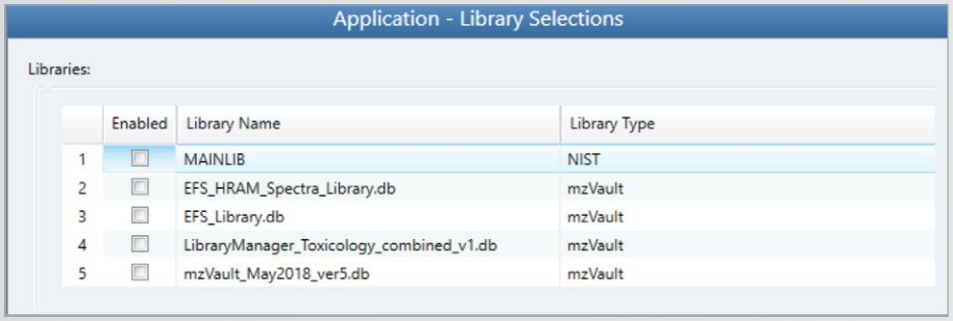
Quickly and easily build targeted screening methods to monitor hundreds of compounds.



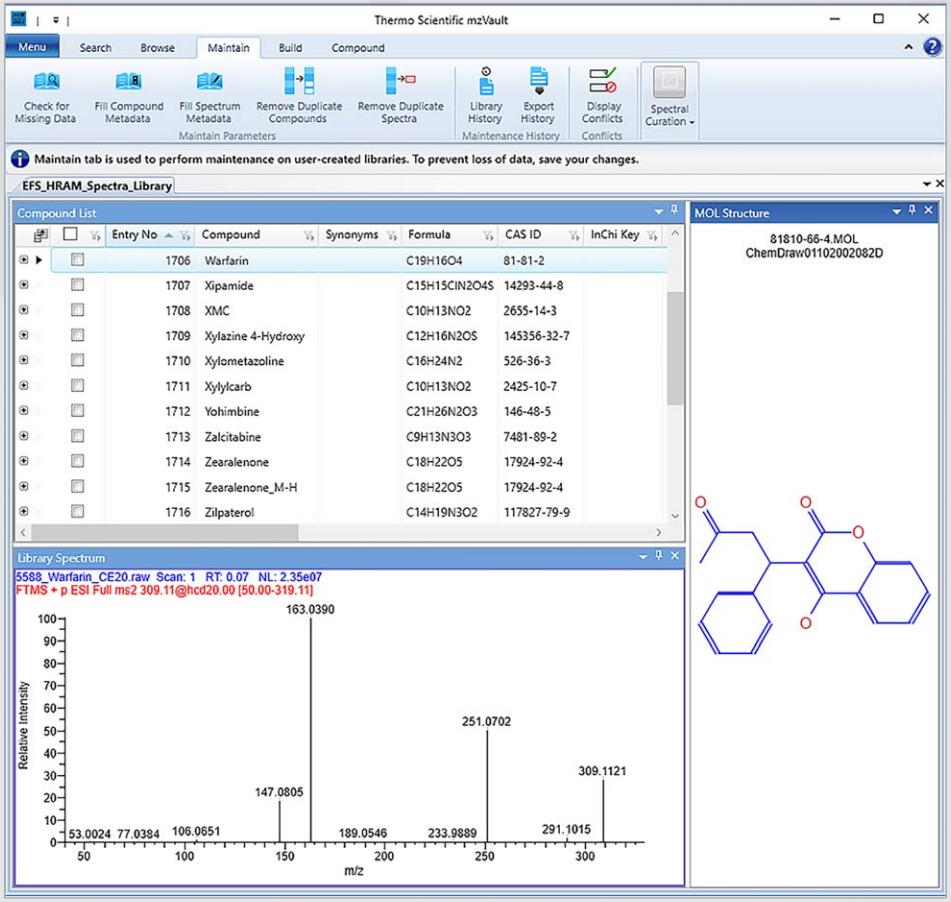
Targeted screening using multiple compound databases is quick and easy, with full flexibility to control identification and additional confirmatory settings such as isotopic pattern and library searching.

Harness the full power of high-resolution accurate-mass spectrometry with mzVault library searching

- High-resolution accurate-mass (HRAM) mass spectrometry is a powerful tool for any screening assay, and when coupled to the highly curated library content of Thermo Scientific™ mzVault™ library you can build unprecedented confidence in your screening results.
- Access the MS²-level content of Thermo Scientific™ mzCloud™ mass spectral fragmentation library offline, through mzVault
- Easily search multiple mzVault libraries for any screening method
- Generate custom mzVault libraries, enabling new and expanded compound search capabilities to support novel research



The ability to search multiple libraries from NIST, through to offline mzCloud contents with mzVault or your own libraries adds confidence to any screening assay.



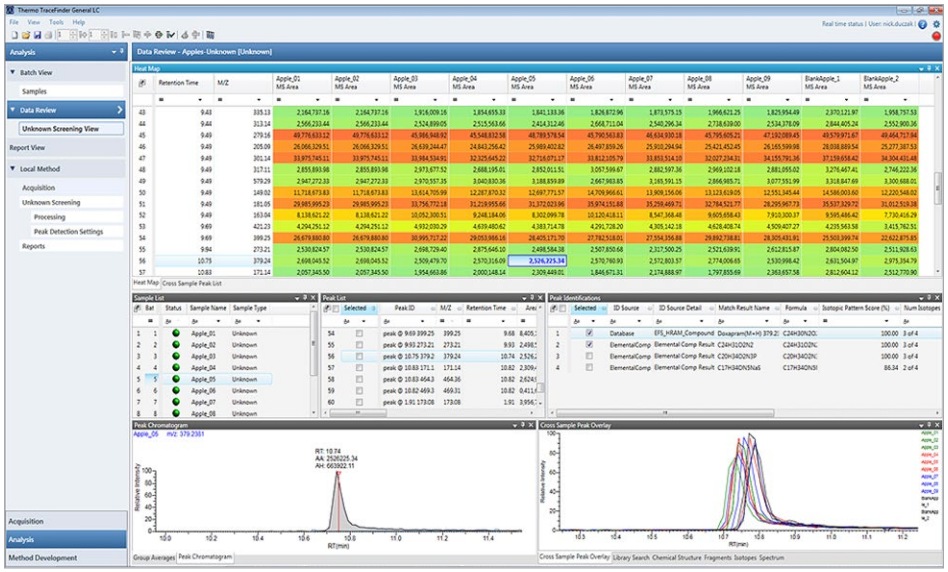
View fragmentation spectra and associated metadata, search, maintain or build your own proprietary libraries to utilize and share your knowledge.

Exploring the unknowns— in any workflow

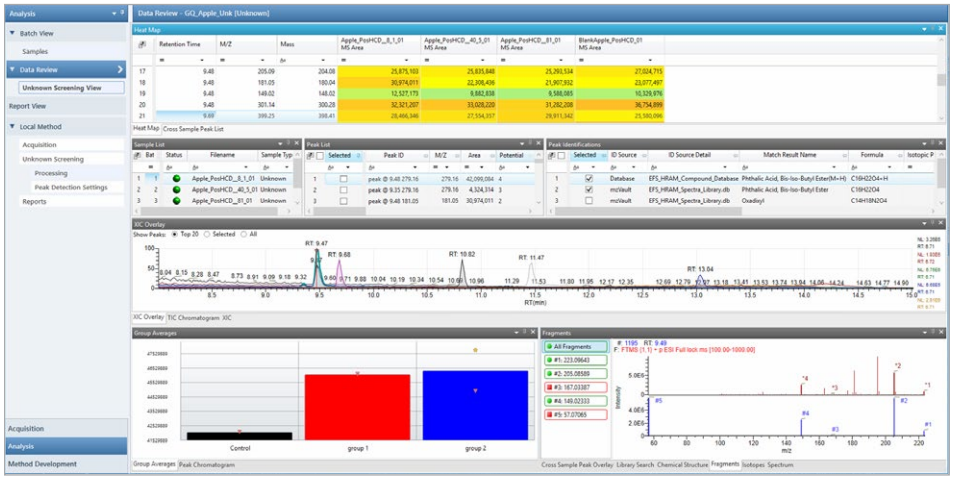
The ability to identify features of interest in a single sample or across a large set of samples requires a wide-ranging set of tools. For unknown screening, TraceFinder has combined best in-class library search capabilities with a comprehensive set of data visualization tools to provide a reliable, straightforward workflow for unknown component detection.

Unknown component investigation is enhanced by a wide array of data visualization tools such as:

- Heat map tools
- Cross sample peak lists
- Group averages
- Cross sample peak overlays
- Isotope matching display



Through customizable options to visualize and interrogate large data sets, such as heat maps for group analysis, user defined retention time alignment, and simultaneous library searching, the process of identification and decision-making is simplified.



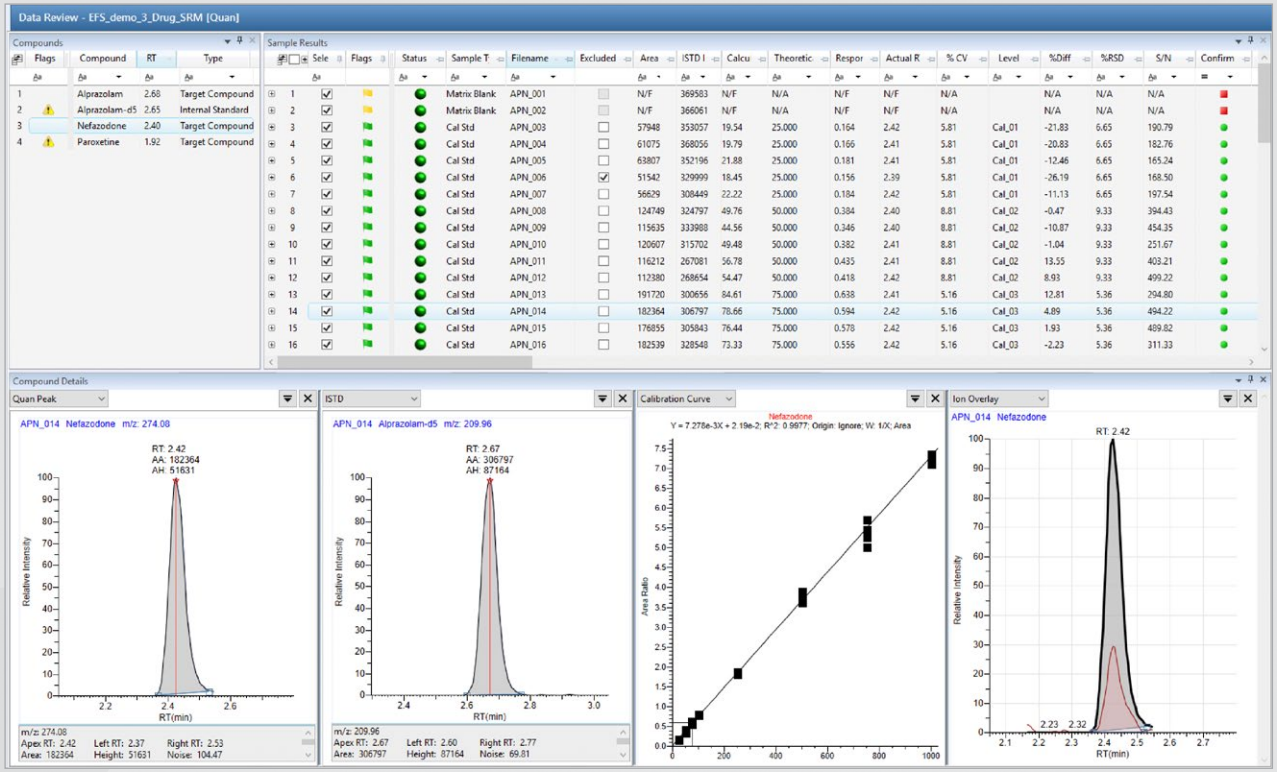
Data visualization tools are easily implemented to highlight features of interest and aid with putative identification. In addition to heat map displays, all identified components can be displayed in a single chromatographic view, sample groups can be averaged and compared to experimental controls, and fragmentation spectra can be searched against multiple mzVault spectral libraries.

Customizable quantitation for maximum results

Comprehesive quantitation tools designed to meet any workflow

TraceFinder software simplifies quantitation across LC, IC and GC-quadrupole and high-resolution mass spectrometers for large and small target lists through:

- Template-driven workflows
- Compound databases for method building
- In-depth data visualization capabilities
- Market specific terminology built into each workflow



Whether quantifying using data from triple quadrupole or high-resolution based mass spectrometers, data review is streamlined through flagging and data quality checks to allow rapid data interrogation and report generation.

Build your workflow to fit the application with a customizable user interface

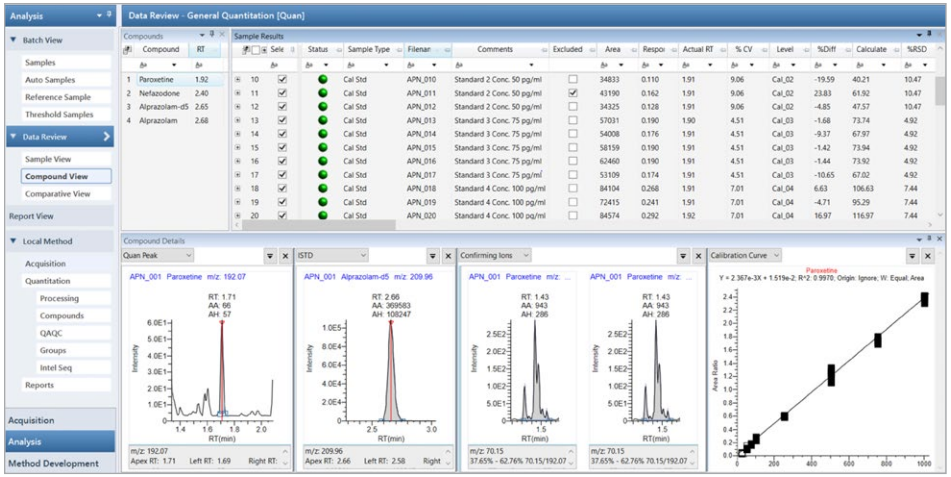
TraceFinder software provides a wide range of features and capabilities, but not all features are required for all experiments. With an application-wide customizable user interface, the workspaces and data display can be configured to visualize as few or as many of the application features as necessary for the analyst and experiment type.

Utilizing a fit for purpose display greatly increases the productivity during system setup, training and SOP development, and assay data review.

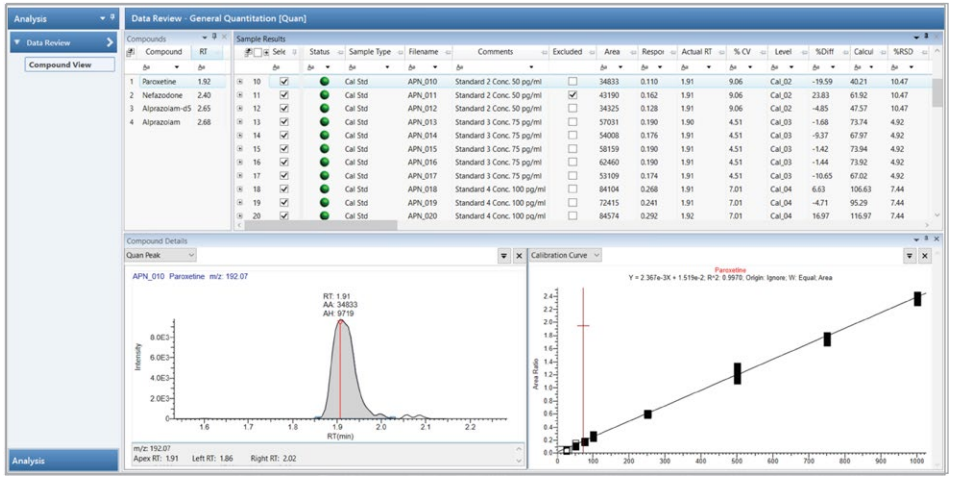
Primarily focusing on targeted and untargeted screening workflows for veterinary drugs, but also screening for other toxicants and contaminates, TraceFinder software has allowed our lab to perform these workflows in a simple and efficient way; we have compound databases allowing us to perform fragment matching and confident compound identification without processing raw data files through complicated workflows across multiple software package.

—Laura Burns, Diagnostic Associate II, Iowa State University Veterinary Diagnostic Laboratory

Full display → **Focused display**



The full view within the navigation tabs (left column) provide access to all functionality within the application, allowing full flexibility and control for method modification, data acquisition, and data visualization.



The customized or focused view provides the capability to display only the required navigation tabs (left column), providing a fit for purpose display for increased operational simplicity.

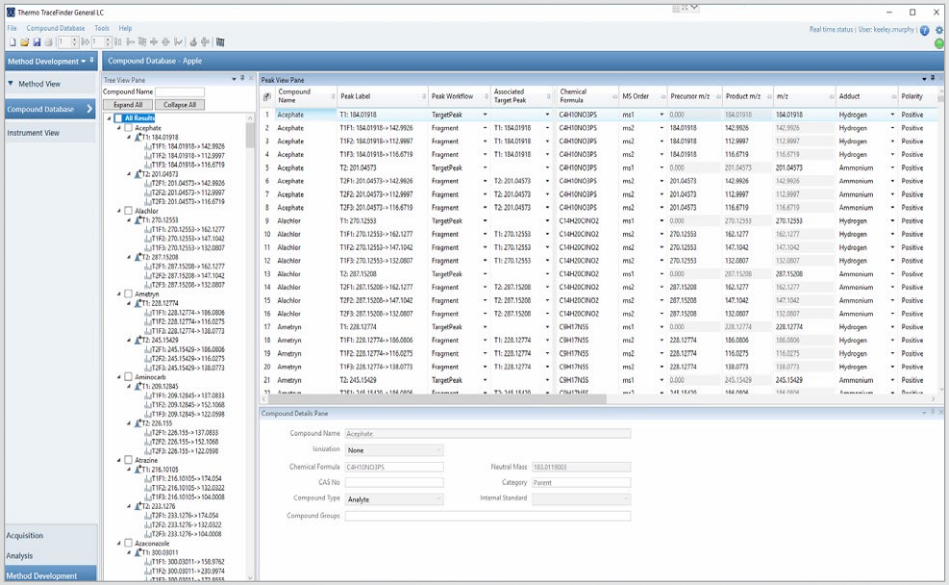
Combine quantitation and targeted screening with TraceFinder software

With TraceFinder software a targeted screening workflow can be built directly into a general quantitation method providing ultimate assay versatility. Target compounds are easily selected from any available TraceFinder compound database creating an easy to view list for all compounds to be screened and quantitated in the assay. Target compounds can be added, removed, or edited all within the processing method.

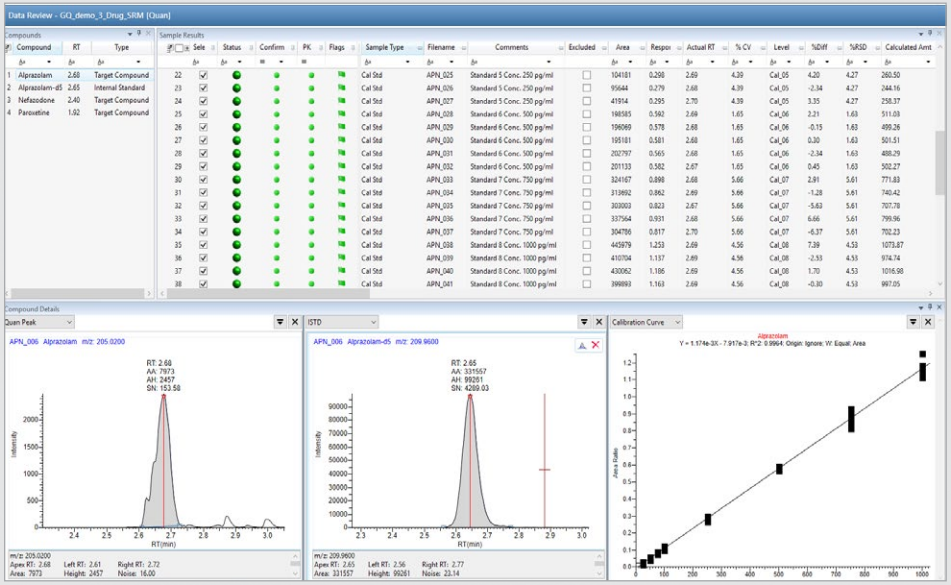
Screening assays built with quantitiation allow for full and single point calibration curves, customizable data review tools and compound flagging.

Navigating within TraceFinder software is intuitive. It is a straightforward process to create master methods and process data. It is very convenient to be able to associate information from a compound database into a master method. The data processing allows for viewing data in different ways all in one screen.

—Dwayne Schrunk, Laboratory Director, Iowa State University Veterinary Diagnostic Laboratory



Target compounds are easily selected from any available TraceFinder compound database, creating an easy-to-view list of all compounds to be screened and quantitated in the assay. Target compounds can be added, removed, or edited all within the processing method, and all necessary targeting information is contained within the database.

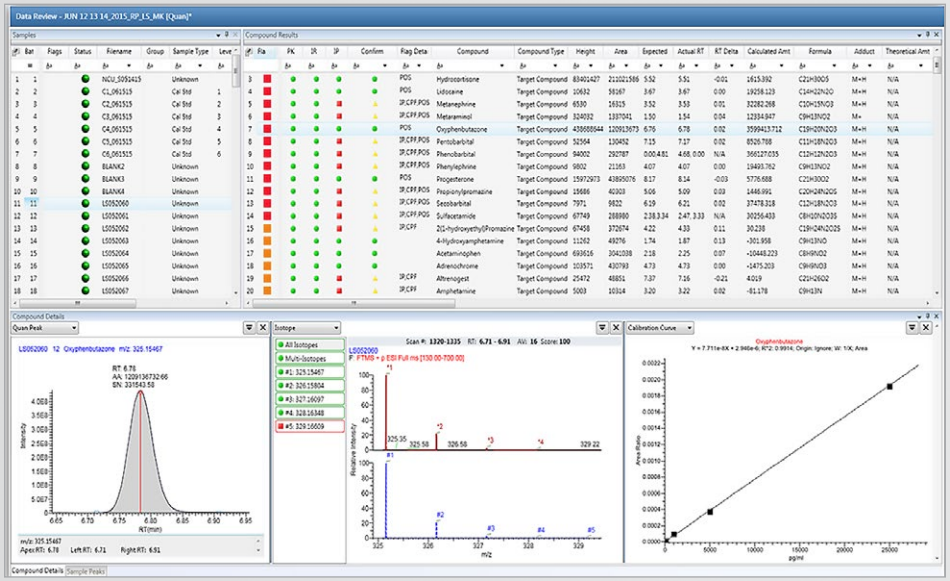


Combining targeted screening and quantitation workflows provides both compound flagging for rapid compound review and calibration curve generation in a single processing method and data review workflow.

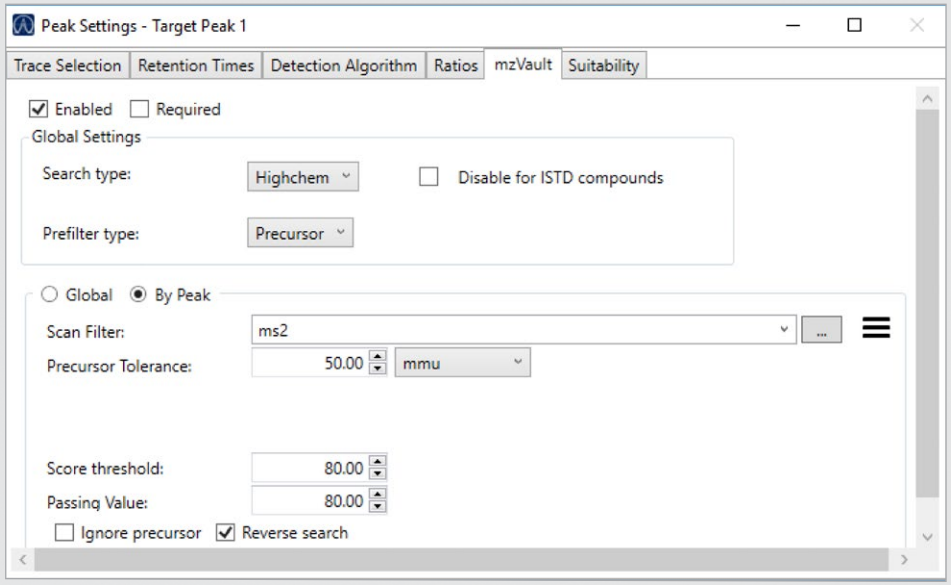

DELL

Taking your quantitative confidence to the next level with mzVault library searching

Quantitation using a high-resolution accurate-mass (HRAM) approach can provide additional benefits and capabilities that increase data quality and confidence in results; to help amplify these benefits, TraceFinder software is fully integrated with Thermo Scientific™ mzVault™ offline library. mzVault provides offline access to the Thermo Scientific mzCloud mass spectral fragmentation library, which is the world's largest, curated spectral fragmentation library. In addition, users can create their own mzVault libraries, and also directly transfer information from Thermo Scientific™ Compound Discoverer™ software to streamline method development from discovery experiments, through to everyday testing.



Utilizing HRAM-MS for screening affords high-confidence target confirmation using spectral isotope matching and fragment confirmation through mzVault spectral library. The resulting matches can added to user-defined flagging to streamline the data review process.

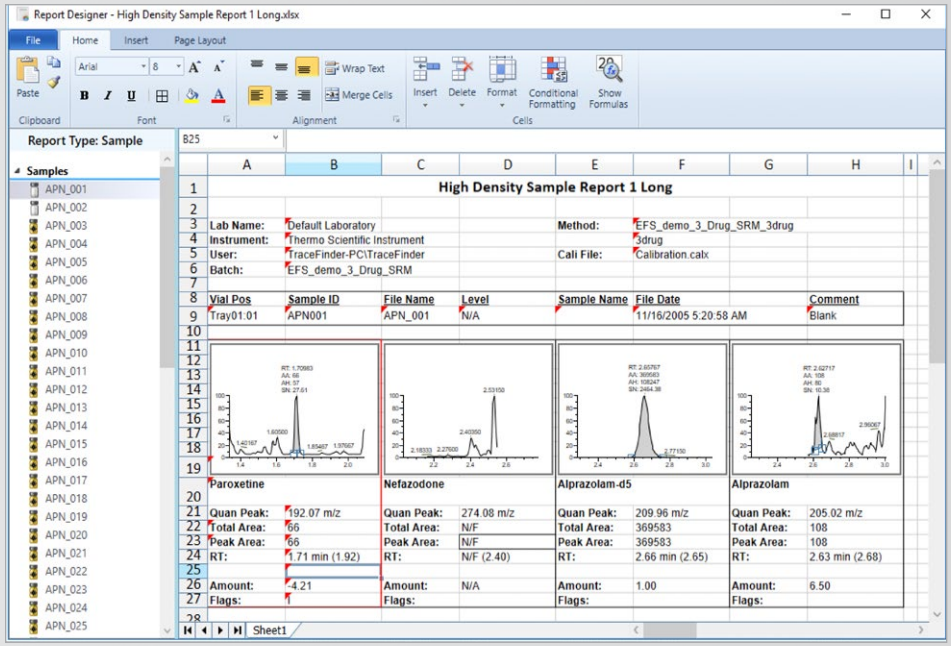


Targeted settings can be global, or specific to a given target, with flexible settings to ensure maximum confidence and consistency in any assignments, and faster time-to-results.

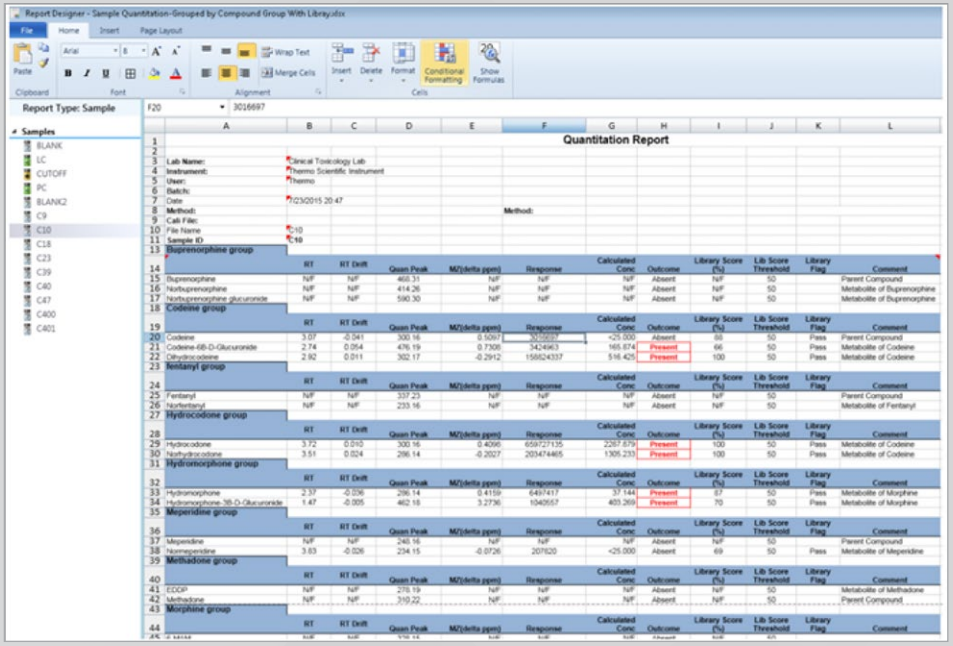
Customizable reporting for crucial results

The ability to easily and accurately report assay results is as essential as the data acquisition itself and is often a laboratory bottleneck. In addition to standard reporting templates, customized report generation is an integrated component within TraceFinder software saving time and resources, minimizing the potential for error, and maximizing throughput.

- Integrated custom report generation saves time and resources, minimizing the potential of error, and maximizing throughput
- A broad selection of pre-configured reports are available and ready for immediate use or can be used to provide a starting template for further report customization



With intuitive and predefined options for inserting chromatograms and building data tables, custom reports can be easily built to meet a wide range of reporting requirements. A broad selection of pre-built reports is available and ready for immediate use or can be used to provide a starting template for further report customization.



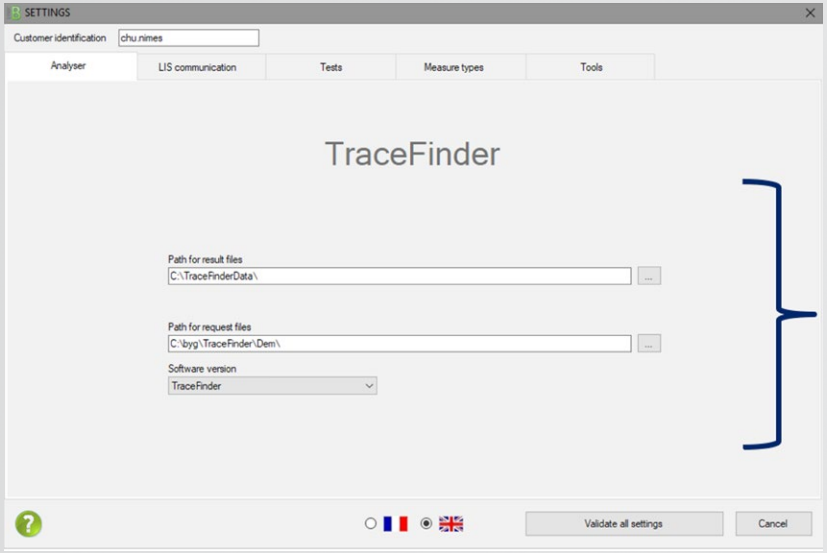
Report generation provides an additional tool for assay evaluation that can built into the overall data review process. Using additional reporting features such as custom logic statements, data filters, and custom calculations, the custom reporting capability can provide a high-level overview of assay results and to identify samples that require additional interrogation all within the data review workspace.

Maximum productivity. Trusted results.

Maximize your connectivity with TraceFinder software and B-Link

TraceFinder software not only has the ability to control multiple inlets (IC, LC, GC and multi-channel LC) and types of instrumentation (single quadrupole, triple quadrupole and high-resolution MS), it also allows bi-directional flow of methods and results from LIS/LIMS (Laboratory Information System/Laboratory Information Management System) to further enhance your productivity.

- Quantitative methods and screening
- Transfer of results and quality control values
- Minimizing user settings and interactions
- Simple to install, maintain and to use



Set-up TraceFinder exchange directories

B-link (BYG INFORMATIQUE, L'UNION France), a universal instrument connector, enables TraceFinder software to connect any LIS, LIMS or middleware, allowing the transfer of requests, information, and results. These requests can be in real time or in batch mode, without any user-action required within B-link once an initial simple system integration has been performed.

Connectivity between B-Link Connector and TraceFinder software

Bi-Directional LIS Connection

Challenge	B-Link LIS/LIMS Connector
Communication between the MS platform and LIS/LIMS • Downloading test requests • Uploading test reports	Software proving bi-directional communication • Between LIS/LIMS and B-Link • Between B-Link and TraceFinder software

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Thermo Scientific™ Compound Discoverer™ software
thermofisher.com/CompoundDiscoverer

Thermo Scientific™ mzVault Offline Mass Spectral database
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Thermo Scientific™ Mass Frontier™ software—Library curation capabilities
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Thermo Scientific™ Chromeleon™ CDS & compliance-ready screening/quan
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