

Frequently asked questions



Comprehensive LC-MS platform for increased confidence in toxicology

What is the Thermo Scientific™ Tox Explorer™ Collection?

Robust LC-MS workstream for toxicology analysis, comprised of:

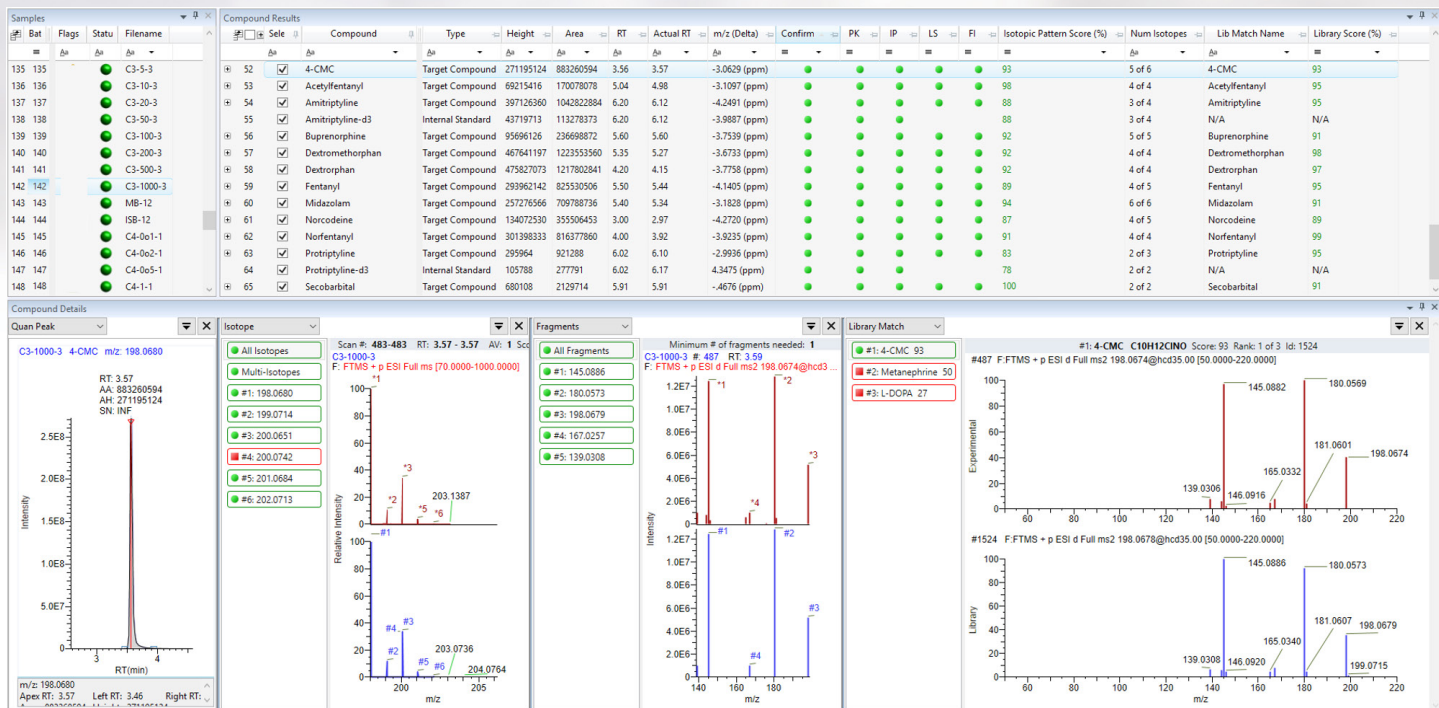
- Reliable liquid chromatography and mass spectrometry (LC-MS) instruments
- An extensive library of drug compounds and their metabolites
- Proven methods that can enable every toxicology laboratory—for every analyte, matrix type, choice of MS, and user expertise level
- Accuracy and reliability, backed by comprehensive training and support

On which MS platform is the Tox Explorer Collection available?

The first platform features the High-Resolution, Accurate-Mass (HRAM) Thermo Scientific™ Q Exactive™ Plus hybrid-quadrupole Orbitrap™ MS, the Thermo Scientific™ Vanquish™ Flex UHPLC, along with supporting instrument control and data analysis software, Compound Database, spectral library, LC-MS method, library, and method, with training and support included.



Q Exactive Plus MS coupled with Vanquish Flex UHPLC system.



Data review of targeted screening using Thermo Scientific™ TraceFinder™ 5.1 software.

What laboratories will this workflow serve?

This workflow serves forensic toxicology, clinical research toxicology, sports anti-doping, and reference laboratories with confident, comprehensive, and concise toxicology screening, identification and confirmation.

Will I receive training and support for the Tox Explorer Collection?

Included in the Tox Explorer Collection bundle are the instrument and enterprise services installation (with an additional day included), along with three days of “on-site or virtual” application-focused training provided by our Center of Excellence.

What Is Included in the Package?

The UHPLC and MS system are sold separately from the method, data package, and training. Your sales personnel will discuss available options if you are currently equipped with Thermo Scientific instrumentation and software.

Is the method optimized and can it be adjusted?

The method contains a proven LC gradient that has been standardized by many laboratories around the world, including several reference laboratories where the users are focused on assays such as: sports anti-doping, clinical

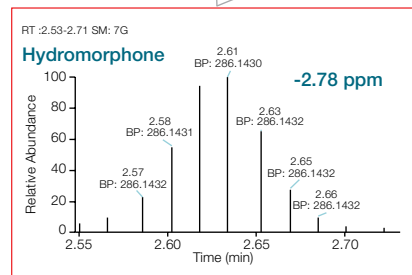
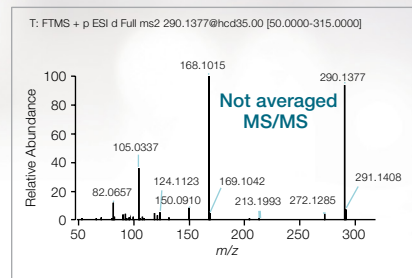
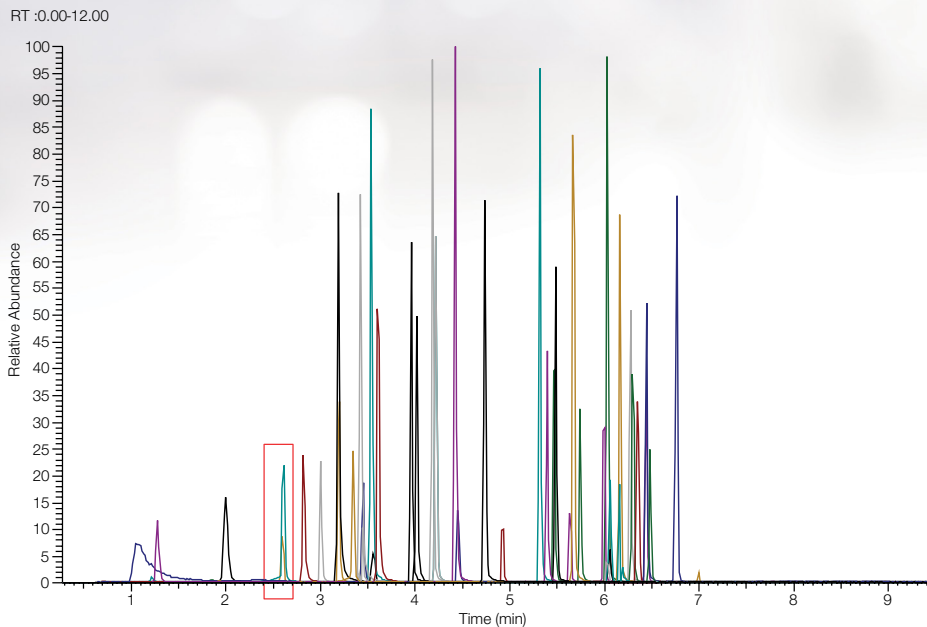
and forensics toxicology. The method could be adjusted, however, any changes in chromatography will cause a shift in the retention times in the Compound Database. Keep in mind the number of compounds in the method. The current chromatographic run length allows for adequate chromatographic separation of the current set of compounds, as well as addition of more compounds in the future. You are free to modify this method as desired, and you will be responsible for determining and updating the database with the new retention times.

Can this method be used with triple quadrupole mass spectrometers?

The current configuration is based upon hybrid-quadrupole Orbitrap technology. Additional platforms are planned to be made available, including a triple quadrupole method, which will contain SRMs and will be suited for fast, targeted analysis of known analytes to suit routine needs.

Can I use different column chemistries?

Other column chemistries would affect retention time, and change the retention times, so we recommend staying with the Thermo Scientific™ Accucore™ phenyl hexyl column, this column is best suited for analyzing a wide range of compounds. (Part No: 179-26-102130)



XIC chromatograms of four mixtures of 54 drugs of abuse compounds (mass accuracy 5 ppm).

Can sample preparation be modified?

Tox Explorer Collection focuses on standardized conditions for LC-MS, consisting of separation and detection parameters with corresponding library and retention times. You may choose to use the sample prep approach you desire.

Different sample prep may lead to better sensitivity, but this method focuses on a quick, efficient process, and this can become time-consuming and more expensive.

Does Tox Explorer Collection work with Chromeleon CDS software?

Methods will be provided for Thermo Scientific™ TraceFinder™ software processing. Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software currently cannot perform screening of MS/MS HRAM data. Until this feature is available, Chromeleon CDS software cannot be used.

Is the Tox Explorer Collection library regularly updated with new compounds?

- The Tox Explorer Collection Compound Database and spectral library will be updated periodically and will be made available for download with the compatible versions of TraceFinder software.
- Users can add their own spectra to the existing library or create their own library.
 - The customer will be responsible for updating the retention times of the new analytes that are added to the database.

- When purchasing TraceFinder software, Thermo Scientific™ mzCloud™ mass spectral libraries that are constantly updated can be downloaded in Thermo Scientific™ mzVault™ mass library format. These analytes, as well as other analytes, can be added directly to the Compound Database in TraceFinder software.

– Do remember to update the new analyte's retention time.

Can the Tox Explorer Collection be used for unknown or discovery-type analyses? Can it be used with Compound Discoverer software?

The method could be altered to acquire unknown data and could be processed with Thermo Scientific™ Compound Discoverer™ software. Additional support may be needed for such a method, and it is not guaranteed that the instrument will detect and find all unknown compounds.

Can DIA analysis be performed under the Tox Explorer umbrella?

This feature is being investigated for use with the Thermo Scientific™ Orbitrap Exploris™ 120 mass spectrometer.

Is Ion Chromatography and Gas Chromatography part of this workflow?

Currently, no. The Compound Database could be used for exact mass, isotopes, and fragment ions, but retention times would have to be re-established.

How is mzCloud mass spectral library being used with this workflow?

Currently, there is no direct route from mzCloud library to TraceFinder software as in Compound Discoverer software. A library from mzCloud library can be downloaded for use in TraceFinder software, but if the analytes are not in the database, retention times need to be assigned.

Can Multi-channel HPLC be used with Tox Explorer Collection?

Retention times were acquired on a single channel Vanquish Flex UHPLC system. Moving to a multi-channel system will alter the retention times, however it is a feasible option.

How many compounds can it quantitate?

Will SIM or PRM work?

- Currently 54 compounds were tested and quantified on concentrations of 0.1 to 1000 ng/ml, and the Tox Explorer Collection library contains over 1,500 compounds.
- Quantitation was performed using the precursor ion m/z . Using this approach, any number of compounds could be quantified with this method. Limits of detection will vary from compound to compound, and the user will be responsible for validation of the method.
- SIM and PRM would work with the same inclusion list, but a different processing method for TraceFinder software would be needed. SIM and PRM data acquisition methods are more time-intensive and will result in fewer scans across a peak.

Can we run Tox Explorer Collection on versions of TraceFinder software prior to version 5.1?

No. the library format will only will work with TraceFinder 5.1 software or higher.

Can All Ion Fragmentation (AIF) be used with this method?

This could be used, however, it would be limited if the concentration of the analyte was low and if many ions eluted at the same time.

What kits could be used with the Tox Explorer Collection?

There are currently no kits that are recommended for use with Tox Explorer Collection.

How many injections can be performed with the Tox Explorer Collection?

Thousands. The UHPLC column can be the limiting factor. Depending on your sample preparation type, we suggest switching out the ion transfer tube at around 500 injections to maintain sensitivity.

Documents of interest

[Current Guidelines for Drugs of Abuse.](#)

[National Forensic Laboratory Information System \(NFLIS\): data collection effort of drug chemistry results from local, State and Federal forensic laboratories](#)

[Tox Explorer Collection Technical Note: Comprehensive, robust LC-MS/MS toxicology method for HRAM screening and quantitation of drugs](#)

Learn more at thermofisher.com/toxexplorer

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