ThermoFisher SCIENTIFIC

Toxicology

Fit for purpose.
Increase productivity.
Consistently accurate results.

Tox Explorer Collection

An all-in-one LC-MS/MS solution for toxicology

thermo scientific

Navigate with ease

An all-in-one LC-MS/MS solution for toxicology

Detect an ever-increasing number of substances at ever-decreasing concentrations. The Thermo Scientific™ Tox Explorer™ Collection helps the world's toxicology community in forensics, clinical research, employee drug testing, and sports anti-doping navigate with ease to solve complex analytical challenges and increase productivity. Now you have a choice of either Thermo Scientific™ Orbitrap HRAM or Thermo Scientific™ TSQ triple quadrupole mass spectrometer platforms. Choose the best option based on your needs.

Keep detection capability one step ahead with high-resolution accurate-mass (HRAM) or triple quadrupole mass spectrometry options of the Tox Explorer Collection.

Streamline your methods using sample preparation guidelines, high performance HPLC columns, intuitive software capabilities, and a comprehensive mass spectral library or compound database.

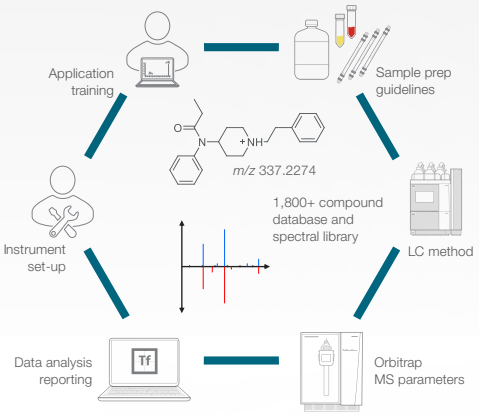
Get excellent dynamic range and highly accurate mass measurements. HRAM option includes over 1,800 compounds of interest in the spectral library.

Increase productivity with SRM acquisition speeds enabling faster polarity switching. Triple quadrupole MS option includes over 1,200 compounds in the compound database.

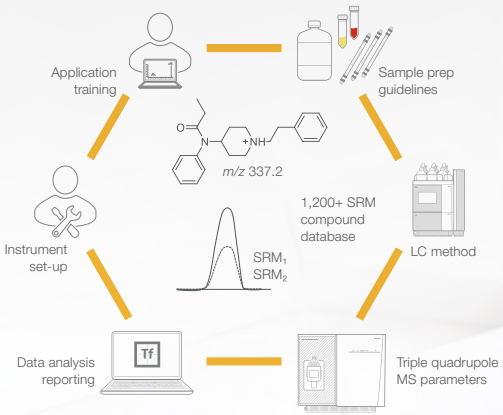
Comprehensive LC-MS solutions

Choose from two LC-MS platforms

Optimized for quick start-up and ease of use, the Tox Explorer Collection is designed to improve efficiency and reduce cost throughout the preparation, separation, detection and analysis of drug compounds in multiple biological matrices such blood, plasma, and urine with unprecedented speed, ease, and confidence, regardless of method complexity or user experience. It is equipped with a standardized LC-MS/MS method, UHPLC column, experimentally obtained database with retention times, and LC-MS/MS instrument set-up and application training enabling smooth start-up and implementation. Choose from two mass spectrometry options; each is a comprehensive LC-MS solution from sample processing to reporting of toxicology analytes.



Tox Explorer Collection for HRAM MS



Tox Explorer Collection for Triple Quad MS

Vanquish Flex Binary UHPLC system

Productivity and quality in chromatography

With confident retention time stability and maximum pressure up to 1,000 bar, the Thermo Scientific™ Vanquish™ Flex UHPLC systems increase productivity without compromising quality of results. The platform shares all the Vanquish system values, such as design focused on uptime, robustness, and quality, enabling every toxicology laboratory to address critical screening and quantitation challenges.

- Designed for maximum flexibility.
- Achieve separations with better reproducibility.
- Increase productivity with high sample throughput.
- Integrates seamlessly with Thermo Scientific mass spectrometers with dedicated software.

UHPLC columns

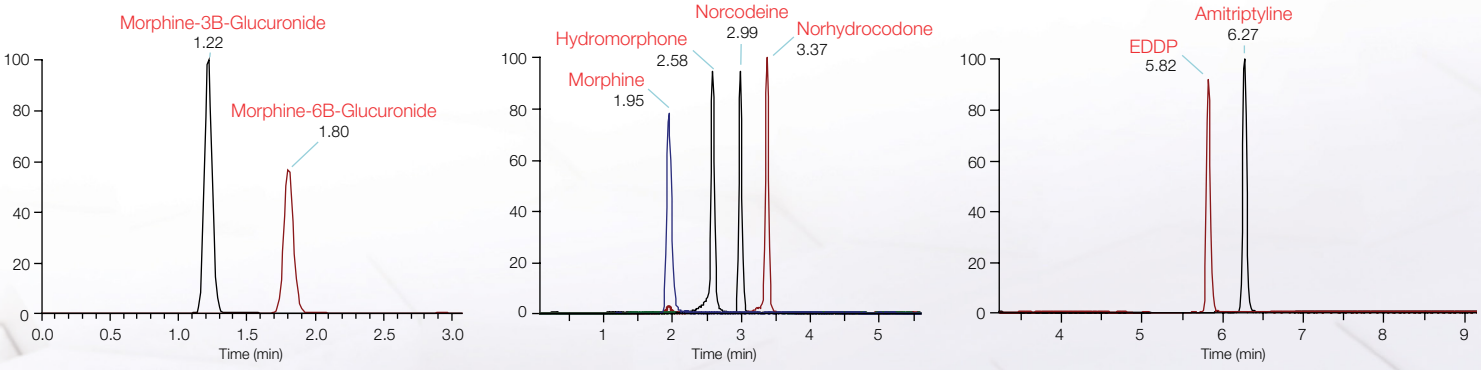
Fast separations with excellent resolution and sensitivity

Based on Core Enhanced Technology, Thermo Scientific™ Accucore™ columns provide fast, high-resolution separations without the elevated backpressures required by sub-2 µm particles.

- Robust columns offer wide separation chemistry for all UHPLC applications.
- Highly efficient, rugged separations are ideal for LC-MS applications.

Chromatographic resolution

The 15-minute LC-MS/MS method of the Tox Explorer Collection is capable of separating drugs of abuse isomers. Screening is based on retention times for each specific isomer.



Commonly found isomers in drugs of abuse screening

Tox Explorer Collection for Orbitrap Exploris 120 mass spectrometer

Tox Explorer Collection for Orbitrap Exploris 120 MS

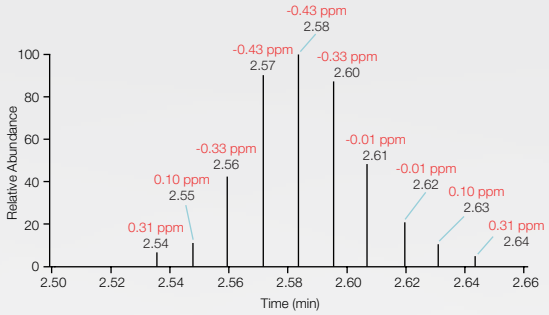
High resolution qualitative and quantitative performance

Navigate with ease using fast scan rates, polarity switching, and an over 1,800-compound database with corresponding high-resolution spectral library. A standardized method and onsite set-up and training ensures less time spent on method development.

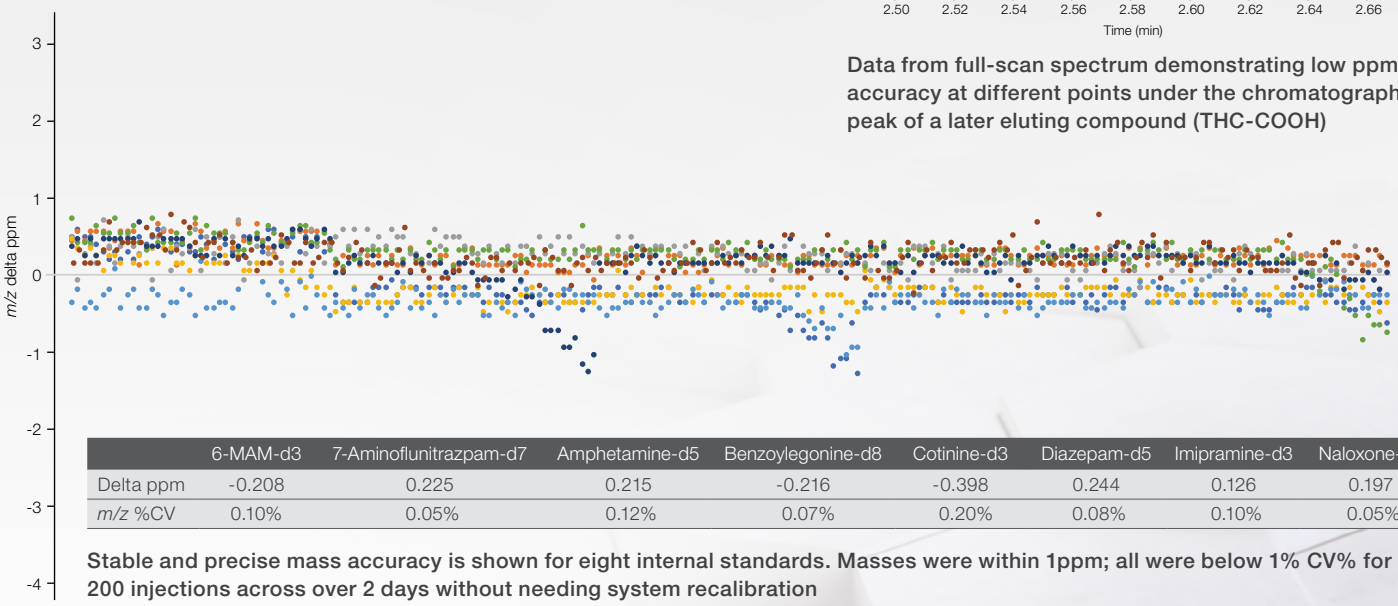
- **Method:** 15-min w/RT for 1,800 compounds (HRAM tubing config.)
- **LC:** Vanquish Flex Binary UHPLC system
- **MS:** Thermo Scientific™ Orbitrap Exploris™ 120 mass spectrometer
- **HRAM resolution:** Full Scan 60K, ddMS^2 15K
- **Pos/neg switching:** standard
- **Column:** Accucore Phenyl Hexyl, 100 × 2.1 mm, 2.6 µm UHPLC column
- **Software:** Thermo Scientific™ TraceFinder™ 5.1 software
- **CDB and library:** 1,800 compounds; experimentally obtained with true standards
- **Mass range:** *m/z* 40–3,000
- **Onsite installation:** included—instrument install and configuration set-up
- **Onsite training:** included—2-days on-site install, support and Tox Explorer Collection application training

High resolution and mass accuracy

Thermo Scientific™ Orbitrap™ technology platforms offer high resolution mass spectrometry and unparalleled mass accuracy without loss of sensitivity and provides positive/negative polarity switching in a single analytical run, saving time and offering greater confidence in data output.



Data from full-scan spectrum demonstrating low ppm mass accuracy at different points under the chromatography peak of a later eluting compound (THC-COOH)



	6-MAM-d3	7-Aminoflunitrazpam-d7	Amphetamine-d5	Benzoylegonine-d8	Cotinine-d3	Diazepam-d5	Imipramine-d3	Naloxone-d5
Delta ppm	-0.208	0.225	0.215	-0.216	-0.398	0.244	0.126	0.197
m/z %CV	0.10%	0.05%	0.12%	0.07%	0.20%	0.08%	0.10%	0.05%

Stable and precise mass accuracy is shown for eight internal standards. Masses were within 1ppm; all were below 1% CV% for over 200 injections across over 2 days without needing system recalibration

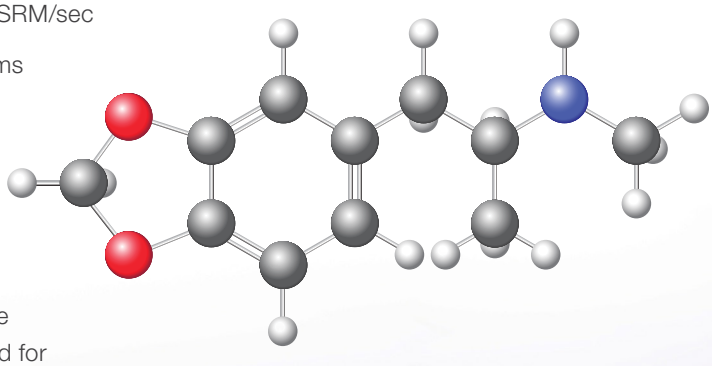
Tox Explorer Collection for TSQ Quantis Plus mass spectrometer

Tox Explorer Collection for TSQ Quantis Plus MS

Accessible quantitative performance

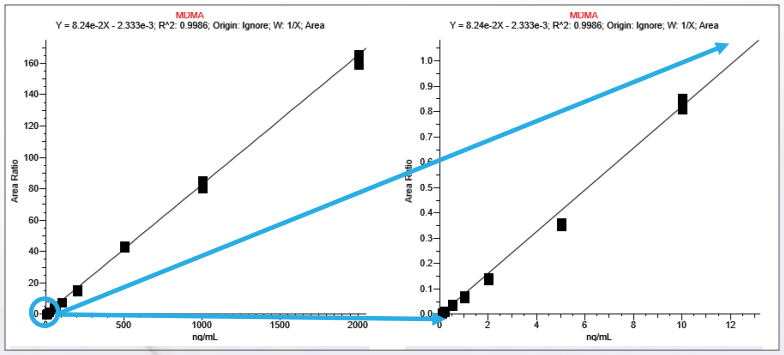
Achieve scientific and business goals by accessing over 1200 compounds with superior acquisition speeds and polarity switching. Quantitative precision and accuracy delivered through innovative product designs enable TSQ Plus mass spectrometers to address the ever-changing drug landscape with consistency and reliability.

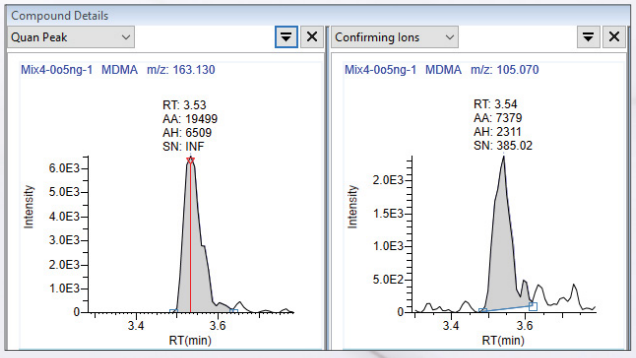
- **Method:** 15-min w/RT for 1,200 compounds (QQQ tubing config.)
- **LC:** Vanquish Flex Binary UHPLC system
- **MS:** Thermo Scientific™ TSQ Quantis™ Plus mass spectrometer
- **SRM acquisition:** 600 SRM/sec
- **Pos/neg switching:** 5 ms
- **Column:** Accucore Phenyl Hexyl, 100 × 2.1 mm, 2.6 µm UHPLC column
- **Software:** TraceFinder 5.1 software
- **CDB and library:** 1,200 compounds; experimentally obtained with true standards
- **Mass range**: *m/z* 2–3,000
- **Onsite installation:** included—instrument install and configuration set-up
- **Onsite training:** included—2-days on-site install, support and Tox Explorer application training



Targeted screening and quantitation

Incorporating the TSQ Quantis Plus mass spectrometer for drugs of abuse testing enables sensitive and reproducible analytical measurement needed for confirmation for compounds covering a range of compound classes and polarities.



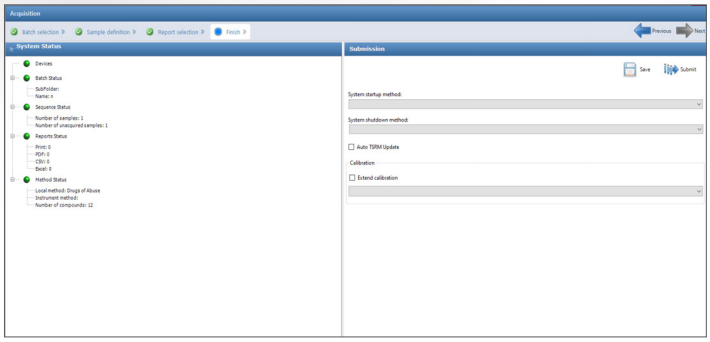


Limits of confirmation (LOC) were determined for MDMA with concentrations ranging from 0.1 to 2000 ng/mL (left) as well as chromatogram results from MDMA at its LOC of 0.5 ng/mL showing quantitation and confirming peaks (right). Calibration curves for quantitation were linear with R^2 values of >0.99 and replicates all <30%.

TraceFinder software for fast actionable results

Simplify high-throughput screening and quantitation

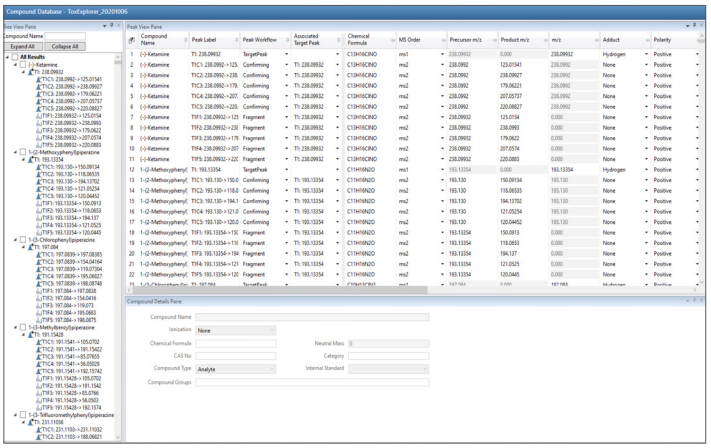
Driven by an intuitive set of acquisition and data processing tools, TraceFinder software provides rapid access to results and increases output across the entire laboratory. Enhance productivity with built-in intelligence such as four-click acquisition and saved templates. A single software platform for method development, acquisition, and processing increases efficiency and confidence. Finally, benefit from increased application productivity using customizable views for reporting, flagging, and screening criteria.



Simplify routine quantitation

Ease of use

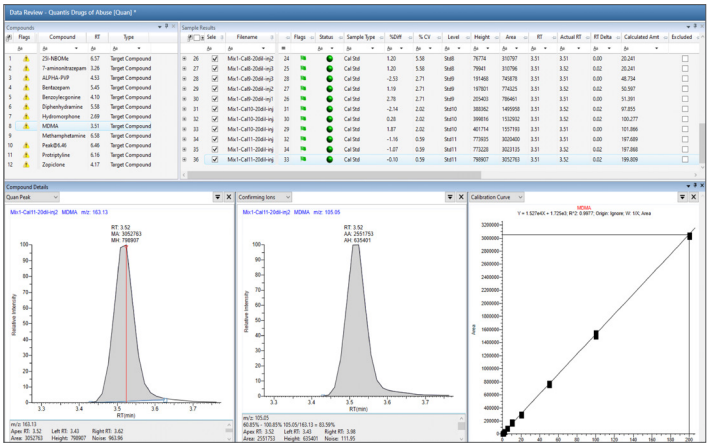
- Four-click acquisition
- Saved templates
- Workflows
  - Quantitation, screening and unknown analysis
  - Small and large molecule analysis



Efficiency and confidence

One software platform

- Method development, acquisition, processing
- Compound databases and spectral libraries
- Auditing/administration



Application productivity

Customization

- Custom report generation
- Customized data viewing
- Smart sample flagging
- Screening criteria
- Auditing/administration

mzVault mass spectral library

Confident identification of toxicology compounds

When using Orbitrap technology, the Thermo Scientific™ mzVault™ mass spectral library seamlessly integrates with the acquisition and processing TraceFinder software while providing an extensive repository of valuable information on critical analytes that enables confident identification of small molecules.

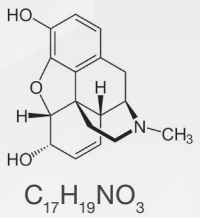
- Includes exact mass of compounds
- Fragmentation data at different collisional energies helps identify unknown compounds

Workflow for adding compounds to the database

Addition of new compounds to a database can be done with ease because manual optimization of individual precursors is not required. New compounds can easily be added to the existing method by collecting full scan data with targeted MS^2 spectra. Once the retention time is known, the information is simply added to the compound database and library. There is no need for revalidation because the cycle time/dwell time does not change in the method.

Users can also add their own spectra to the existing library or create their own library. The customer will need to update the retention times of the new analytes that are added to the database.

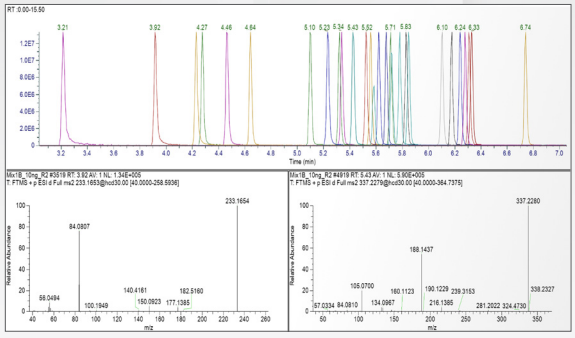
1



$C_{17}H_{19}NO_3$

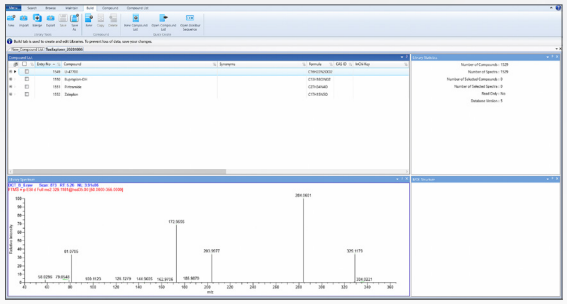
Known data: *m/z* and empirical formula to calculate isotope pattern

2



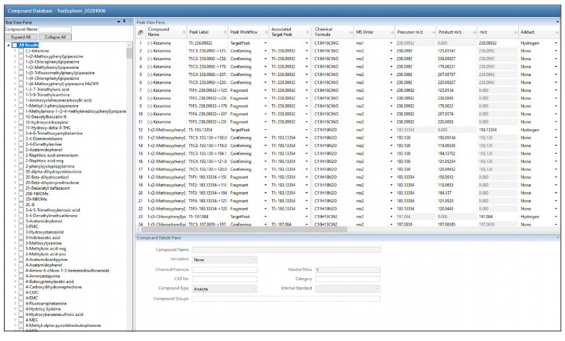
Run standard and obtain RT and MS^2 spectrum (includes fragments)

3



Import MS spectrum in mzVault

4



Export to compound database

5

	Mass [m/z]	Formula [M]	Species	CS [z]	Polarity	Start [min]	End [min]	(N)CE	MSX ID	
1	238.09932				Positive	3.44	4.44			(-)-Ketamine
2	193.13354				Positive	2.85	3.85			1-(2-Methoxyphenyl)piperazine
3	197.08400				Positive	3.56	4.56			1-(3-Chlorophenyl)piperazine
4	191.15428				Positive	1.96	2.96			1-(3-Methylbenzyl)piperazine
5	231.11036				Positive	4.12	5.12			1-(3-Trifluoromethylphenyl)piperazine
6	197.08400				Positive	3.47	4.47			1-(4-Chlorophenyl)piperazine
7	193.13354				Positive					1-(4-Methoxyphenyl) piperazine MeOPP
8	545.23812				Positive					10-Deacetylbaccatin III
9	255.11280				Positive	4.44	5.44			10-hydroxycarbazepine
10	331.22677				Positive	8.39	9.39			11-Hydroxy-delta-9-THC
11	209.06801				Negative	2.58	3.58			1-3-7-Trimethyluric acid
12	195.08765				Positive	2.15	3.15			1-3-9-Trimethylxanthine
13	144.10191				Positive	0.45	1.45			1-Aminocyclohexanecarboxylic acid
14	177.13863				Positive	0.30	1.30			1-Methyl-3-phenylpiperazine
15	194.11756				Positive	3.25	4.25			1-Methylamino-1-(3-4-methylenedioxyphenyl)propane
16	363.21660				Positive	4.86	5.86			20-Alpha-dihydroprednisolone
17	365.23225				Positive	5.04	6.04			20-Beta-dihydrocortisol
18	363.21660				Positive	5.00	6.00			20-Beta-dihydroprednisolone
19	400.21185				Positive	5.50	6.50			21-Deacetyl deflazacort

Export compound database to inclusion list

Ordering information

Tox Explorer Collection for Orbitrap Exploris 120 mass spectrometer	
Catalog number	WFLOW-62002
Type	Tox Explorer Collection
Mass spectrometer interface	Orbitrap Exploris 120 mass spectrometer (Sold separately)*
Liquid chromatography system	Vanquish Flex Binary UHPLC system (Sold separately)*
Methods	LC-MS/MS w/RT (HRAM tubing config.)
Software	TraceFinder 5.1 software
Description	Tox Explorer Collection for Orbitrap Exploris 120 mass spectrometer
For use with (application)	High resolution QUALITATIVE and QUANTITATIVE performance in: Forensic toxicology, clinical research toxicology, employee drug testing, and anti-doping applications
Includes	Standardized LC-MS/MS method, (U)HPLC column, experimentally obtained database with retention times, and LC-MS/MS instrument set-up and Tox Explorer application training by dedicated experts
Unit size	Each
Tox Explorer Collection for TSQ Quantis Plus mass spectrometer	
Catalog number	WFLOW-62003
Type	Tox Explorer Collection
Mass spectrometer interface	TSQ Quantis Plus mass spectrometer (Sold separately)*
Liquid chromatography system	Vanquish Flex Binary UHPLC system (Sold separately)*
Methods	LC-MS/MS w/RT (QQQ tubing config.)
Software	TraceFinder 5.1 software
Description	Tox Explorer Collection for TSQ Quantis Plus mass spectrometer
For use with (application)	Accessible QUANTITATIVE performance in: Forensic toxicology, clinical research toxicology, employee drug testing, and anti-doping applications
Includes	Standardized LC-MS/MS method, (U)HPLC column, experimentally obtained database with retention times, and LC-MS/MS instrument set-up and Tox Explorer application training by dedicated experts
Unit size	Each

* The Orbitrap Exploris 120 (HRAM) or TSQ Quantis Plus (triple quadrupole) mass spectrometers and Vanquish Flex Binary UHPLC system can be ordered separately in case you already own these instruments and are looking to purchase only the method, data package, and training components of Tox Explorer Collection.

Learn more at **thermofisher.com/ToxExplorer**