

Confident.  
Comprehensive.  
Concise.

## Tox Explorer Collection: Resolute sensitivity enabled by Orbitrap technology

The Thermo Scientific™ Tox Explorer™ Collection features a robust LC-MS/MS platform with class-leading Thermo Scientific™ Orbitrap™ technology and proven methods for toxicology analysis. This workflow provides forensic toxicology, clinical research toxicology, sports anti-doping, and reference laboratories with confident, comprehensive, and concise toxicology screening, identification and confirmation—all with one instrument.

- Confident, robust, and reliable analytical methods featuring the Thermo Scientific™ Q Exactive™ Plus mass spectrometer and the Thermo Scientific™ Vanquish™ Flex UHPLC system
- Streamline your methods using sample preparation guidelines, high performance HPLC columns, intuitive software capabilities, and comprehensive mass spectral library
- Utilize over 1,500 compounds of interest in the spectral library including compound details, such as exact mass, retention time, and fragment ions encompassing a wide range of drug classes and analytes, and gain access to regular compound updates
- Step up productivity, reduce costs, and achieve high quality analysis of data with confidence—all backed by application support and training

# Confident, comprehensive, concise method

## Robust LC-MS/MS platform for toxicology analysis

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 as blood, plasma, and urine with unprecedented speed, ease, and confidence, regardless of the method complexity or user experience level.

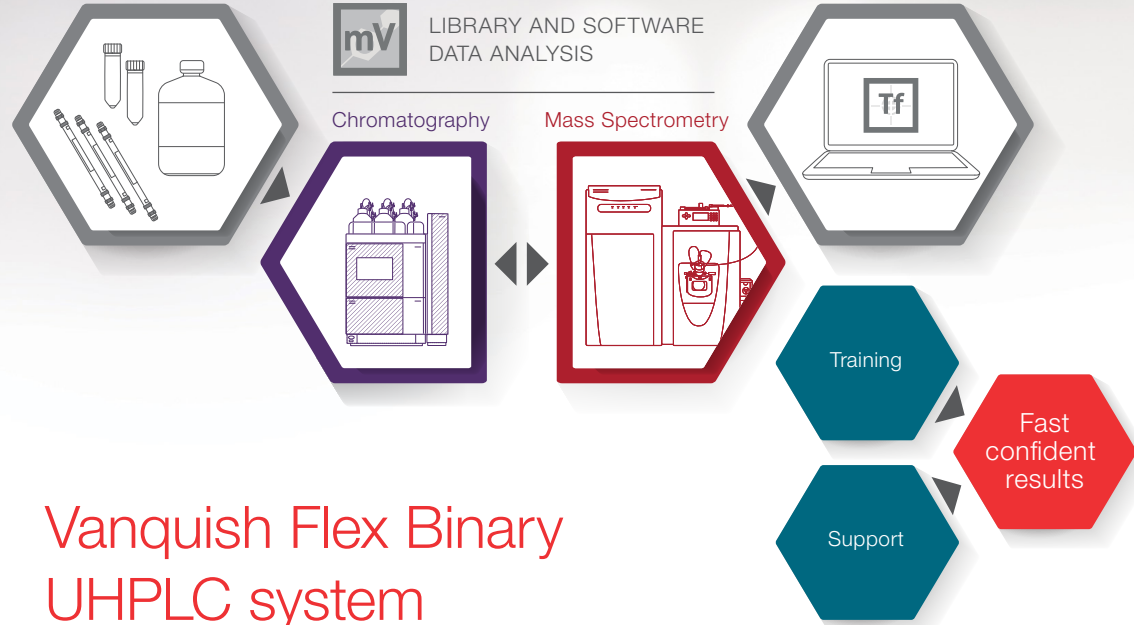
Sample Preparation Guidelines

**mV** LIBRARY AND SOFTWARE DATA ANALYSIS

Chromatography

Mass Spectrometry

Reporting



## Vanquish Flex Binary UHPLC system

### Productivity and quality in chromatography



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

- System designed for maximum flexibility
- Separations with better reproducibility
- High sample throughput with fast analysis
- Better connectivity of LC-MS with dedicated software

## HPLC 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 with wide separation chemistry for all UHPLC applications
- Highly efficient, rugged separations for LC-MS applications



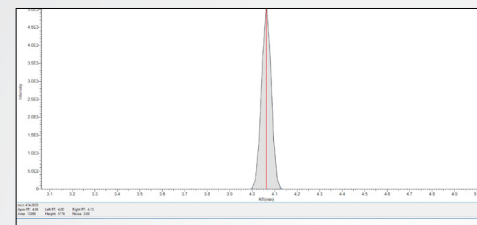
## Screening

Over 1,500 compounds in the mass spectral library

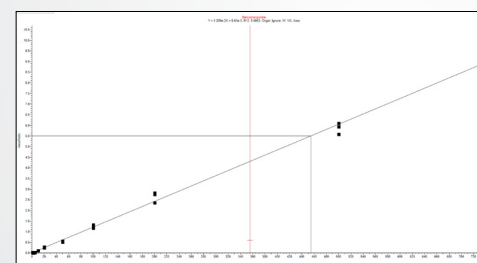
### Accurate compound identification

Compound	Formula	m/z (Delta ppm)	RT (min)	Match Result Name	Similarity Pattern Score (%)	
1	4-Methyl-alpha-pyrrolidinoethamphetamine	C10H17NO	-2.376	-0.33	4-Methyl-alpha-pyrrolidinoethamphetamine@Tf 4.61	100
2	7-Desoxy-7-oxococaine	C19H21NO2	-2.260	-0.28	7-Desoxy-7-oxococaine@Tf 3.18	93
3	7-Desoxy-7-oxococaine	C19H21NO2	-2.102	0.04	7-Desoxy-7-oxococaine@Tf 3.18	93
4	Carbamidol	C21H29O2	-1.4123	-0.18	Carbamidol@Tf 8.89	86
5	Delta-9-tetrahydrocannabinol	C21H30O2	-1.4123	-0.30	Delta-9-tetrahydrocannabinol@Tf 8.89	86
6	Delta-9-THC	C21H30O2	-1.4123	-0.36	Delta-9-THC@Tf 8.89	86
7	MDMA	C11H15NO2	-1.9875	0.00	MDMA@Tf 3.42	100
8	Mephentermine	C10H17N	-1.8207	0.20	Mephentermine@Tf 3.87	100
9	Nonoxonylin	C18H17N	-1.1081	0.00	Nonoxonylin@Tf 6.03	88
10	Propylamine	C3H9N	-1.1081	0.00	Propylamine@Tf 6.03	88
11	Ziprasidone	C21H27NO3	-4.2029	-0.04	Ziprasidone@Tf 4.03	76

## Quantitation



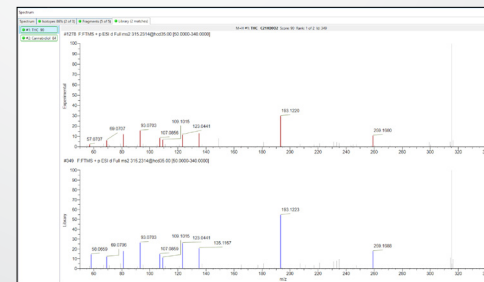
Low levels of detection: 1 ng/mL



Linear calibration curves

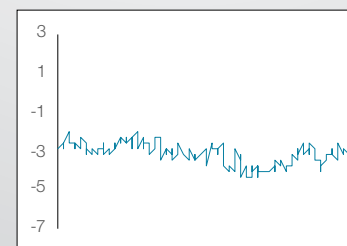
## Confirmation

### Library matching



## Robustness

### Mass accuracy over 400 injections



## HRAM mass spectrometer

### Screen, identify, confirm, and quantitate with Orbitrap technology

The Q Exactive Plus hybrid quadrupole-Orbitrap mass spectrometer is equipped with the ability to routinely and confidently identify, quantify, and confirm in a single analysis using a single mass spectrometer. Take your screening, quantitation, and confirmation to a new level with increased performance meeting toxicology requirements.

- Screen, identify, confirm, and quantitate—all with one instrument
- Analyze a broad spectrum of compounds in one run
- Perform retrospective analysis without requiring additional experiments
- Comprehensive MS/MS spectra without the need to average, while allowing accessibility to positive and negative compounds in one run
- Utilize data-dependent acquisition for the identification of unknown structures via MS/MS spectra
- Exceptional mass accuracy and stability within and between runs—even at low mass ranges—to ensure confidence in results



## Intuitive software

### Simplify high-throughput screening and quantitation

Driven by a powerful and intuitive set of acquisition and data processing tools, Thermo Scientific™ TraceFinder™ software provides rapid access to your results and increases output across the entire laboratory. Drive your productivity with built-in intelligence provided through TraceFinder software acquisition and data processing.

- Simplify sample analysis at each step of the process
- Smart sample flagging, flexible data review, and custom report generation
- Streamline and standardize operating procedures, minimizing training requirements and simplifying lab operations



## mzVault mass spectral library

### Confident identification of toxicology compounds

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

- Includes exact mass of compounds
- Includes fragmentation data at different collisional energies to help identify unknown compounds

## Tox Explorer Collection components

- Thermo Scientific Q Exactive Plus hybrid quadrupole-Orbitrap mass spectrometer
- Thermo Scientific Vanquish Flex UHPLC system
- Thermo Scientific Accucore column and consumables configured for high performance separations
- Thermo Scientific TraceFinder software
- A 1,500+ compound HRAM spectral library and database with streamlined data processing and reporting
- LC-MS hardware parameters
- Step-by-step walkthrough guide for quick start-up and method installation
- Application support and training

## Additional resources

- Brochure: Tox Explorer LC-MS Collection
- Technical Note: Comprehensive, robust LC-MS/MS toxicology platform and method for high-resolution, accurate mass (HRAM) detection, screening, and quantitation of drugs

## Comprehensive service and application support

### Proven method and quick start guide

- Refer to a comprehensive start-up guide, which includes installation and method instructions

### Comprehensive training

- Receive customized instrument and application training for users of all expertise levels

### Application support

- From regional demonstration laboratories to centers of excellence support
- From global marketing teams to special solution centers
- Enable your workflows via an extensive network of experienced and expert scientists

### Unity™ Lab Services

- Single source for integrated lab service, support, and supply management
- Complete portfolio of services and support solutions
- Enabling users to improve productivity, reduce total cost of ownership, and ensure performance

## Ordering information

Product	Part number
Thermo Scientific Q Exactive Plus mass spectrometer	0726030
Thermo Scientific Vanquish Flex Binary UHPLC system	5400.0225
Thermo Scientific Tox Explorer Bundle - KIT, TOX EXPLORER COLLECTION	OPTON-31039

Facing limitations with immunoassay testing? Need to screen for the presence of many different drugs and metabolites, with lower limits of detection at lower costs? LC-MS/MS is becoming the analytical method of choice for comprehensive drug screening in the toxicology laboratory.

Find out more at [thermofisher.com/toxexplorer](https://thermofisher.com/toxexplorer)