

Mass spectrometry



## Simplify the complexity of dioxin analysis

Thermo Scientific dioxin analysis with GC-MS/MS

thermo scientific





## Dioxin analysis portfolio: compliance, productivity and robustness

The Thermo Scientific™ dioxin analysis portfolio allows analysts to meet the most rigorous of challenges associated with dioxin analysis. The portfolio includes worldwide compliant magnetic sector technology, high resolution accurate mass spectrometry for comprehensive characterization of samples and GC triple quadrupoles for an easy-to-implement analytical workflow for dioxin analysis.

The Thermo Scientific™ TSQ™ 9610 GC-MS/MS system is part of an integrated, sample-to-result GC-MS/MS-based analytical workflow developed to deliver robust and sensitive quantitation of polychlorinated dibenzo-p-dioxins (PCDD), polychlorinated dibenzo furans (PCDF) and dioxin-like polychlorinated biphenyls (dl-PCBs), in food and feed samples in compliance with the latest EU regulations (EU Regulation 664/2017).

Recent advances in GC-MS/MS technology have enabled lower detection limits and improved automated selected reaction monitoring (SRM) performance. This, in turn, has led the European Commission to update regulations to permit the use of GC-MS/MS, in addition to magnetic sector technology, as a confirmatory method for enforcing maximum levels (ML) and action levels (AL) for dioxins/furans and dl-PCBs in foodstuffs and animal feeds. Combining the technological advances of the TSQ 9610 GC-MS/MS system with ease of use, laboratories are able to produce a comprehensive workflow for dioxin analysis with accelerated implementation that includes a user deployment guide, quality check standards, a pre-loaded acquisition method, as well as data processing and reporting templates—all in a single analytical package from a single vendor.

### The immediate benefits for the laboratories are:

- **Compliance** with EU requirements for dioxin/furan and dl-PCBs in food and feed samples and ultimate confidence in results.
- **Productivity** ensured by out-of-box implementation and operational simplicity, supported by a comprehensive suite of Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) tools, tailored to dioxin analysis. These are aimed at reducing training needs and increasing productivity immediately after installation.
- **Robustness** of the instrumentation for a large variety of sample types and extended uptimes (less unscheduled downtime) producing consistent high-quality results.

## The most comprehensive GC-MS portfolio for dioxins and POPs analysis

Thermo Fisher Scientific offers complementary technology for the analysis of dioxins/furans and persistent organic pollutants (POPs). Each solution has specific advantages and collectively offer the most comprehensive GC-MS portfolio available on the market.



### Magnetic Sector GC-HRMS

The Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS System offers worldwide compliance with any official Dioxin, PCB or PBDE method (e.g., EPA 1613, 1668, 1614). Laboratories measuring not only the maximum levels, but also low background levels in food and animal feed, can exploit the benefits of unmatched sensitivity for dioxin/furan and dl-PCB and robustness, delivered by the most established dioxin solution.



### Orbitrap GC-MS/MS

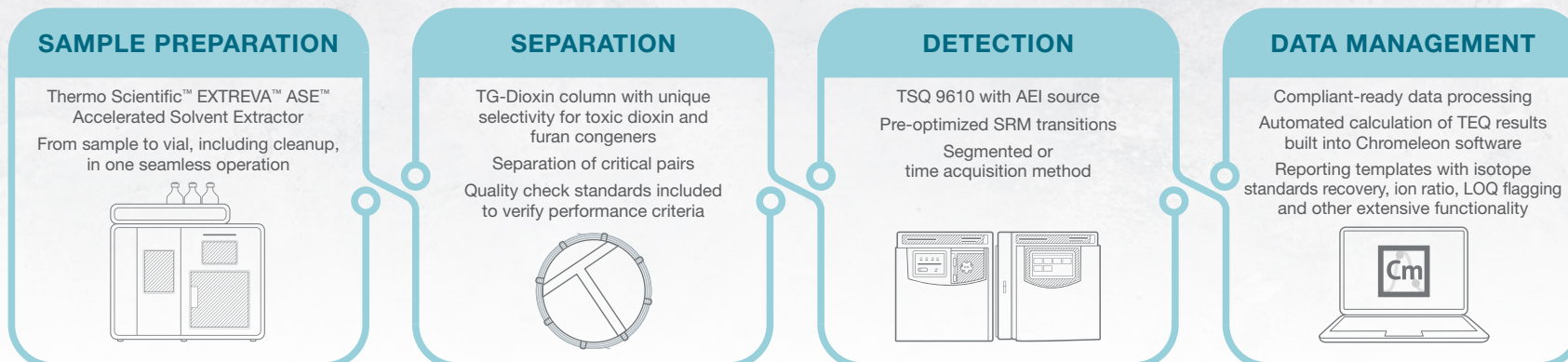
The Thermo Scientific™ Orbitrap Exploris™ GC mass spectrometer is a high-resolution, accurate-mass (HRAM) benchtop GC-MS system that provides the highest confidence for screening and quantitation of legacy and emerging contaminants. This performance-based testing is achieved through the superior resolving power, mass accuracy and sensitivity that only Orbitrap technology can deliver.



### TSQ 9610 GC-MS/MS

The Thermo Scientific TSQ 9610 GC-MS/MS system is easy to implement with a full analytical workflow developed to deliver robust and sensitive quantitation of polychlorinated dibenzo-p-dioxins (PCDD), polychlorinated dibenzo furans (PCDF) and dioxin-like polychlorinated biphenyls (dl-PCBs), in food and feed samples in compliance with the latest EU regulations (EU Regulation 664/2017).

## DIOXIN WORKFLOW





## Full compliance with EU criteria at the lowest LOQ level

Gain cost-effective high sample-throughput for monitoring maximum levels and action levels of dioxins/furans and dl-PCBs in foodstuffs and animal feeds. To support the validity of data reported within the framework of official controls, testing laboratories are required for each analytical sequence, to demonstrate compliance with method performance criteria, ranging from sensitivity to accuracy. In particular, the limit of quantitation (LOQ) for each of the most toxic congeners needs to be confirmed by checking the consistency of the response at the lowest concentration level of a calibration curve. Leveraging benchmark sensitivity of the Thermo Scientific TSQ 9610 triple quadrupole GC-MS/MS system with the Advanced Electron Ionization (AEI) source provides the confidence to meet all EU compliance criteria at the lowest LOQ levels.

TSQ 9610 triple quadrupole GC-MS/MS system including a Thermo Scientific™ TRACE™ 1610 Gas Chromatograph and Thermo Scientific™ TriPlus™ RSH SMART Autosampler

## PERFORMANCE CRITERIA

Separation of isomers shall be <25% peak to peak between  
**1,2,3,4,7,8-HxCDF**  
 and  
**1,2,3,6,7,8-HxCDF**

Resolution for each quadrupole to be set equal to or better than  
**unit mass resolution**  
 (sufficient resolution to separate two peaks one mass unit apart)

Maximum permitted tolerance of relative ion intensities of **±15 %** for selected transition product ions in comparison to theoretical or measured values

Response Factor deviation of the lowest concentration shall be **<30%** from average value throughout the sequence, in order to use this point to calculate LOQ

Limit of Quantification (LOQ) shall be **20%** of the maximum level in the corresponding food and feed stuffs

EU quality performance criteria for routine use of GC-MS/MS for confirmational analysis

## Enhanced productivity from day one



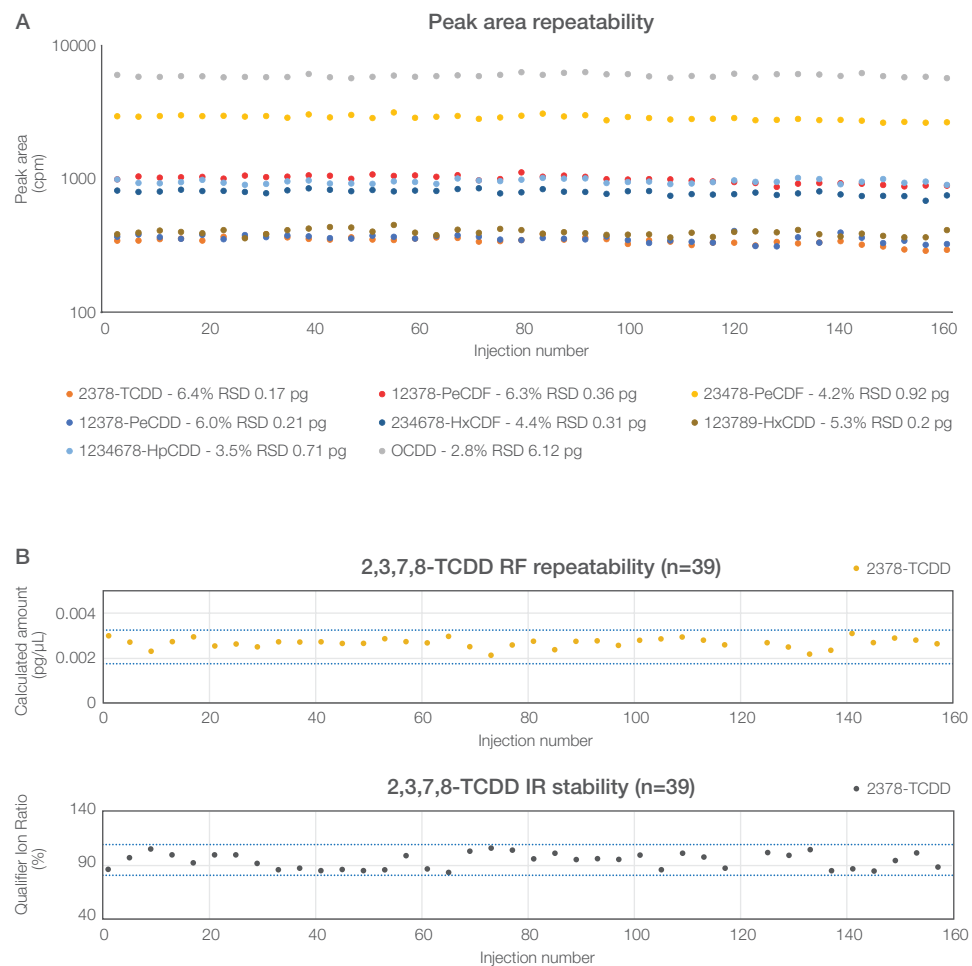
All instrument components, capillary GC column, system suitability check standard solutions, software and comprehensive user guidelines are included for seamless implementation and enablement of ongoing optimum performance immediately after installation. Complex data

calculation and automatic generation of results is made easier through the Chromleon CDS productivity tools. This suite of software tools supports and facilitates all steps, from creating the analytical sequence with all quality checks and performance criteria, to the interactive monitoring of the analysis progress, automatic calculation of concentrations based on isotope dilution calculations and reporting the Toxic Equivalent (TEQs) results in compliance with the EU Regulation. Thus, giving back to the user, valuable time to be invested in other more profitable activities.

## Robust workflow for unstoppable uptime

Take advantage of the robust, productive and reliable quantitation, in compliance with EU method performance criteria, in every analysis sequence. The new ultra-robust AEI source design of TSQ 9610 GC-MS/MS system provides extremely high tolerance to the matrix. This enables the user to set up complete sample sequences with hundreds of injections—alternating samples with blanks and multiple level standard solutions—with the confidence to deliver consistent and trusted results. As an example, Figures A and B show the excellent robustness of an injection sequence over a period of two weeks, with no maintenance such as: source cleaning, liner replacement, tuning or analytical column trimming, performed during the sequence despite the high number of injections and matrix complexity.

## Consistent results over continuous analysis



(A) Absolute peak area repeatability over two weeks of analysis, for selected PCDD/F congeners in pooled matrix sample. Relative standard deviations and amounts on-column (pg) are annotated for each selected congener. (B) LOQ Response Factor (RF) deviation (upper plot, calculated as deviation from target amount) and Ion Ratio, IR, (lower plot) for the 10 fg on-column 2,3,7,8-TCDD congener (2.5 fg/µL, 4 µL injection).



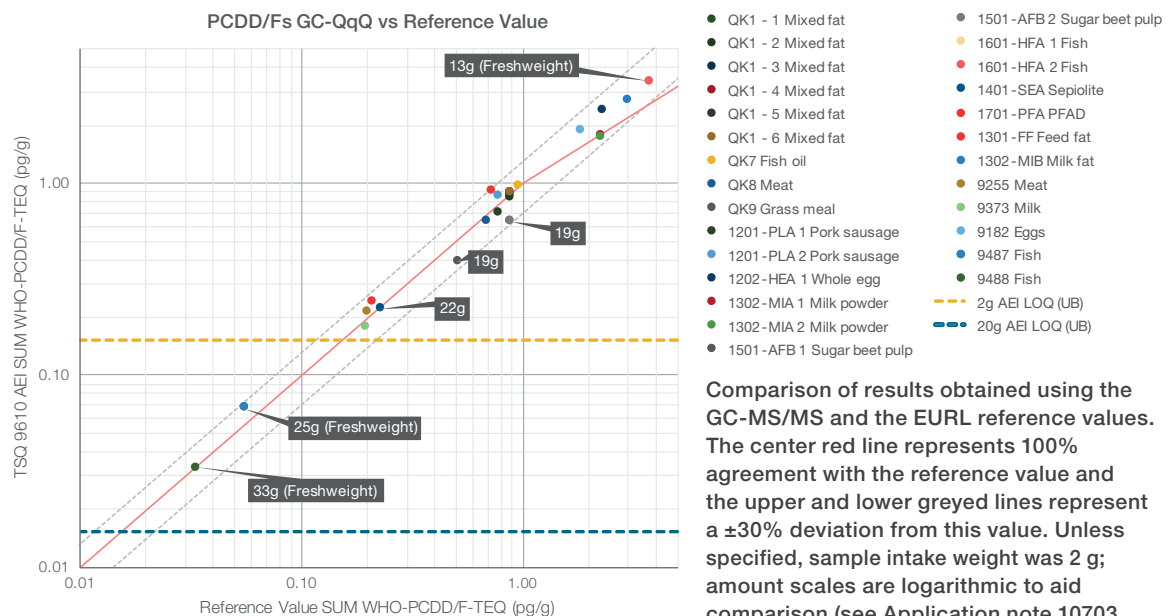
# Increase your laboratory productivity

The analysis of dioxins with GC-MS/MS addresses the high cost and complexity faced by scientists testing food and animal feeds for low levels of dioxins/furans and dl-PCBs. This package includes all components needed – consumables, hardware, software and built-in instrument and data processing methods. All components are pre-configured and tested from your single trusted supplier, Thermo Fisher Scientific.

## Lower cost per sample

The TSQ 9610 triple quadrupole GC-MS/MS system, with fully automated SRM transitions optimization, allows the method to be easily implemented into any laboratory. The system delivers reproducible data at high sensitivity to meet all compliance criteria at the lowest LOQ level. This level of sensitivity enables users to lower sample weights, reducing both the cost of sample preparation and system maintenance.

## Excellent match with EURL results on supplied samples



## Reduce instrument downtime

Using Thermo Scientific™ NeverVent™ technology, planned maintenance, such as changing a column and ion source cleaning, can be performed without venting the mass spectrometer, increasing uptime. NeverVent technology is available with the AEI source.



TSQ 9610 NeverVent AEI system

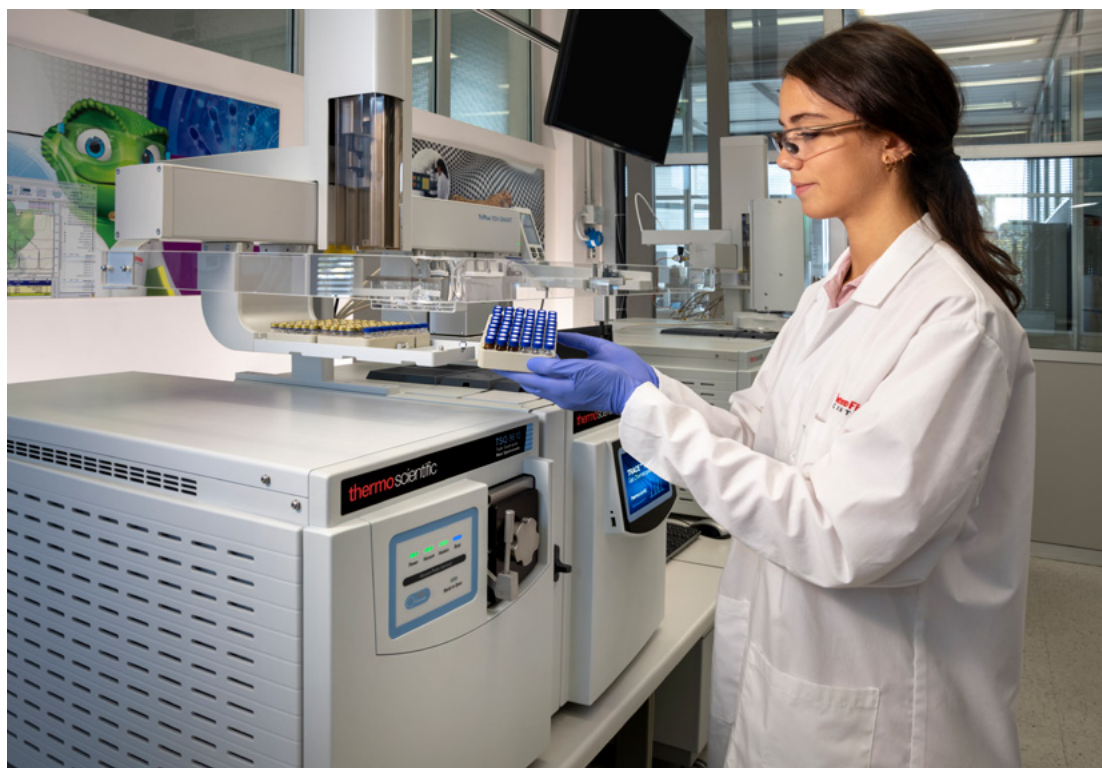


## Quality results with a large variety of sample types and lower sample weights

Impeccable results start with correct GC injection and chromatographic separation. High quality Thermo Scientific™ iConnect™ PTV and SSL injector modules, available with the TRACE 1600 Series GC, ensure a high quality start to the chromatographic separation process even with splitless injection of several microliters. Best-in-class serviceability and ease of operational use add unmatched high lab productivity to the delivery of quality results. The TriPlus RSH SMART Autosampler offers the unique capability for accurate micro-sampling and injection of extracts (few hundred of microliters) resulting from extraction, clean-up and fractionation, thus maximizing results with your most precious samples. Additionally, it brings together technological innovations through SMART consumables ID recognition and usage tracking, offering a fully documented usage-based approach for consumable management and operation traceability.



Accurate micro-sampling and injection



TRACE 1600 GC coupled with the TriPlus RSH SMART Autosampler and TSQ 9610 GC-MS/MS system

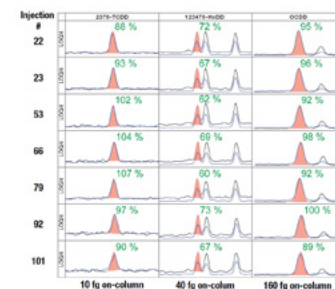


## Rapid and consistent implementation

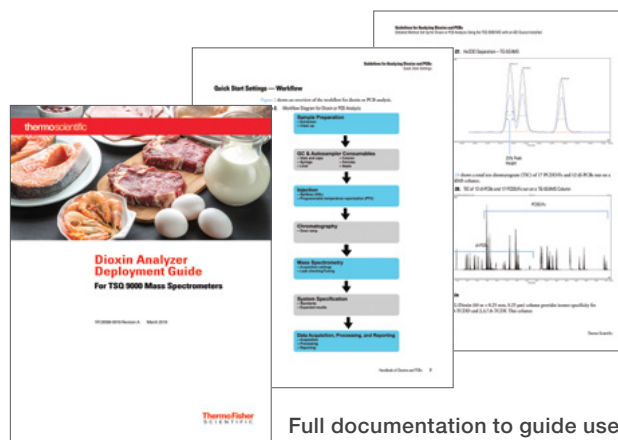
Included with the package are documents and quality check standards to assist the rapid and consistent implementation of this workflow in the lab. The document guides the user step by step through all phases to implement a pre-configured method or to customize a new user-defined method.

The deployment guide is based on an extended validation undertaken to test the suitability of GC-MS/MS, especially for the long-term routine analysis of hundreds of samples. Successful validation of method performance criteria (LOQ, precision, accuracy and calibration) was carried out using three different TSQ 9610 AEI GC-MS systems, in three geo-locations, providing perfectly aligned results. This validation also demonstrated that implementation of the method could be deployed with ease in any laboratory across the world—giving piece of mind to analysts wanting to quickly integrate the analysis of dioxins into their laboratory.

## LOQ repeatability during the UK-based validation



Overlaid extracted ion chromatograms are displayed (quantification and confirmation ions) for selected TCDD, HxCDD, and OCDD congeners. IRs (as displayed in green) and RRFs were within the allowable tolerances.



Full documentation to guide user step-by-step through all phases of this workflow



## Excellent chromatographic separation for dioxin analysis

The proprietary phase of the Thermo Scientific™ TraceGOLD™ TG-Dioxin Capillary GC Column provides excellent separation of toxic dioxin, furan and PCB congeners within 45 minutes. This is critical to eliminate any quantitation errors resulting from co-elution of critical pairs of congeners. The TG-Dioxin column also facilitates compliance with all required chromatographic quality performance criteria.

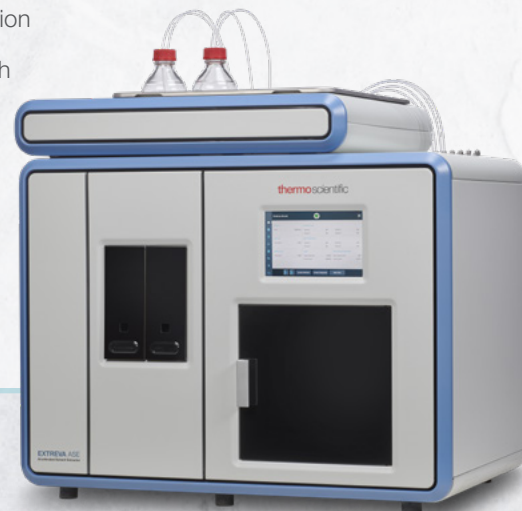


## Extract more efficiently with walk-away automation from sample to vial

The Thermo Scientific EXTREVA ASE Accelerated Solvent Extractor is the perfect partner for your chromatography. This fully automated system combines the extraction and evaporation capabilities in one instrument, providing true walk-away automation for unattended operations and high productivity for any laboratory.

### EXTREVA ASE Accelerated Solvent Extractor provides:

- Parallel and serial extraction using up to six solvents allow for maximum flexibility in the daily schedule
- Completely unattended extraction and evaporation of up to 16 samples in one analytical batch
- Patented gas-assisted extraction helps achieve sustainability goals by reducing solvent consumption
- Collection of the extracts in vials and bottles for evaporation to dryness or in easy-to-use assemblies for direct concentration into gas or liquid chromatography vials
- Concentration with fully automated end point detection through artificial intelligence machine vision
- Sample tracking through a 2D bar-code reader



EXTREVA ASE Accelerated Solvent Extractor



# Powerful tools to simplify complexity of dioxin analysis

Chromeleon software is fully scalable, from a single workstation to an enterprise-wide installation, and can provide control of more than 500 modules from Thermo Fisher Scientific and many other vendors, using the same intuitive user interface. Chromeleon CDS simplifies all data processing and reporting using a comprehensive suite of software tools and pre-loaded acquisition, calculation and reporting templates designed to meet EU requirements for confirmatory analysis of dioxin/furan and PCBs—all with ultimate confidence of the highest data integrity and compliance-ready data processing.



## Error-free execution of routine analysis

The eWorkflow™ procedures provide a pre-loaded template that captures the unique aspects of a chromatography workflow and guides the operator through a minimal number of choices needed to create a finalized sequence with predefined files and a well-defined method structure. The dioxin analysis eWorkflow includes all pre-optimized SRM transitions, isotope dilution calculation and reporting templates for an error-free execution of the analysis to meet compliance requirements.

## Interactive results pane with real-time updates

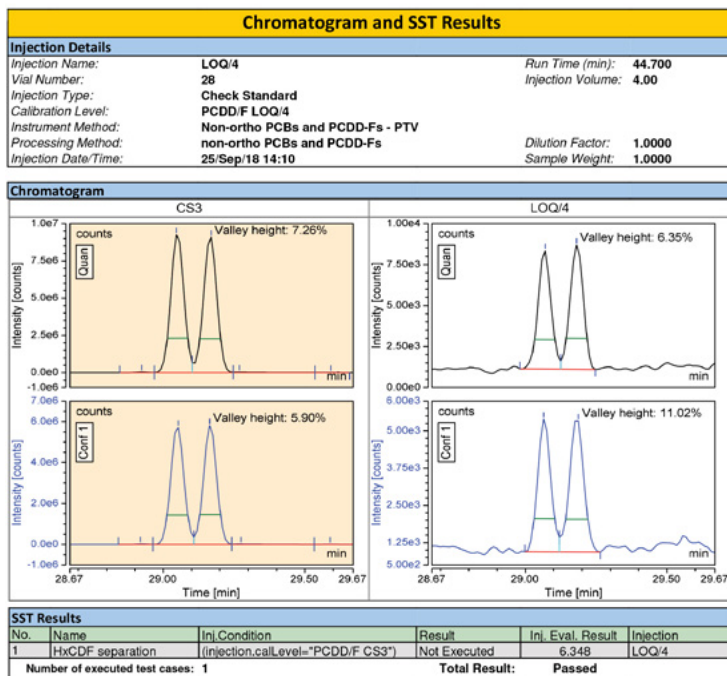
Interactive results pane showing ISTD recovery and ion ratio deviation (flagged red if outside limits) and upper, middle and lower-bound congener specific results. Sum WHO-PCDD/F-TEQ result and flag to indicate above/below maximum limit (top right). Ion ratio deviation and congener specific contribution to the WHO-PCDD/F-TEQ (bottom right).



## Compliance control at a glance

Compliance tools are available in the results pane and dynamically updated during the data acquisition for easy and immediate checking of results, thus saving time. This template shows for instance, internal standard (ISTD) recovery and ion ratio deviation, using a color-coded flag to visually highlight compliance/noncompliance throughout the sequence. Dynamically updated calculation results for sample Toxicity Equivalent (TEQ) are also shown and color flagged for faster action in case the results are outside of the acceptable limits.

## System suitability test report

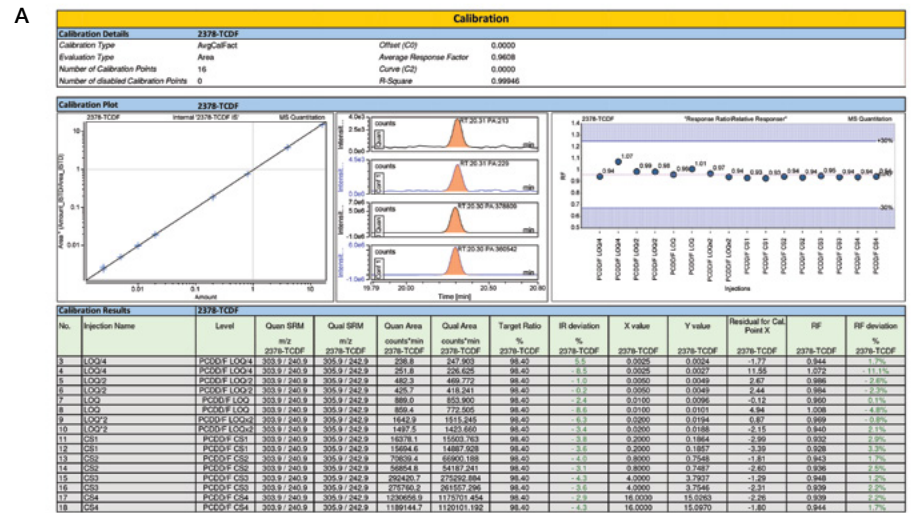


System suitability results built into the method allow for intelligent run control, ensuring samples are only analyzed if the system passes specification, saving repeat analysis time, acquisition and processing of non-compliant data

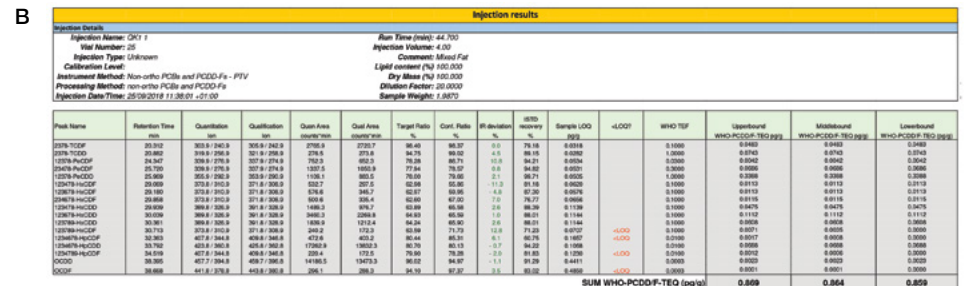
## Built-in reporting tool

To simplify data reporting, eWorkflow offers a comprehensive template that includes the required results and calculations to meet all quality and compliance requirements. This includes recovery for <sup>13</sup>C-labeled standards, ion ratio, sum parameters, and LOQ flagging amongst other features. If needed, the Report Designer enables further customization to meet all reporting and charting requirements.

## Comprehensive calibration report



## Comprehensive sample report template



A. Key information includes average response factor, response factor deviation and ion ratio  
 B. Key results include <sup>13</sup>C-labeled standards recovery, ion ratio, sum parameters, LOQ flagging

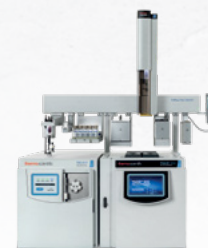
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Orbitrap Exploris GC  
mass spectrometer

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Thermo Scientific  
TSQ 9610 GC-MS/MS  
system

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DFS Magnetic Sector  
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