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Streamline

compliance, productivity and robustness for anionic pesticides analysis with an IC-MS/MS workflow

Thermo Scientific Anionic Pesticides Explorer



Anionic Pesticides Explorer: compliance, productivity and robustness The Thermo Scientific[™] Anionic Pesticides Explorer is an integrated IC-MS/MS workflow. In a single analysis, it addresses the challenge of obtaining reliable quantitation of low concentrations of polar anionic pesticides, such as glyphosate, glufosinate, fosetyl and metabolites, without the need for derivatization.

This analytical workflow is delivered as an off-the-shelf package offering fast implementation and optimum performance for routine testing laboratories. This workflow includes all instruments, software, necessary consumables, suitability check standard and a detailed deployment guide for fast implementation, higher productivity and consistent high-level performance during routine analysis.

For routine laboratories, the Anionic Pesticides Explorer offers:

- Compliance with regulations and method performance guidelines
- Productivity by consolidation of multiple methods into one analysis
- **Robustness** underpinned by the high capacity and high matrix tolerance of anion exchange columns enabling routine analysis of analytes at low concentration, even in complex matrices







Thermo Scientific Dionex Integrion HPIC system coupled with Thermo Scientific TSQ Altis triple-stage quadrupole mass spectrometer

Full compliance with EU criteria at the lowest LOQ level

Gain cost-effective high sample-throughput for monitoring maximum residue levels and tolerance levels of anionic polar pesticides in food samples. To support the validity of data reported, testing laboratories are required to demonstrate compliance with method performance criteria. Leveraging benchmark sensitivity of the Thermo Scientific[™] TSQ[™] Altis triple-stage quadrupole LC-MS/MS system, the Anionic Pesticides Explorer provides the confidence to meet all EU SANTE/11813/2017 compliance criteria at the LOQ levels.

Performance criteria



VALIDATION PARAMETERS



EU compliance criteria at the LOQ levels according to SANTE/11813/2017

Convenient, easy, and effective: Modified QuPPe sample extraction

The most popular extraction method for polar pesticides is the original Quick Polar Pesticides Extraction (QuPPe) method based on the extraction with methanol/water, without liquid/liquid partition or solid phase extraction clean-up. Consequently, the extracts can contain high levels of co-extractives that can contaminate the system and suppress the MS response.

The Modified QuPPE sample preparation method, with cartridge SPE clean-up, provides a time-saving, yet extremely effective approach for the extraction and clean-up of polar anionic pesticide residues in food matrices. Pre-validated sample preparation procedures are included for wheat, leek, and baby food matrices. With the Explorer kit, users can easily extract and analyze samples with confidence.







Summary of recovery data



% Recovery at 10 ng/g in different sourced leek samples using procedural standard calibration (n=5 per sample; RSD% <9%). Full compliance with EU SANTE guideline criteria

The power of ion chromatography



Thermo Scientific Dionex Integrion HPIC system

Optimized for anionic analysis

Ion chromatography with electrolytic ion suppression coupled to MS (IC-MS/MS) offers a number of advantages for the multi-residue analysis of polar anionic pesticides and their metabolites without the need for derivatization.

The metal-free IC system eliminates the issue of chelation caused by metal ions leaching from LC systems and provides excellent chromatographic retention and resolution in a wide range of matrices.

Automated eluent generation (EG) eliminates error-prone manual eluent preparation to achieve better method reproducibility

Optimized system components

- PEEK configuration
- No metals contamination of column
- No chelation of analytes

Maximum flexibility and ease of use

- Electrolytic eluent generation
- Reproducible KOH gradients
- Reagent free—just-add-water technology



Excellent chromatographic separation for polar anionic pesticides

Expand scope, increase robustness and reduce method variability

Polar anionic pesticides have poor retention in reversed-phase LC-MS/MS, which is widely used for multi-residue determination of pesticides in food. Pre- or post-column derivatization can increase chromatographic retention and selectivity for glyphosate and glufosinate, but is not generally favored because of the limited scope, additional labor, and high method variability.

Alternative approaches to achieve greater retention of wider-range polar compounds have included ion-pair reversed-phase LC, HILIC and graphitized carbon columns, with some success. By contrast, ion exchange chromatography with post column ion suppression provides even more control of retention and chromatographic resolution. Furthermore, the proven robustness of high capacity ion exchange columns which permit higher sample loading and lower LOQs for even the most complex samples.

counts





Peak shapes of Fosetyl-Al and Perchlorate after 500 injections of matrix

Perchlorate





Thermo Scientific[™] Dionex[™] IonPac[™] AS19-4µm 2 × 250 mm IC column

Rapid and consistent implementation

Included with the Anionic Pesticides Explorer are documents and quality check standards to assist the rapid and consistent implementation of this workflow in the laboratory. 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 IC-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 the Dionex Integrion HPIC system coupled with the TSQ Altis triple-stage quadrupole mass spectrometer, in multiple geo-locations, providing perfectly aligned results. This validation also demonstrates 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 Anionic Pesticides Explorer into their laboratory.



Powerful tools to simplify complexity of anionic pesticides analysis

Error-free execution of routine analysis

Thermo Scientific[™] Chromeleon[™] 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 Anionic Pesticides eWorkflow includes all pre-optimized SRM transitions and reporting templates for an error-free execution of the analysis to meet compliance requirements.





Five clicks to success: TraceFinder software

Thermo Scientific[™] TraceFinder[™] software includes pre-optimized SRM transitions; ability to quantitate and identify the targeted analytes; streamlined data review; customized, editable report templates; and automaticallygenerated reports—specifically tailored for pesticides applications. From data acquisition to the final report, TraceFinder software makes workflows fast and simple.



Superior sensitivity and confident quantitation: TSQ Altis mass spectrometer

The TSQ Altis triple-stage mass spectrometer enables food safety testing laboratories to address regulatory requirements with confidence and ease. Users become productive quickly with built-in automated compound optimization and application-specific methods and reports. Outstanding sensitivity in the negative ion mode permits simultaneous quantitation of 15 compounds at regulatory levels. The ability to change the ion transfer tube without venting simplifies maintenance and reduces downtime.



Enhanced productivity from day one

All instrument components, anion exchange column, system suitability check standard solutions, software and comprehensive user guidelines are fully optimized for seamless implementation immediately after installation. Data calculation and automatic generation of results are made easier through the Chromeleon CDS and TraceFinder 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. Thus, giving back to the user, valuable time to be invested in 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 high-capacity anion exchange columns provide extremely high tolerance to the matrix, enabling the user to set up sample sequences with hundreds of injections with the confidence that it will deliver consistent and trusted results. 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, tuning or analytical column cleaning.



Repeatability and stability



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The most comprehensive portfolio for pesticide analysis

In addition to the IC-MS, Thermo Fisher Scientific offers complementary technology for the analysis of pesticides. Each solution has specific advantages and collectively offers the most comprehensive portfolio available on the market.



TSQ triple-stage quadrupole LC-MS/MS

Thermo Scientific[™] TSQ Altis[™], TSQ Quantis[™] and TSQ Fortis[™] LC-MS systems provide LODs and LOQs unrivalled in their class. Each offers rugged and reliable operation 24/7, regardless of sample type or matrix complexity. The pre-tested and pre-validated Pesticides Explorer is available for over 400 pesticides to get started from day one.



Orbitrap LC-MS/MS

The sensitivity, selectivity, flexibility and ease of use provided by hybrid quadrupole-Orbitrap mass spectrometers has genuinely set the standard for non-targeted screening and the targeted quantitation and identification of pesticides. It simplifies method development, saving time and decreasing costs, while reliably delivering unsurpassed results.



TSQ triple quadrupole GC-MS/MS

Satisfy your current and future analytical needs for pesticide residues testing with truly unstoppable performance. The Thermo Scientific[™] TSQ[™] 9000 triple quadrupole GC-MS/MS system delivers high sensitivity with routine-grade robustness and maximum uptime. With pre-optimized methods, easy-to-use routine workflows and powerful reporting tools designed for optimal productivity, you can achieve quality results for pesticides residues on time, every time.



Orbitrap GC-MS/MS

The Thermo Scientific[™] Q Exactive[™] and Exactive[™] GC systems bring the power of HRAM to routine pesticides analysis. Non-targeted full scan acquisition and comprehensive libraries enable screening and quantitative workflows which provide the highest confidence in the detection, quantitation and identification of pesticide residues, even in the most complex samples.

Find out more at thermofisher.com/anionicpesticides

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