Application brief | 004196

Food safety

Precision pesticide residue detection in food: Unleashing the power of dual channel LC - Orbitrap Exploris EFOX mass detector

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Keywords

Pesticide residues analysis, QuEChERS, targeted quantitation, HRMS, Orbitrap mass analyzer, food analysis, organic food contaminants, EURL pesticides list, EFOX

Application benefits

- **Combine quantitation and screening capabilities:** Precise quantitation of an extensive range of pesticide compounds using full-scan high-resolution acquisition, enabling both targeted and suspect screening, with capabilities for retrospective analysis.
- **Regulatory compliance:** Exceptional sensitivity, selectivity, repeatability, and robustness, ensuring consistent and accurate results to meet stringent quality control criteria.
- **Quality:** Engineered to meet stringent quality control criteria, including EC SANTE guidelines.[1]
- **Simple data processing and time savings:** Simplifies method development by using full-scan data acquisition, thus eliminating the need to experimentally determine SRM transitions or maintain narrow retention time windows for a large number of compounds.

Goal

To demonstrate the quantitation capabilities of the Thermo Scientific™ Orbitrap Exploris™ EFOX Mass Detector in Full Scan mode for analyzing pesticide residues in acetonitrile extracts. The analytical qualification of the method is demonstrated with results on the limit of quantitation, linearity, reproducibility, and robustness. This method is aimed at food analysis.

Introduction

The World Health Organization reports that over one thousand different pesticides are used to protect crops from pests, boost yields, and reduce deterioration of agricultural products during post-harvest storage and transportation. However, improper pesticide use can contaminate the food supply, making it crucial to define and monitor pesticide residue targets to protect consumer health, support trade, and establish food regulatory controls.

As a result, laboratories must develop methods to detect, accurately identify, and quantify hundreds of different pesticides and their transformation products across various sample matrices, in compliance with maximum residue levels (MRLs) set by regulatory authorities.

Therefore, it is essential that workflows cover a broad range of pesticides, are sensitive and robust, and are as productive and efficient as possible to achieve regulatory compliance while meeting business goals such as return on investment (ROI), sample turnaround times, and cost-per-sample targets.

Analytical approach and methodology

Liquid chromatography coupled with mass spectrometry provides high sensitivity and specificity for detecting a wide range of pesticide compounds. Leveraging the high resolution and sensitivity of the Orbitrap Exploris EFOX mass detector, the analytical method has been developed with a low-volume food extract injection to ensure robustness while complying with regulatory limits of quantitation (LOQs). The strong solvent loop allows direct injection of QuEChERS extracts (acetonitrile) and reduces sample preparation time, as neither dilution nor reconstitution steps are required. The strong solvent loop also improves peak shape and reproducibility (stable retention times), given the highly aqueous initial mobile phase conditions, by reducing solvent mismatch effects. Using our dual channel LC system with two different column geometries for dedicated gradients, positive and negative compounds elute separately from each other. This maximizes overall sensitivity of the method as constant polarity switching is not required. The Thermo Scientific™ Vanquish™ Duo System and Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) streamline this process, delivering a combined data file for compounds analyzed in both positive and negative modes, thereby facilitating data processing.

Workflow method performance and package

This application brief outlines our method for quantifying 577 pesticides (Table A1 in the Appendix). Method performance is evaluated based on the LOQ, linear dynamic range, accuracy, precision, and robustness with real sample extracts.

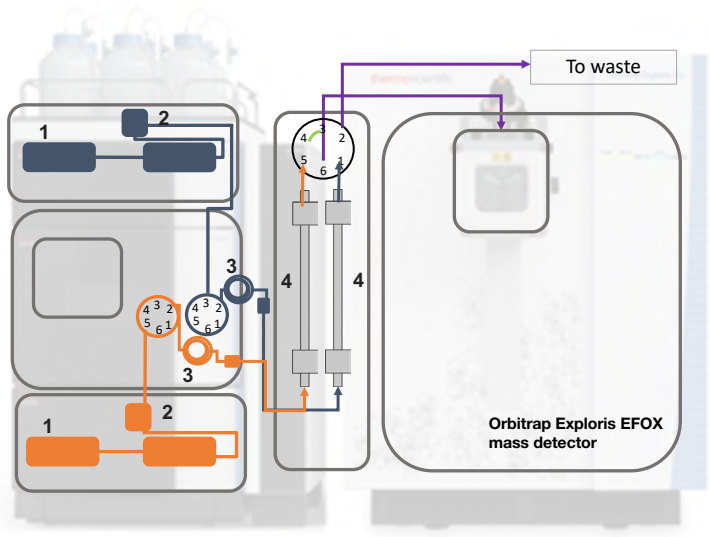

Figure 1. System fluidic configuration used for pesticides analysis: Binary pump (1), Capillary static mixer (2), Strong solvent loop (3), Analytical column (4).

Table 1. References of configuration utilized for pesticides analysis.

Cat. No.	Instrument
VF-P10-A-01	Thermo Scientific™ Vanquish™ Flex Binary UHPLC Pump
VF-A40-A-02	Thermo Scientific™ Vanquish™ Dual Split Sampler
VH-C10-A-03	Thermo Scientific™ Vanquish™ Flex Column Compartment
BRE725557	Orbitrap Exploris EFOX Mass Detector
6044.3870	Thermo Scientific™ Vanquish™ 35 µL Mixer Set, Vanquish F Pumps
6036.2200	Thermo Scientific™ Strong Solvent Loop
25002-152130	Thermo Scientific™ Hypersil GOLD™ C18 Column, 150 × 2.1 mm, 1.9 µm
25002-102130	Thermo Scientific™ Hypersil GOLD™ C18 Column, 100 × 2.1 mm, 1.9 µm

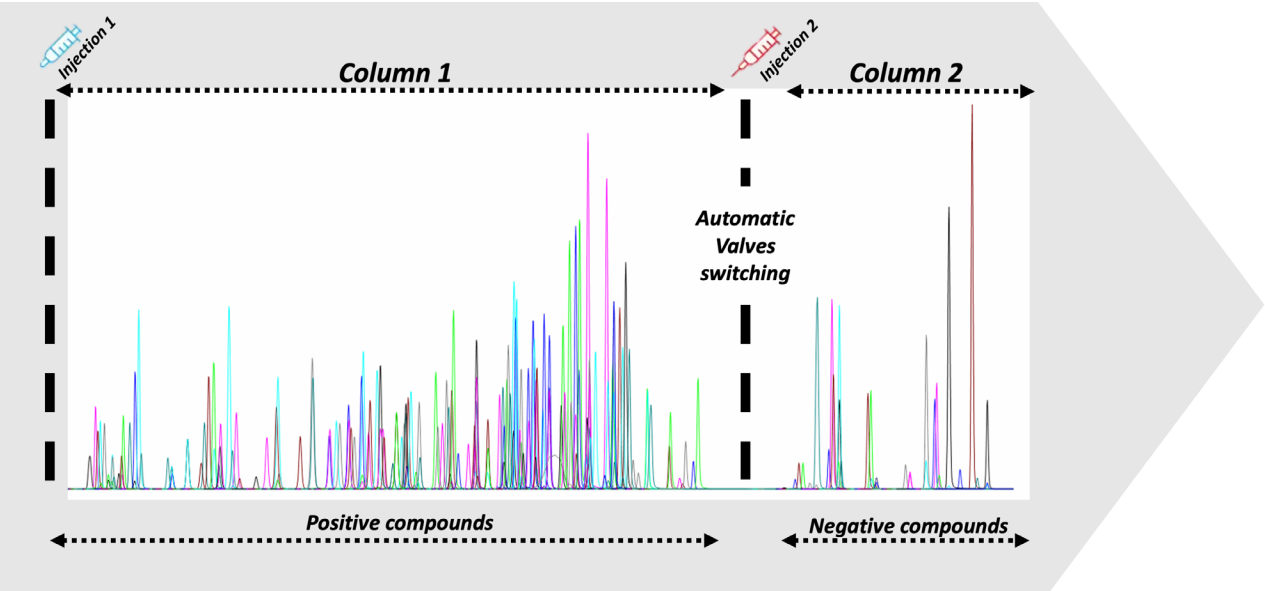

Figure 2. The unique Vanquish Duo system provides two independent binary pumps, injection ports, and flow paths. One pump was dedicated to positive pesticides analysis gradient and the second was dedicated to negative pesticides analysis. Samples are alternately injected in column N°1 and column N°2 thanks to automatic valves switching, resulting in only a single flow directed to the MS.

Our workflow is comprehensively documented and includes:

- A standard operating procedure (SOP) that specifies hardware, viper, consumables, and reagents.
- A software package that includes the instrument method and processing methods, with view settings for guided, fast, and compliant data review and reporting using the Chromeleon 7.3.2 CDS.
- A data set featuring examples and performance demonstrations.

Experimental

Instrument configuration and method

The LC setup consists of two Thermo Scientific™ Vanquish™ Flex UHPLC Binary Pumps connected each to one of the two injection valves within the Thermo Scientific™ Vanquish™ Duo Autosampler. The Orbitrap Exploris EFOX mass detector MS is used to obtain HRMS data in Full Scan mode and analyze the combined gradient runs for dedicated injections of positive and negative ionizing pesticides in the same data file. This is achieved automatically through Chromeleon CDS and by two separate injections in time of the same sample, each onto an analytical column with a different geometry.

Table 2. Instrument parameters.

Parameter	Value
Column 1 (Positive mode injection)	Hypersil GOLD C18 Selectivity, 150 × 2.1 mm, 1.9 µm
Column 2 (Negative mode injection)	Hypersil GOLD C18 Selectivity, 100 × 2.1 mm, 1.9 µm
Mobile phase A	0.1 mM ammonium fluoride and 0.1% formic acid in water
Mobile phase B	0.1 mM ammonium fluoride and 0.1% formic acid in methanol
Total run time (Injection POS + NEG)	19.5 min
Injection volume	1 µL
Acquisition type	Full Scan
Scan range	*m/z* 70–1,000
Resolution	60,000
Source type	HESI
LC peak width	4 s

The mobile phases were the same for both injections (positive and negative mode scan). It simplifies operation and minimizes the risk of preparation errors.

The same mobile phase (combination of water and methanol) and comparable gradients were used for both injections. A switching valve in the column compartment directed a single LC flow to the mass spectrometer, timed in accordance with the elution of compounds of interest from either one or the other column, resulting in a single combined MS data file (Figure 2). The hardware configuration schemes can be seen in Figure 1 and Table 1. Table 2 recaps the main instrument parameters.

Method qualification results

To verify that the method is suitable for analyzing food samples and to evaluate its reliability, an analytical qualification of the method was conducted.

Sample preparation

The 577 pesticides were divided into three different mixtures and were prepared in acetonitrile. Using these three pesticides mixtures, three distinct calibration curves were prepared in acetonitrile with concentrations ranging from 1 ppb up to 100 ppb.

All custom-made commercial pesticide solutions were purchased from Cluzeau Info Labo and Analytical Standard Solutions (A2S) laboratory.

For the robustness study, three different matrices (apple, tomato, carrot) were extracted using the Thermo Scientific™ QuEChERS AOAC 2007.01 Method Extraction Kit (Cat. No. S1-15-AOAC-POT). A cleanup step is necessary before injection using the Thermo Scientific™ QuEChERS AOAC 2007.01 Method Clean-Up Kit (Cat. No. S2-2-GFV-AOAC-KIT).

Results of qualification

Linearity

Linearity was assessed by injecting five calibration sets with varying parameters such as operator and day for the preparation of each set of solutions.

Each compound was qualified using at least five different calibration curves, and each curve met the validation criteria ($R^2 > 0.990$ and a relative amount deviation of less than 40% for the LOQ and less than 20% for other levels).

Calibration curves were produced in the range of 1–100 ppb, with the lower limit varying (1, 2, 5, or 10 ppb) depending on the compound.

Examples of compound calibration curves are presented in Table 3 and Figure 3, while the charts for relative amount deviation checks are shown in Figure 4.

Table 3. Results of calibration qualification for eight representative pesticides.

Name	CAS number	Polarity	Calibration type	Range (ppb)
Pymetrozine	123312-89-0	Positive	Lin, WithOffset, 1/A	1–100
3-OH-carbofuran	16655-82-6	Positive	Lin, WithOffset, 1/A	1–100
Chlorsulfuron	64902-72-3	Positive	Quad, WithOffset, 1/A	1–100
Valifenalate	283159-90-0	Positive	Lin, WithOffset, 1/A	1–100
Dalapon	75-99-0	Negative	Quad, WithOffset, 1/A	5–100
Bromoxynil	1689-84-5	Negative	Lin, WithOffset, 1/A	1–100
Fenoxaprop-p	113158-40-0	Negative	Quad, WithOffset, 1/A	2–100
Dinoterb	1420-07-1	Negative	Quad, WithOffset, 1/A	1–100

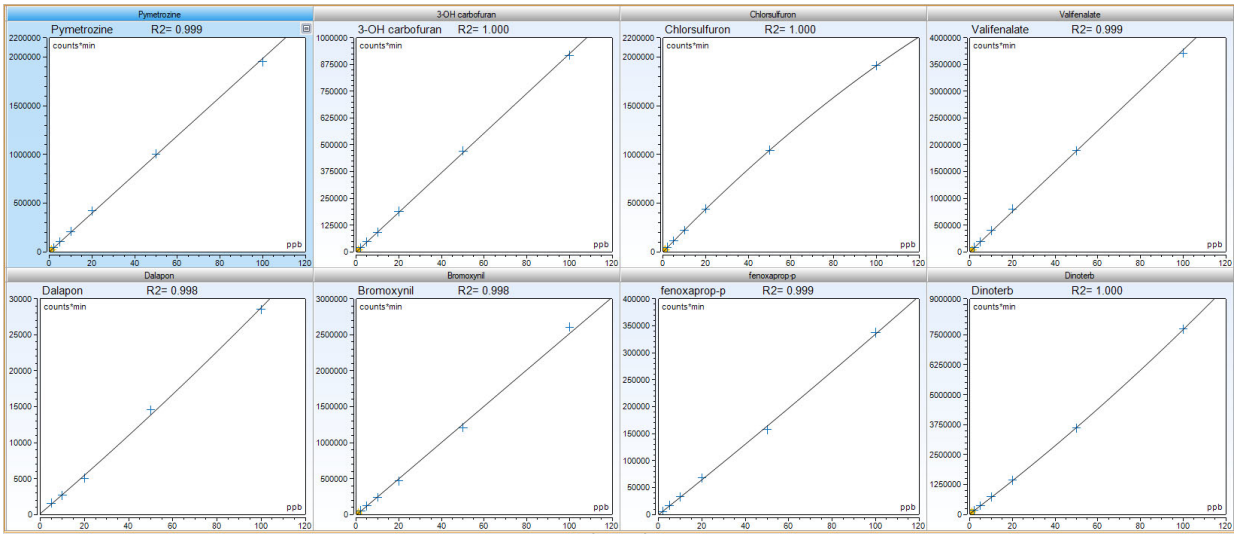

Figure 3. Calibration curves from 1 ppb or 2 ppb or 5 ppb to 100 ppb, for eight representative pesticides.

Figure 4 shows the relative amount deviation for each of the five calibration standards and each calibration level (purple squares) across repeated curves. The white area represents the acceptable deviation limit (%), while the red area indicates deviations beyond the tolerance limit. The criteria of less than 40% deviation at LOQ and less than 20% for other levels were consistently met in the calibration curve.

A

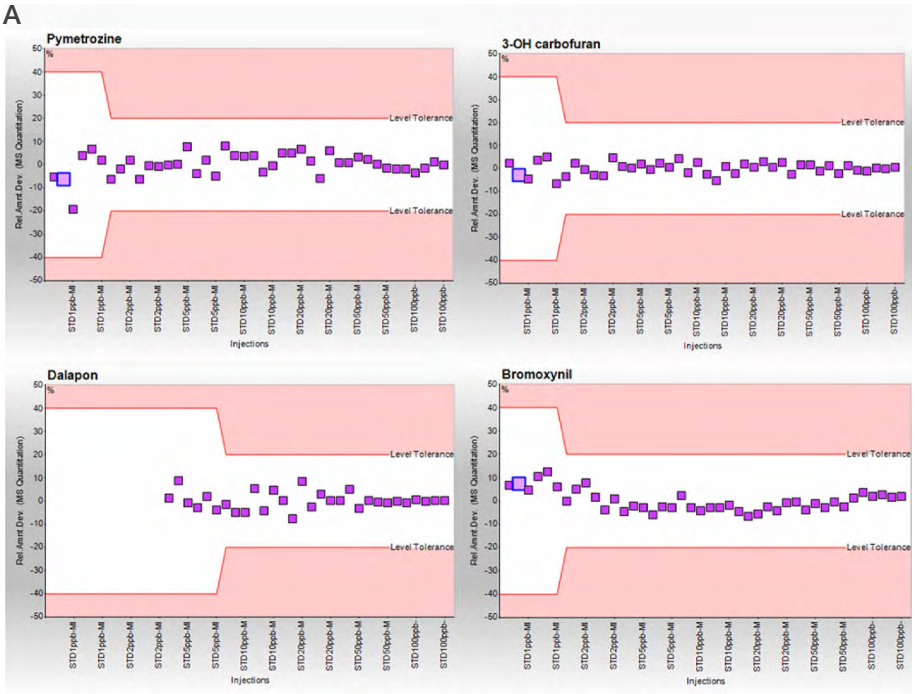

Figure 4A. Example of charts illustrating the relative amount deviation according to criteria for eight representative pesticides. The LOQ is set at 1 ppb for pymetrozine, 3-OH-carbofuran, chlorsulfuron, valifenalate, bromoxynil, and dinoterb. The LOQ is set at 5 ppb for dalapon and at 2 ppb for fenoxaprop-p.

B

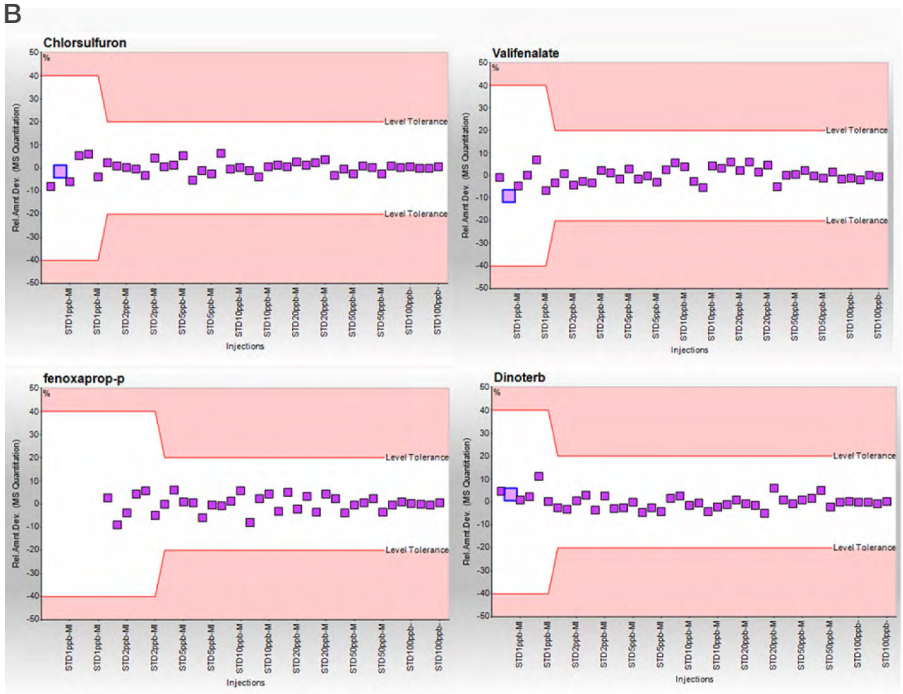

Figure 4B. Example of charts illustrating the relative amount deviation according to criteria for eight representative pesticides. The LOQ is set at 1 ppb for pymetrozine, 3-OH-carbofuran, chlorsulfuron, valifenalate, bromoxynil, and dinoterb. The LOQ is set at 5 ppb for dalapon and at 2 ppb for fenoxaprop-p.

Limit of quantification

The chromatograms in Figures 5, 6, and 7 illustrate examples of eight representative pesticides at the LOQ in solvent, showcasing excellent resolution and peak shape. Each LOQ was reproduced and measured for stability using five replicate injections (Table 4).

The overlays correspond to the base peak plus the second most intense ion in the full scan, which can be an adduct ion, a fragment ion, or an isotope ion depending on the specific structural and chemical characteristics of the selected pesticide.

Table 4. Results of stability and repeatability for eight representative pesticides.

Name	CAS number	Polarity	LOQ (ppb)	RSD (n=5)
Pymetrozine	123312-89-0	Positive	1	3%
3-OH-carbofuran	16655-82-6	Positive	1	1%
Chlorsulfuron	64902-72-3	Positive	1	4%
Valifenalate	283159-90-0	Positive	1	5%
Dalapon	75-99-0	Negative	5	15%
Bromoxynil	1689-84-5	Negative	1	2%
Fenoxaprop-p	113158-40-0	Negative	2	6%
Dinoterb	1420-07-1	Negative	1	2%

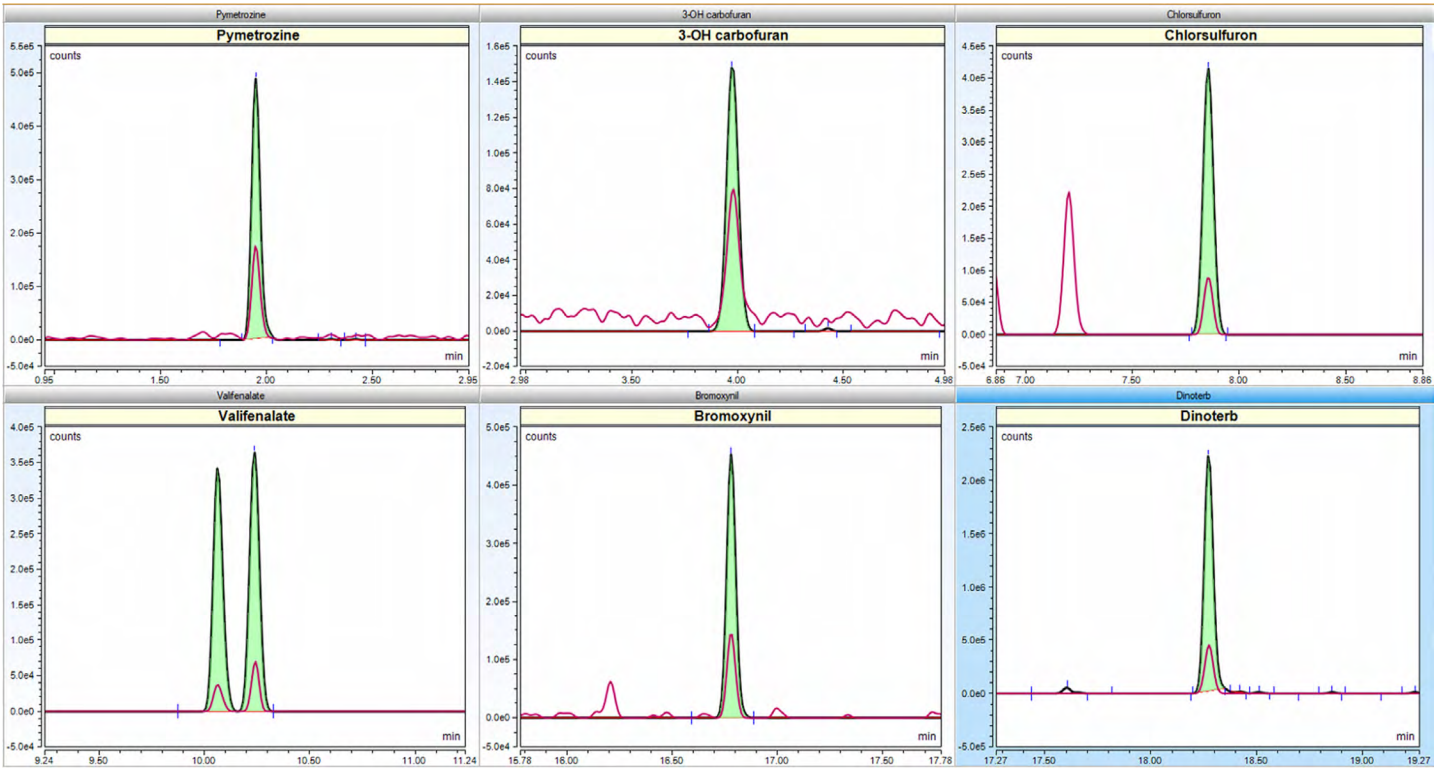

Figure 5. Overlaid full scan at the LOQ (1 ppb) for pymetrozine, 3-OH-carbofuran, chlorsulfuron, valifenalate, bromoxynil, and dinoterb.

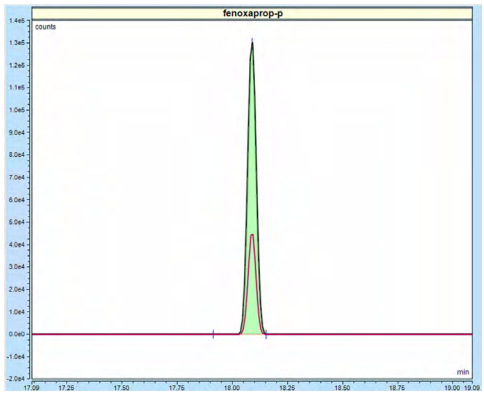

Figure 6. Overlaid full scan at the LOQ (2 ppb) for fenoxaprop-p.

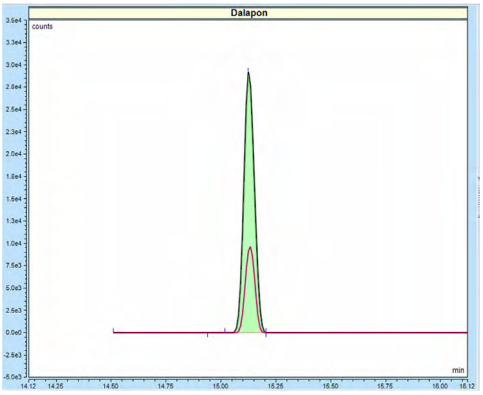

Figure 7. Overlaid full scan at the LOQ (5 ppb) for dalapon.

Robustness

The method robustness was assessed by injecting a QC in solvent at the LOQ after every 10 matrix samples (extract of apple, tomato, and carrot). After 40 consecutive injections, the data presented in Table 5 demonstrated good robustness for injections on both methods (positive and negative injection). The quantification results remained within acceptable accuracy limits, and all relative amount deviations (Rel. Amnt. Dev.) were clearly below 40%.

It is important to note that no maintenance or MS tuning was conducted during the evaluation of robustness. The method is robust against matrix load as shown by continuous injections over several days.

Table 5. Stability of three different LOQs for an example of eight pesticides for both methods (positive and negative) under robustness test.

Name	CAS number	Polarity	LOQ (ppb)	Rel. Amnt. Dev. (%) LOQ-R1	Rel. Amnt. Dev. (%) LOQ-R2	Rel. Amnt. Dev. (%) LOQ-R3	Rel. Amnt. Dev. (%) LOQ-R4
Asulam	3337-71-1	Positive	1	4	-6	11	3
Phosmet-oxon	3735-33-9	Positive	1	-4	-2	-6	1
Simeconazole	149508-90-7	Positive	1	1	0	6	2
Flubendiamide	272451-65-7	Negative	1	-3	5	-11	-5
Dodine	2439-10-3	Positive	2	-19	-17	-22	-17
TFNG	207502-65-6	Negative	2	-13	-1	17	9
AvermectineB1a	65195-55-3	Positive	5	-9	-17	22	26
Spinosad (Spinosyn D)	131929-63-0	Positive	5	-20	-23	-26	4

Conclusions

- **Accurate pesticides quantitation:** The method enables the precise quantitation of 577 pesticides using full-scan high-resolution acquisition in a targeted approach. Additionally, this configuration opens the door to suspect screening and provides the capability for retrospective analyses when new pesticides targets are added to regulatory lists.
- **Regulatory compliance:** The method demonstrated the ability to meet the limit of quantification required by regulations. This signifies that our workflow is capable of accurately and precisely determining the presence of pesticides at levels that comply with regulatory standards.
- **Robust method:** Proven robustness with consistent performance across multiple injections and different matrices (apple, tomato, and carrot extract), maintaining accuracy and stability without the need for maintenance or MS tuning.
- **Validated performance:** The method meets stringent validation criteria, including linearity ($R^2 > 0.990$), accuracy, precision, and robustness, with relative amount deviations well within acceptable limits.

For an alternative approach of this workflow, please refer to its twin application brief, run with the Thermo Scientific™ TSQ Altis™ Plus EFOX Edition Mass Spectrometer.

For further information, contact your local commercial representative.

References

1. European Commission. Directorate General for Health and Safety. Guidance document on analytical quality control and method validation procedures for pesticide residues and analysis in food and feed. SANTE/11312/2021. Implemented January 1, 2022. (accessed January 11, 2024)
2. Chromeleon CDS - pesticides solution (accessed January 11, 2024)
3. Thermo Fisher Scientific Application Brief 002783: An advanced integrated GC-MS/MS and LC-MS-MS workflow for the comprehensive analysis of pesticide residues in food

Appendix

Table A1. Pesticides included in the LC-Orbitrap Exploris EFOX mass detector method.

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
2008-58-4	2,6-Dichlorobenzamide	1	1
2686-99-9	3,4,5-Trimethacarb	1	1
584-79-2	Allethrin	5	5
834-12-8	Ametryn	1	1
2032-59-9	Aminocarb	1	1
64249-01-0	Anilofos	10	10
1912-24-9	Atrazine	1	1
86-50-0	Azinphos-methyl	1	1
113614-08-7	Beflubutamid	1	1
71626-11-4	Benalaxyl	1	1
22781-23-3	Bendiocarb	1	1
82560-54-1	Benfuracarb	1	1
15310-01-7	Benodanil	1	1
98730-04-2	Benoxacor	1	1
741-58-2	Bensulide	1	1
29104-30-1	Benzoximate	1	1
149877-41-8	Bifenazate	1	1
55179-31-2	Bitertanol	5	5
188425-85-6	Boscalid	1	1
116255-48-2	Bromuconazole	1	1
23184-66-9	Butachlor	1	1
134605-64-4	Butafenacil	1	1
2008-41-5	Butylate	1	1
95465-99-9	Cadusafos	1	1
63-25-2	Carbaryl	1	1
16118-49-3	Carbetamide	1	1
1563-66-2	Carbofuran	1	1
5234-68-4	Carboxin	1	1
13360-45-7	Chlorbromuron	1	1
1967-16-4	Chlorbufam	5	5
470-90-6	Chlorfenvinphos	1	1
1698-60-8	Chloridazon	1	1
101-21-3	Chlorpropham	1	1
2921-88-2	Chlorpyrifos-ethyl	1	1
5598-13-0	Chlorpyrifos-methyl	1	1
142891-20-1	Cinidon-ethyl	1	1
105512-06-9	Clodinafop-propargyl	1	1
99607-70-2	Cloquintocet-mexyl	1	1
56-72-4	Coumaphos	1	1
535-89-7	Crimidine	1	1
120116-88-3	Cyazofamid	1	1
101205-02-1	Cycloxydim	1	1
52315-07-8	Cypermethrin	1	1
94361-06-5	Cyproconazole	1	1
121552-61-2	Cyprodinil	1	1
1014-69-3	Desmetryn	1	1
333-41-5	Diazinon	1	1
62-73-7	Dichlorvos	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
75736-33-3	Diclobutrazole	1	1
51338-27-3	Diclofop-methyl	1	1
141-66-2	Dicrotophos	1	1
87130-20-9	Diethofencarb	1	1
119446-68-3	Difenoconazole	1	1
35367-38-5	Diflubenzuron	1	1
87674-68-8	Dimethenamid	1	1
66840-71-9	Dimethyl amino sulfotoluidide (DMST)	1	1
149961-52-4	Dimoxystrobin	1	1
83657-24-3	Diniconazole	1	1
957-51-7	Diphenamid	1	1
2497-07-6	Disulfoton sulfoxide	1	1
17109-49-8	Edifenphos	1	1
60207-93-4	Etaconazole	1	1
29973-13-5	Ethiofencarb	1	1
13194-48-4	Ethoprophos	1	1
153233-91-1	Etoxazole	1	1
38260-54-7	Etrimphos	1	1
131807-57-3	Famoxadone	1	1
161326-34-7	Fenamidone	1	1
22224-92-6	Fenamiphos	1	1
60168-88-9	Fenarimol	1	1
120928-09-8	Fenazaquin	1	1
114369-43-6	Fenbuconazole	1	1
3983-45-7	Fenchlorphosoxon	1	1
126833-17-8	Fenhexamid	1	1
3766-81-2	Fenobucarb	1	1
72490-01-8	Fenoxycarb	1	1
67564-91-4	Fenpropimorph	1	1
473798-59-3	Fenpyrazamine	1	1
134098-61-6	Fenpyroximate	1	1
115-90-2	Fensulfothion	1	1
55-38-9	Fenthion	1	1
6552-12-1	Fenthion-oxone	1	1
14086-35-2	Fenthion-oxonsulfone	1	1
3761-42-0	Fenthion-sulfone	1	1
3761-41-9	Fenthion-sulfoxide	1	1
120068-37-3	Fipronil	1	1
120068-36-2	Fipronil sulfone	1	1
158062-67-0	Flonicamid	1	1
79241-46-6	Fluazifop-P-butyl	1	1
131341-86-1	Fludioxonil	1	1
142459-58-3	Flufenacet	1	1
103361-09-7	Flumioxazine	1	1
361377-29-9	Fluoxastrobin	1	1
136426-54-5	Fluquinconazole	1	1
56425-91-3	Flurprimidole	1	1
96525-23-4	Flurtamone	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
85509-19-9	Flusilazole	1	1
958647-10-4	Flutianil	1	1
66332-96-5	Flutolanil	1	1
76674-21-0	Flutriafol	1	1
907204-31-3	Fluxapyroxad	1	1
944-22-9	Fonofos	1	1
2540-82-1	Formothion	1	1
98886-44-3	Fosthiazate	1	1
3878-19-1	Fuberidazole	1	1
65907-30-4	Furathiocarb	1	1
23560-59-0	Heptenophos	1	1
79983-71-4	Hexaconazole	2	2
51235-04-2	Hexazinone	1	1
86598-92-7	Imibenconazole	1	1
24353-61-5	Isocarbofos	1	1
2631-40-5	Isoprocarb	1	1
34123-59-6	Isoproturon	1	1
143390-89-0	Kresoxim-methyl	1	1
2164-08-1	Lenacil	1	1
121-75-5	Malathion	1	1
173662-97-0	Mandestrobin	1	1
1417782-03-6	Mefentrifluconazole	1	1
110235-47-7	Mepanipyrim	1	1
55814-41-0	Mepronil	1	1
57837-19-1	Metalaxyl	1	1
41394-05-2	Metamitron	1	1
67129-08-2	Metazachlor	1	1
125116-23-6	Metconazole	5	5
18691-97-9	Methabenzthiazuron	1	1
62610-77-9	Methacrifos	1	1
950-37-8	Methidathion	1	1
3060-89-7	Metobromuron	1	1
220899-03-6	Metrafenone	1	1
21087-64-9	Metribuzin	1	1
1746-81-2	Monolinuron	1	1
88671-89-0	Myclobutanil	1	1
60397-77-5	N-(2,4-Dimethylphenyl) formamide	1	1
27314-13-2	Norflurazon	1	1
76738-62-0	Paclobutrazol	1	1
2597-03-7	Phenthoate	1	1
2588-03-6	Phorate-sulfoxide	1	1
2310-17-0	Phosalone	10	10
732-11-6	Phosmet	1	1
137641-05-5	Picolinafen	1	1
30614-22-3	Pirimarb desmethyl	1	1
27218-04-8	Pirimicarb-desmethyl-formamido	2	2
29232-93-7	Pirimiphos-methyl	1	1
41198-08-7	Profenofos	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
2631-37-0	Promecarb	1	1
1610-18-0	Prometon	1	1
7287-19-6	Prometryn	1	1
709-98-8	Propanil	1	1
2312-35-8	Propargite	1	1
139-40-2	Propazine	1	1
31218-83-4	Propetamphos	1	1
114-26-1	Propoxur	1	1
23950-58-5	Propyzamide	1	1
189278-12-4	Proquinazid	1	1
52888-80-9	Prosulfocarb	1	1
175013-18-0	Pyraclostrobin	1	1
129630-19-9	Pyraflufen-ethyl	1	1
13457-18-6	Pyrazophos	1	1
55512-33-9	Pyridate	10	10
53112-28-0	Pyrimethanil	1	1
688046-61-9	Pyriofenone	1	1
76578-14-8	Quizalofop-ethyl	1	1
83-79-4	Rotenone	1	1
7286-69-3	Sebuthylazine	1	1
175217-20-6	Silthiofam	1	1
122-34-9	Simazine	1	1
1014-70-6	Simetryn	1	1
283594-90-1	Spiromesifen	1	1
118134-30-8	Spiroxamine	1	1
3689-24-5	Sulfotep	1	1
107534-96-3	Tebuconazole	1	1
119168-77-3	Tebufenpyrad	1	1
83121-18-0	Teflubenzuron	1	1
5902-51-2	Terbacil	1	1
13071-79-9	Terbufos	2	2
33693-04-8	Terbumeton	1	1
5915-41-3	Terbuthylazine	1	1
30125-63-4	Terbuthylazine desethyl	1	1
886-50-0	Terbutryn	1	1
22248-79-9	Tetrachlorvinphos	1	1
112281-77-3	Tetraconazole	1	1
7696-12-0	Tetramethrin	1	1
39184-59-3	Thiofanox-sulfone	1	1
57018-04-9	Tolclofos-methyl	5	5
55219-65-3	Triadimenol	1	1
2303-17-5	Tri-allate	1	1
112143-82-5	Triazamate	1	1
24017-47-8	Triazophos	1	1
41814-78-2	Tricyclazole	1	1
141517-21-7	Trifloxystrobin	1	1
68694-11-1	Triflumizole	1	1
131983-72-7	Triticonazole	1	1
83657-22-1	Uniconazole	1	1
86-86-2	1-Naphthylacetamide	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
93-76-5	2,4,5-T	1	1
94-75-7	2,4-D	2	2
94-82-6	2,4-DB	5	5
95-68-1	2,4-Dimethylaniline	1	1
912654-91-2	4,6-Dihydroxytembotrione	5	5
122-88-3	4-CPA	5	5
135410-20-7	Acetamiprid	1	1
34256-82-1	Acetochlor	1	1
135158-54-2	Acibenzolar-S-methyl	1	1
15972-60-8	Alachlor	1	1
150114-71-9	Aminopyralid	1	1
348635-87-0	Amisulbrom	2	2
140-57-8	Aramite	1	1
1007-28-9	Atrazinedeisopropyl	1	1
65195-55-3	Avermectine B1b	5	5
60207-31-0	Azaconazole	1	1
2642-71-9	Azinphos-ethyl	1	1
131860-33-8	Azoxystrobin	1	1
101-27-9	Barban	1	1
25057-89-0	Bentazone	1	1
60374-42-7	Bentazone-6-hydroxy	10	10
149878-40-0	Bifenazate-diazene	1	1
82657-04-3	bifenthrin	1	1
125401-92-5	Bispyribac sodium	1	1
28772-56-7	Bromadiolone	10	10
33089-74-6	BTS27271 (metabolite of mitraz)	2	2
41483-43-6	Bupirimate	1	1
69327-76-0	Buprofezin	1	1
33629-47-9	Butralin	1	1
128621-72-7	Carfentrazone	1	1
128639-02-1	Carfentrazone-ethyl	1	1
143-50-0	Chlordecone	5	5
1918-13-4	Chlorthiamid	5	5
38083-17-9	Climbazole	1	1
114420-56-3	Clodinafop	1	1
81777-89-1	Clomazone	1	1
210880-92-5	Clothianidin	1	1
21725-46-2	Cyanazine	1	1
1031756-98-5	Cyclaniliprole	1	1
1134-23-2	Cycloate	1	1
122008-85-9	Cyhalofop-butyl	5	5
57966-95-7	Cymoxanil	1	1
66215-27-8	Cyromazine	1	1
533-74-4	Dazomet	1	1
52918-63-5	Deltamethrin	2	2
919-86-8	Demeton-S-methyl	1	1
17040-19-6	Demeton-S-methylsulfone	1	1
13684-56-5	Desmedipham	1	1
2303-16-4	Di-allate	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
1918-00-9	Dicamba	5	5
37764-25-3	Dichlormid	1	1
120-36-5	Dichlorprop	1	1
134-62-3	Diethyl-N'N-toluamide-m (DEET)	1	1
83164-33-4	Diflufenican	1	1
50563-36-5	Dimethachlor	1	1
60-51-5	Dimethoate	1	1
110488-70-5	Dimethomorph	1	1
39300-45-3	Dinocap	2	2
88-85-7	Dinoseb	1	1
122-39-4	Diphenylamine	2	2
2497-06-5	Disulfotonsulfone	1	1
1593-77-7	Dodemorph	1	1
133855-98-8	Epoxiconazole	1	1
759-94-4	EPTC	1	1
563-12-2	Ethion	2	2
26225-79-6	Ethofumesate	1	1
27512-72-7	Ethylchlozate	1	1
80844-07-1	Etofenprox	1	1
31972-44-8	Fenamiphossulfone	1	1
93-72-1	Fenoprop	1	1
74738-17-3	Fenpiclonil	1	1
39515-41-8	Fenpropathrin	1	1
67306-00-7	Fenpropidin	1	1
120067-83-6	Fipronilsulfide	1	1
52756-25-9	Flamprop-methyl	2	2
174514-07-9	Fluazolate	5	5
70124-77-5	Flucythrinate	1	1
162320-67-4	Flufenzine	1	1
2164-17-2	Fluometuron	1	1
239110-15-7	Fluopicolide	1	1
77501-90-7	Fluoroglycofene	1	1
70441-63-3	Fluorophenyl-N-isopropyl	1	1
31251-03-3	Fluotrimazole	1	1
61213-25-0	Flurochloridone	1	1
69377-81-7	Fluroxypyr	10	10
81406-37-3	Fluroxypyr-methylheptyl	1	1
117337-19-6	Fluthiacet-methyl	1	1
69409-94-5	Fluvalinate	1	1
57646-30-7	Furalaxyl	1	1
943831-98-9	Halauxifenmethyl	1	1
35554-44-0	Imazalil	1	1
114311-32-9	Imazamox	1	1
104098-48-8	Imazapic	1	1
81334-34-1	Imazapyr	1	1
138261-41-3	Imidacloprid	1	1
87-51-4	Indolylaceticacid	1	1
144171-61-9	Indoxacarb	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
1689-83-4	Ioxynil	1	1
140923-17-7	Iprovalicarb	1	1
42509-80-8	Isazophos	1	1
25311-71-1	Isofenphos	2	2
99675-03-3	Isofenphos-methyl	1	1
50512-35-1	Isoprothiolane	1	1
163520-33-0	Isoxadifen-ethyl	1	1
77501-63-4	Lactofen	1	1
330-55-2	Linuron	1	1
1634-78-2	Malaoxon	1	1
94-74-6	MCPA	1	1
94-81-5	MCPB	5	5
2595-54-2	Mecarbam	1	1
135590-91-9	Mefenpyr-diethyl	1	1
2032-65-7	Methiocarb	1	1
51218-45-2	Metolachlor (+ S-Metolachlor)	1	1
1129-41-5	Metolcarb	1	1
7786-34-7	Mevinphos	1	1
2212-67-1	Molinate	1	1
6923-22-4	Monocrotophos	1	1
15299-99-7	Napropamide	1	1
121451-02-3	Noviflumuron	1	1
63284-71-9	Nuarimol	1	1
1113-02-6	Omethoate	1	1
248593-16-0	Orysastrobin	1	1
39807-15-3	Oxadiargyl	1	1
19666-30-9	Oxadiazon	1	1
77732-09-3	Oxadixyl	1	1
30558-43-1	Oxamyl-oxime	1	1
1003318-67-9	Oxathiapiprolin	1	1
53716-50-0	Oxfendazole	1	1
311-45-5	Paraoxon	1	1
950-35-6	Paraoxon-methyl	1	1
1114-71-2	Pebulate	1	1
66246-88-6	Penconazole	1	1
66063-05-6	Pencycuron	1	1
40487-42-1	Pendimethalin	1	1
106700-29-2	Pethoxamid	1	1
13684-63-4	Phenmedipham	1	1
26002-80-2	Phenothrin	2	2
298-02-2	Phorate	10	10
2600-69-3	Phorate-oxon	1	1
13171-21-6	Phosphamidon	1	1
1918-02-1	Picloram	2	2
117428-22-5	Picoxystrobin	1	1
243973-20-8	Pinoxaden	1	1
51-03-6	Piperonyl butoxide	1	1
23103-98-2	Pirimicarb	1	1
23505-41-1	Pirimiphosethyl	1	1
67747-09-5	Prochloraz	1	1
139542-32-8	Prochloraz desimidazole-amino BTS44596	1	1
1918-16-7	Propachlor	1	1
24579-73-5	Propamocarb	2	2
111479-05-1	Propaquizafop	1	1
122-42-9	Propham	1	1
60207-90-1	Propiconazole	1	1
86763-47-5	Propisochlor	1	1
178928-70-6	Prothioconazole	5	5
96489-71-3	Pyridaben	1	1
179101-81-6	Pyridalyl	5	5
337458-27-2	Pyrifluquinazone	1	1
105779-78-0	Pyrimidifen	1	1
95737-68-1	Pyriproxyfen	1	1
13593-03-8	Quinalphos	1	1
84087-01-4	Quinclorac	1	1
90717-03-6	Quinmerac	1	1
2797-51-5	Quinoclamine	1	1
124495-18-7	Quinoxyfen	1	1
76578-12-6	Quizalofop	1	1
10453-86-8	Resmethrin	1	1
122836-35-5	Sulfentrazone	1	1
35400-43-2	Sulprofos	1	1
34643-47-5	Sulprofos-sulfoxide	1	1
335104-84-2	Tembotrione	1	1
149979-41-9	Tepraloxydim	1	1
158062-71-6	TFNAAM	1	1
111988-49-9	Thiacloprid	1	1
317815-83-1	Thiencarbazone-methyl	1	1
28249-77-6	Thiobencarb	1	1
129558-76-5	Tolfenpyrad	1	1
210631-68-8	Topramezone	1	1
87820-88-0	Tralkoxydim	1	1
43121-43-3	Triadimefon	1	1
72459-58-6	Triazoxide	1	1
52-68-6	Trichlorfon	1	1
55335-06-3	Triclopyr	2	2
1263133-33-0	Triflumezopyrim	1	1
2275-23-2	Vamidothion	1	1
2655-14-3	XMC	1	1
156052-68-5	Zoxamide	1	1
51-28-5	2,4-DNOP	1	1
496925-02-1	2-Hydroxypropoxycarbazone	1	1
120-23-0	2-Naphthyloxyaceticacid	5	5
16655-82-6	3-OH-carbofuran	1	1
1967-25-5	4-Bromophenyluree	1	1
1214-39-7	6-Benzyladenine	1	1
30560-19-1	Acephate	1	1
35272-27-6	Acibenzolaracid	5	5

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
50594-66-6	Acifluorfen	1	1
116-06-3	Aldicarb	1	1
1646-88-4	Aldicarb-sulfone	1	1
1646-87-3	Aldicarbsulfoxide	1	1
865318-97-4	Ametoctradin	1	1
120923-37-7	Amidosulfuron	1	1
3337-71-1	Asulam	1	1
65195-55-3	Avermectine B1a	5	5
11141-17-6	Azadirachtin	1	1
120162-55-2	Azimsulfuron	1	1
83055-99-6	Bensulfuron-methyl	1	1
60374-43-8	Bentazone-8-hydroxy	5	5
413615-35-7	Benthiavalicarb	1	1
177406-68-7	Benthiavalicarb-isopropyl	1	1
1072957-71-1	Benzovindiflupyr	1	1
581809-46-3	Bixafen	1	1
1689-84-5	Bromoxynil	1	1
34681-24-8	Butocarboxim sulfoxide	1	1
10605-21-7	Carbendazim	1	1
55285-14-8	Carbosulfan	1	1
17757-70-9	Carboxin sulfoxide	1	1
104030-54-8	Carpropamid	1	1
500008-45-7	Chlorantraniliprole	1	1
71422-67-8	Chlorfluazuron	1	1
6339-19-1	Chloridazon-desphenyl	1	1
15545-48-9	Chlorotoluron	1	1
1982-47-4	Chloroxuron	1	1
64902-72-3	Chlorsulfuron	1	1
143807-66-3	Chromafenozide	1	1
99129-21-2	Clethodim	1	1
74115-24-5	Clofentezine	5	5
84496-56-0	Clomeprop	1	1
101-10-0	Cloprop	2	2
13067-93-1	Cyanofenphos	5	5
736994-63-1	Cyantraniliprole	1	1
113136-77-9	Cyclanilide	1	1
180409-60-3	Cyflufenamid	2	2
400882-07-7	Cyflumetofen	1	1
39515-40-7	Cyphenothrin	2	2
75-99-0	Dalapon	5	5
6190-65-4	Desethyl-atrazine	1	1
40843-25-2	Diclofopacid	5	5
14214-32-5	Difenoxuron	1	1
143701-75-1	Diketonitrile	1	1
34205-21-5	Dimefuron	1	1
61432-55-1	Dimepiperate	1	1
644-64-4	Dimetilan	1	1
165252-70-0	Dinotefuran	1	1
1420-07-1	Dinoterb	1	1
330-54-1	Diuron	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
534-52-1	DNOC	1	1
2439-10-3	Dodine	2	2
97780-06-8	Ethametsulfuron-methyl	1	1
53380-22-6	Ethiofencarbsulfoxide	1	1
181587-01-9	Ethiprole	1	1
23947-60-6	Ethirimol	1	1
91-53-2	Ethoxyquin	5	5
126801-58-9	Ethoxysulfuron	1	1
31972-43-7	Fenamiphos-sulfoxide	1	1
113158-40-0	Fenoxaprop-P	2	2
517875-34-2	Fenpicoxamid	1	1
3761-41-9	Fenthion-PO-sulfoxid	1	1
104040-78-0	Flazasulfuron	1	1
145701-23-1	Florasulam	1	1
1390661-72-9	Florpyrauxifen-benzyl	1	1
83066-88-0	Fluazifop-P	2	2
79622-59-6	Fluazinam	1	1
86811-58-7	Fluazuron	1	1
272451-65-7	Flubendiamide	1	1
113036-88-7	Flucycloxuron	1	1
101463-69-8	Flufenoxuron	10	10
42835-25-6	Flumequine	1	1
658066-35-4	Fluopyram	1	1
951659-40-8	Flupyradifurone	1	1
144740-53-4	Flupyrsulfuron-methyl	1	1
131549-75-2	FM-6-1 (metabolite of triflumizole)	1	1
72178-02-0	Fomesafen	1	1
173159-57-4	Foramsulfuron	1	1
68157-60-8	Forchlorfenuron	1	1
23422-53-9	Formetanate HCL	1	1
123572-88-3	Furametpyr	1	1
943832-60-8	Halauxifen	1	1
100784-20-1	Halosulfuron methyl	1	1
69806-34-4	Haloxyfop	1	1
86479-06-3	Hexaflumuron	2	2
78587-05-0	Hexythiazox	1	1
10004-44-1	Hymexazol	1	1
81335-37-7	Imazaquin	1	1
81335-77-5	Imazethapyr	1	1
122548-33-8	Imazosulfuron	1	1
950782-86-2	Indaziflam	1	1
133-32-4	Indolylbutyricacid	1	1
144550-36-7	Iodosulfuron-methyl	1	1
125225-28-7	Ipconazole	1	1
875915-78-9	Isofetamid	1	1
881685-58-1	Isopyrazam	1	1
55861-78-4	Isouron	2	2
82558-50-7	Isoxaben	1	1

CAS number	Compound name	LOQ* (ppb)	LOQ** (µg/kg)
141112-29-0	Isoxaflutole	1	1
103055-07-8	Lufenuron	1	1
1246768-30-8	M800H11	1	1
1246768-31-9	M800H35	1	1
374726-62-2	Mandipropamid	1	1
93-65-2	Mecoprop	2	2
131-72-6	Meptyldinocap	5	5
208465-21-8	Mesosulfuron-methyl	1	1
104206-82-8	Mesotrione	1	1
139968-49-3	Metaflumizone	1	1
172960-62-2	Metazachlor ESA	5	5
1231244-60-2	Metazachlor	5	5
10265-92-6	Methamidophos	1	1
2179-25-1	Methiocarb-sulfone	1	1
2635-10-1	Methiocarb sulfoxide	1	1
16752-77-5	Methomyl	1	1
161050-58-4	Methoxyfenozide	1	1
139528-85-1	Metosulam	1	1
19937-59-8	Metoxuron	1	1
74223-64-6	Metsulfuron-methyl	1	1
51596-10-2	Milbemectin A3	1	1
51596-11-3	Milbemectin A4	1	1
150-68-5	Monuron	1	1
555-37-3	Neburon	1	1
111991-09-4	Nicosulfuron	1	1
150824-47-8	Nitenpyram	1	1
116714-46-6	Novaluron	1	1
58810-48-3	Ofurace	1	1
19044-88-3	Oryzalin	1	1
23135-22-0	Oxamyl	2	2
144651-06-9	Oxasulfuron	1	1
153197-14-9	Oxaziclomefone	1	1
5259-88-1	Oxycarboxin	1	1
301-12-2	Oxydemetonmethyl	1	1
66063-15-8	Pencycuron-PB-amine	1	1
494793-67-8	Penflufen	1	1
219714-96-2	Penoxsulam	1	1
183675-82-3	Penthiopyrad	1	1
3735-33-9	Phosmetoxon	1	1
14816-18-3	Phoxim	1	1
139520-94-8	Prochloraz desimidazole-amino BTS44595	2	2
139001-49-3	Profoxydim	1	1
181274-15-7	Propoxycarbazone	1	1
94125-34-5	Prosulfuron	1	1
120983-64-4	Prothioconazole-desthio	1	1
123312-89-0	Pymetrozine	1	1
129630-17-7	Pyraflufen	1	1
40020-01-7	Pyridafol	1	1
422556-08-9	Pyroxsulam	1	1
122931-48-0	Rimsulfuron	1	1
372137-35-4	Saflufenacil	1	1
874967-67-6	Sedaxane	1	1
74051-80-2	Sethoxydim	1	1
149508-90-7	Simeconazole	1	1
130561-48-7	Sintofen	1	1
87392-12-9	S-Metolachlor + Metolachlor	1	1
935545-74-7	Spinetoram	5	5
131929-60-7	Spinosad (Spinosyn A).2	1	1
131929-63-0	Spinosad (Spinosyn D).1V2	5	5
203313-25-1	Spirotetramat	1	1
203312-38-3	Spirotetramat-enol	1	1
1172614-86-6	Spirotetramat-enol-glucoside	1	1
1172134-11-0	Spirotetramat-keto-hydroxy	1	1
1172134-12-1	Spirotetramat-mono-hydroxy	1	1
141776-32-1	Sulfosulfuron	1	1
946578-00-3	Sulfoxaflor	1	1
112410-23-8	Tebufenozide	1	1
107-49-3	TEPP	1	1
10548-10-4	Terbufos-sulfoxide	1	1
158063-66-2	TFNA	1	1
207502-65-6	TFNG	2	2
148-79-8	Thiabendazole	1	1
153719-23-4	Thiamethoxam	1	1
79277-27-3	Thifensulfuron-methyl	1	1
59669-26-0	Thiodicarb	1	1
39184-27-5	Thiofanoxsulfoxide	1	1
23564-05-8	Thiophanate-methyl	1	1
82097-50-5	Triasulfuron	1	1
101200-48-0	Tribenuronmethyl	1	1
81412-43-3	Tridemorph	1	1
64628-44-0	Triflumuron	1	1
126535-15-7	Triflusulfuron-methyl	1	1
26644-46-2	Triforine	1	1
143294-89-7	Trinexapac	2	2
95266-40-3	Trinexapac-ethyl	2	2
142469-14-5	Tritosulfuron	1	1
283159-90-0	Valifenalate	1	1
70898-34-9	Vamidothion-sulfone	1	1
81-81-2	Warfarin	1	1
2425-10-7	Xylylcarb	1	1

*Limit of quantification in solvent (acetonitrile)

**Limit of quantification in matrices (fruits, vegetables, cereals) based on QuEChERS method

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