Wide-scope screening of multi-class contaminants in seafood using a novel sample preparation (QuEChUP) procedure coupled with UHPLC-Q-TOF-MS: application for semi-quantitation of real seafood samples

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Abstract

A high-resolution mass spectrometry screening method was developed and validated based on EU SANTE/11312/2021 guidelines for the analysis of 850 multi-class contaminants in commercial seafood samples. Samples were extracted using a novel sequential QuEChUP preparation method that combines the QuEChERS and QuPPe procedures. The screening detection limits (SDLs) and limits of identification (LOIs) were equal to or lower than 0.01 $mg.kg^{-1}$ for 92% and 78% of contaminants, respectively. This screening procedure was ultimately applied for a target screening analysis of 24 seafood samples. The concentrations of identified contaminants were assessed using semi-quantitative approach. Two identified contaminants, diuron and diclofenac, showed the highest estimated average concentrations: 0.076 and 0.068 $mg.kg^{-1}$ respectively in mussel samples. Suspect screening was also performed. Target and suspect screening led to the identification of mixtures of contaminants (pesticides, veterinary products, industrial chemicals and personal care products) and the assessment of their frequencies of appearance (FoA).

Keywords

LC-HRMS, Emerging contaminants, Fishery/aquaculture products, Semi-quantitation, Eco-exposome, QuEChUP

1. Introduction

Currently, there is heightened awareness of the toxicity of certain chemical compounds, such as pesticides, whose presence in the environment has been or is regulated by various legislation (Teysseire et al., 2021). Along with pesticide use, veterinary drug use has increased dramatically in recent years (Casado et al., 2019). This latter group of substances, which includes antimicrobials, hormones and non-steroidal anti-inflammatory drugs (NSAIDs), is one of the major classes of emerging contaminants (Samal et al., 2022). The main route of entry of veterinary drugs into the aquatic environment is via wastewater (including urban, industrial, agricultural and livestock wastewater), whereas pesticides enter the aquatic ecosystem via runoff, vaporisation into the atmosphere, agricultural returns, intrusion into groundwater or by adsorption or uptake by plants (Tudi et al., 2021). Once pesticides, veterinary drugs and various mixtures of contaminants enter the water, aquatic species absorb them — e.g. fish take them up through their gills — and they can accumulate and undergo metabolism in tissues (van der Oost et al., 2003). In addition, other species such as bivalves filter a large volume of water and can bioaccumulate xenobiotics in their digestive glands, making bivalves good sentinel species of environmental quality (Breitwieser et al., 2018) and therefore relevant for eco-exposome assessment. Pesticides, veterinary drugs and other contaminants that enter the food chain through aquatic ecosystems can indirectly threaten human health (Breitwieser et al., 2018; van der Oost et al., 2003). Contaminant residues in seafood are therefore a critical public health issue that needs to be addressed not only in the context of the advocated 'One Health' approach but also to amend the limited information available on the mixtures of contaminants to which humans are exposed. Nevertheless, few maximum residue limits (MRLs) have been set for currently employed contaminants to ensure safe seafood consumption.

Seafood contains a large quantity of lipids (up to 17%) and proteins (up to 27%) (ANSES, 2020) that can affect the analysis of target contaminant compounds, especially because when the analytes are present at low concentrations. These usually result in signal suppression or enhancement, which affects the accuracy of the results obtained (Diallo et al., 2023). Therefore, appropriate extraction and clean-up methods must be developed to limit the presence of matrix interferents during analysis. The current popular generic solid-phase extraction method is the QuEChERS (which stands for 'quick, easy, cheap, effective, rugged and safe') method, owing to its rapid protocol, reliable results and affordable cost (Barbieri et al., 2019). Acetonitrile is the most widely used organic solvent for QuEChERS extraction,

because it can extract a wide range of non-polar and medium polar pesticides from several animal and plant foodstuffs (Kim et al., 2019). Some extraction methods use methanol as the extraction solvent, such as the quick polar pesticides (QuPPe) method (Jansons et al., 2021). This method, which was originally designed to extract polar and highly polar pesticide residues — i.e. non-QuEChERS-amenable — , has already been tested for the analysis of antiviral drugs (Douillet et al., 2022).

Food sample preparation for the analysis of pesticides and veterinary drugs normally involves an extraction and purification step. To achieve the best extraction performance, many parameters need to be optimised, including sample amount, extraction solvent, pH, partition salt, clean-up, and concentration/dilution of the extracts, which makes optimisation complex and time consuming. The orthogonal array design, also known as the Taguchi orthogonal array (TOA) design, is a simple and effective strategy for the simultaneous optimisation of multiple experimental conditions at multiple levels (Narenderan et al., 2019). It can greatly simplify the experimental optimisation without reducing the quality of the results. The TOA method has been used to optimise the QuEChERS method for wide-scope multi-residue analysis of 129 and 204 pesticides in beef (Pang et al., 2021) and bivalves (Diallo et al., 2022), respectively.

Most current analytical methods for the separation and detection of pesticides and veterinary drug in seafood are based on liquid or gas chromatography coupled to triple quadrupole mass spectrometry (LC-MS/MS or GC-MS/MS, respectively) operated in multiple reaction monitoring (MRM) mode due to their selectivity and sensitivity (Barbieri et al., 2019). However, the use of these instruments has proven to have some limitations, including the limited number of target compounds that can be included in the analysis. For large-scale screening purposes, an alternative to MRM is the application of full-scan techniques based on high-resolution mass spectrometry (HRMS), using Orbitrap MS-based instruments and time-of-flight (ToF) MS systems (Rajski et al., 2021). This analytical technique can perform simultaneous (*via* data treatment) target, suspect and non-target analyses to increase the number of analytes that can be included in multi-residue approaches (Rajski et al., 2021). In addition, retrospective analyses are possible because data can be reprocessed and the digitised samples (mass spectra) can be used in future studies without having to re-inject them (Arroyo-Manzanares et al., 2021).

One of the greatest challenges of HRMS is to obtain good quality MS/MS spectra for unequivocal identification of contaminants in complex matrices. The main methods for

acquiring a MS/MS mass spectrum are data-dependent acquisition (DDA) and data-independent acquisition (DIA) (Diallo et al., 2022). The choice of acquisition mode may depend on the instrument and software available to each user, although the HRMS acquisition mode that provides the best quality and easiest-to-interpret spectra is DDA, also called information-dependent acquisition (IDA), in Sciex instruments (Diallo et al., 2022). However, only the most intense precursor ions selected by the user (Top*N*) are fragmented in IDA, which can lead to difficulties in complex matrices or low concentrations. The Top*N* must therefore be optimised to avoid or minimise the loss of pertinent MS/MS data, especially for suspect and non-targeted analyses. For targeted analyses, a precursor inclusion list (PIL) can be added. In IDA-PIL mode, the targeted precursor ions have the highest priority for fragmentation, regardless of whether these precursor ions are the most intense (Diallo et al., 2022; Makni et al., 2022).

The aim of this study was to develop a wide-scope screening approach for 850 multi-class chemical contaminants in 12 different commercial seafood products using a novel sample preparation method combining QuEChERS and QuPPe (called QuEChUP), followed by UHPLC-QTOF-MS analysis. The list of target contaminants included pesticides, veterinary drugs, their transformation products (TPs) and industrial chemicals from different families with very distinct physicochemical properties, used as a templates for suspect screening. To our knowledge, this study is the first to perform simultaneous analysis by HRMS for such a comprehensive list of contaminants in so many different seafood species. The TOA method was used to evaluate the optimal parameters for the sample extraction step. The developed method was validated in accordance with the criteria set by European Union SANTE/11312/2021 guidelines for qualitative multi-residue methods (European Commission, 2021). For each contaminant, screening detection limits (SDLs) were established. Although not required for the validation of the qualitative screening method according to SANTE guidelines, the limits of identification (LOIs) were also established. The number of false positives was assessed using non-spiked seafood samples. To test its applicability, the screening method was applied to the analysis (target screening) of real seafood samples, including mussels, oysters, sole, horse mackerel, spiny lobster and crayfish from South-West France and the French West Indies. The concentration of the identified contaminants was estimated using different semi-quantitative strategies. To test the versatility of the method on contaminants other than those included in the validation, a suspect screening approach was

also performed. This study reports the first comprehensive data on the occurrence of a large number of multi-class chemical contaminants in real seafood samples.

2. Materials and methods

2.1. Chemical substances and analytical standards

A kit of 745 pesticide and industrial chemical standards, divided into five mixtures (5 $mg.L^{-1}$ of each compound in either acetonitrile (ACN) or methanol (MeOH)), was obtained from LGC Standards (Molsheim, France). The analytical standards of 180 veterinary drugs, divided into 10 mixtures (10 $mg.L^{-1}$ of each compound in either ACN or MeOH)), was obtained from the ANSES Fougères Laboratory (France). ACN, MeOH, purchased from Fisher Scientific (Illkirch, France), and ultrapure water (18.2 MΩ.cm), obtained by purifying distilled water with a Milli-Q system from Merck Millipore (Saint-Quentin-en-Yvelines, France), were used for the mobile phases and sample preparation. Formic acid (FA) was supplied by Fisher Scientific to prepare the LC-MS mobile phases and the extraction solvent. QuEChERS extraction pouches based on the original method (4.0 g of magnesium sulphate ($MgSO_4$), 1.0 g of sodium chloride (NaCl)) was provided by Agilent Technologies (Santa Clara, CA, USA). A dispersive solid-phase extraction (dSPE) kit containing 900 mg of $MgSO_4$, 150 mg of primary and secondary amines (PSA) and 150 mg of octadecylsilane (C18), Enhanced Matrix Removal-lipid (EMR-lipid) dSPE, and a dispersive kit for veterinary drugs containing 900 mg Na_2SO_4, 50 mg PSA and 150 mg C18 end-capped (C18EC), were obtained from Agilent Technologies. Ethylenediaminetetraacetic acid disodium salt dihydrate ($Na_2EDTA.H_2O$), citric acid (≥99.5% purity) and disodium phosphate (HNa_2PO_4; ≥99.0% purity) were obtained from Fisher Scientific. $Na_2EDTA.H_2O$ (37.18 g), citric acid (12.9 g) and HNa_2PO_4 (10.9 g) were dissolved in 1 L of ultrapure water to prepare a 0.1 $mol.L^{-1}$ Na_2EDTA-McIlvaine buffer solution.

2.2. Equipment and apparatus

A Genie 2 vortex mixer (Scientific Industries, Bohemia, NY, USA) and an Eppendorf 5810 centrifuge (Eppendorf, Hamburg, Germany) were used for the extraction procedure. An IKA Ultra-Turrax T25 digital homogeniser and a GM 200 Grindomix (Retsch Technology GmbH, Haan, Germany) were also used for the extraction procedure.

An UHPLC Thermo Fisher Scientific U3000 system with a binary pump and autosampler (Waltham, MA, USA) coupled with a 5600 Q-TOF AB Sciex mass spectrometer (Darmstadt, Germany) with an electrospray ionisation source (ESI) was used for analyses.

2.3. Selection and use of the contaminants

Of the initial 920 contaminants, 850 could be analysed in solvent at 0.2 $mg.L^{-1}$ and were therefore selected for this study (Table S1); of these 364 (204 pesticides and 160 veterinary drugs) were used for optimisation of sample preparation. These substances are representative of the rest of the contaminants in terms of retention time (t_R), mass-to-charge ratio (*m/z*) and range of polarity (LogP) (Table S1). The optimised method was then validated on 850 contaminants to demonstrate its relevance and applicability on a wide scope of multi-class contaminants. The contaminants used for method validation included pesticides, veterinary drugs and industrial chemicals, as well as their TPs (Table S1).

2.4. Selection and use of seafood samples

Twelve of the most widely consumed seafood species in France, namely oysters, mussels, scallops (*Pecten maximus* and *Mimachlamys varia*), clams, cod, salmon, sole, anchovies and tuna, as well as spiny lobster and crayfish, used to optimise and validate the method (including to asses false positives), were purchased from local markets in March and April 2022 (Maisons-Alfort, France). These 12 seafood samples were pooled and used to optimise sample preparation. To validate the method, two groups were randomly formed for each of the 12 seafood species, for a total of 24 seafood samples. To test the applicability of the screening method using target and suspect screening, two species of bivalves (mussels (n = 6) and oysters (n = 6)) and two species of fish (sole (n = 3) and horse mackerel (n = 3)) were collected in the Pertuis-Charentais area (South-West France), and two species of crustaceans (lobster (n = 3) and crayfish (n = 3)) were collected in Martinique (French West Indies). Before shucking (bivalves) or dissection (fish), the seafood samples were stored at 4°C overnight and then brought to room temperature. The samples were homogenised and kept at -20°C until analysis.

2.5. Development of a homemade LC-MS/MS compound database and MS/MS library

A homemade MS/MS library of 850 contaminants was built using AB Sciex LibraryView™ software, version 1.0.3 (Les Ulis, France). The library was acquired in IDA mode by injecting mixtures of compound analytical standards, diluted to 0.1 $mg.L^{-1}$ in ACN. The injections of

the standards were performed in both ESI^+ and ESI^- mode. The information on molecular formulae, retention time (T_R), accurate m/z of the precursor ion, isotopic pattern and the MS/MS fragmentation spectrum of each of the studied contaminants were recorded and taken as reference for the automated detection and identification process in matrix samples. In total, 744 and 247 spectra in ESI^+ and ESI^-, respectively, were recorded. Data were processed and evaluated using PeakView® software version 2.2 comprising the AB Sciex MasterView™ module. The MasterView™ module is inter-connected to LibraryView™ software and compares the experimental fragmentation spectra to those recorded in the homemade database. The term 'detection' was employed when a contaminant did not exceed the following thresholds: (i) T_R variation ± 0.1 min and (ii) mass accuracy ± 5 ppm on the precursor ion (European Commission, 2021). The term 'identification' was based on the same thresholds as detection, and also satisfied an MS/MS library score of spectral similarity of >70% between the experimental and reference MS/MS fragmentation spectra using the Fit MS/MS search algorithm (Makni et al., 2022). The Fit algorithm represents the degree of similarity of the peaks and intensities of the reference spectrum with those of the experimental spectrum, ignoring the other interfering peaks in the experimental spectrum.

2.6. Orthogonal array design for optimisation of sample preparation

The factors affecting the detection rates (%) were simultaneously optimised by adopting an analysis of mean (ANOM) approach, using the Taguchi method. Three factors (extraction solvent, dSPE and dilution ratio) were considered for extraction and clean-up optimisation. Three levels were defined for each factor, as described in Table 1.

In the conventional full-factorial method of optimisation, the total number of experiments for three parameters with three levels is 27. If each experiment is replicated three times, the total number of experiments would be equal to 81 (i.e. 3 × 27). Taguchi method of optimisation significantly reduces the number of experiments using orthogonal arrays. Using an L9 orthogonal array, with each experiment replicated three times, the total number of experiments reduces to 27 (i.e., 9 × 3). The L9 orthogonal array (Table S2) was used to design the experiments. The response assessed was the detection rate (%) of the contaminants.

2.7. Optimisation of sample preparation

Extraction solvent, dSPE and dilution ratio were simultaneously optimised using L9 TOA. To obtain a pesticide supplementation at a concentration of 0.01 $mg.kg^{-1}$, 7.5 µL of the mix containing 364 contaminants were added to 50-mL polypropylene centrifuge tubes, which

contained 1.50 ± 0.05 g of pooled seafood sample. The tubes were stored at 4°C for 24 h to allow the contaminants to bind to the matrix. Then, 8.5 mL of the aqueous phase (Na_2EDTA-McIlvaine buffer (0.1 $mol.L^{-1}$)) was added to each tube, and the sample was then ground using an IKA Ultra-Turrax mixer for 3 min at 5000 rpm. Then, 10 mL of organic solvent was added to each centrifuge tube and vortexed again for 1 min. After that, a mixture of 4.0 g of $MgSO_4$ and 1.0 g of NaCl were added to the fortified samples, and the resulting mixture was centrifuged for 5 min at 4000 rpm.

For the purification step, there were two cases. When EMR-lipid was used as the dSPE reagent, the sorbent was activated by adding 5 mL of water to a 15 mL centrifuge tube containing the EMR-lipid and vortexed for 3 s. Then, 5 mL of the extract supernatant (50 mL polypropylene centrifuge tube) was transferred to the activated 15 mL centrifuge tube. The mixture was immediately vortexed for 1 min. The tube was centrifuged at 4000 rpm for 5 min, and 5 mL of the supernatant was transferred to the polishing tube containing 0.5 g NaCl and 1.5 g $MgSO_4$ to remove excess water. When using the other dSPE reagents, 6 mL of the supernatant was transferred to a 15-mL centrifuge tube containing the dSPE reagent. The tube was vortexed for 1 min, and then centrifuged for 5 min at 4000 rpm. The supernatant was then combined with ACN according to the dilution ratio. The mixture was then vortexed, filtered and deposited into a 2-mL autosampler vial for injection in the UHPLC-QTOF system.

To check for cross-contamination, matrix-free ACN was subjected to the same extraction and purification protocols as previously described.

2.8. UHPLC-Q-TOF-MS conditions

Reversed-phase liquid chromatography separation was performed using a Phenomenex Aqua® C18 column (150 × 2 mm, 3 µm particle size, 125 Å pore diameter; Phenomenex Inc, Torrance, CA, USA). The UHPLC-Q-TOF-MS conditions were the same as in previous work by Diallo et al. (2022), Makni et al. (2022) and are summarised in Table S3. The instrument was tuned and calibrated manually before each batch, in high-sensibility mode using the APCI positive or negative calibration solutions for the 5600 system (AB Sciex technology). The automated calibration device system (CDS) was scheduled to perform automatic calibration every five injections to avoid as much as possible a mass deviation over 5-ppm during the run analysis.

Data acquisition was performed using a combination of full scan TOF-MS and IDA mode. The mass range of full-scan TOF-MS acquisition was 50–1000 Da, the collision energy (CE) was 10 eV (-10 eV in ESI⁻) and the accumulation time was set to 490 ms. In IDA mode, the declustering potential (DP) was 80 eV (-80 eV in ESI⁻) and the collision energy (CE) was 40 eV with ±20 eV (-40 eV in ESI⁻ with ±20 eV). The 10 highest intensity precursors (i.e. ion intensity greater than 50 cps and ion tolerance ≤ 10 ppm) (Top10) were monitored in every cycle, and dynamic background subtraction was turned on. Data acquisition with the UHPLC-Q-TOF system was performed using Analyst® software (version 1.7) of AB Sciex.

2.9. Method validation

The screening method was validated according to EU SANTE/11312/2021 guidelines (European Commission, 2021). For this purpose, 24 commercial seafood samples were used (see section 2.4). Samples (1.5 g) were spiked before extraction with a mixture containing 850 contaminants at 0.001, 0.01, and 0.1 $mg.kg^{-1}$ (in a total of 24 samples for each concentration level). The SDL was established as the lowest concentration level at which a contaminant was detected in at least 95% of the samples (i.e., 23 out of 24 samples analysed) (European Commission, 2021). SDL was estimated as the concentration level at which the thresholds of (i) T_R (variation ±0.1 min) and (ii) mass accuracy (±5 ppm) of the precursor ion were satisfied (European Commission, 2021). The LOI (not required according to SANTE guidelines) was established as the lowest concentration tested for which a contaminant was satisfactorily identified in at least 95% of the samples. LOI used the same thresholds as for SDL, and also satisfied an MS/MS library score (Fit > 70%). Non-spiked samples were also extracted and analysed to assess the number of false positives out of the 850-targeted contaminants.

2.10. Data processing for real sample analysis

2.10.1. Target screening

For target analyses, data processing was performed using PeakView® software version 2.2 comprising the AB Sciex MasterView™ module. The contaminants were detected and identified using the previously developed homemade database for automated screening of samples against a target list of 850 contaminants. The criteria for detection and identification are the same as those described in Section 2.5.

The concentration of positively identified contaminants was estimated using a semi-quantitative approach. Calibration curves were constructed only for positively identified

contaminants. To construct the calibration curve, the areas obtained for each contaminant in the 24 validation samples (spiked at 0.001, 0.01 and 0.1 $mg.kg^{-1}$) were used. For normalisation purposes, the areas obtained in the matrices for each contaminant were divided by the area of the same contaminant in solvent (injected in each batch) at 0.1 $mg.L^{-1}$ to obtain area ratios. Three calibration curves, constructed on general, broad and specific taxon groups, were established for each positive contaminant as follows.

Calibration strategy A: average area ratios for each contaminant were calculated using the values for all 24 samples. These average area ratios (n = 24) were used to establish the final calibration curve for each contaminant to estimate their concentration in the real seafood samples.

Calibration strategy B: average area ratios for each contaminant were calculated for each broad taxon group (bivalves, fish and crustaceans). These average area ratios for each species (n = 10, n = 10 and n = 4 for bivalves, fish and crustaceans, respectively) were used to establish the final calibration curve for each contaminant to estimate their concentration in the real seafood samples.

Calibration strategy C: average area ratios for each contaminant were calculated for each specific matrix (oysters, mussels, sole, spiny lobster and crayfish). These average area ratios for each matrix (n = 2 for all matrices) were used to establish the final calibration curve for each contaminant to estimate their concentration in the real seafood samples. When the matrix type of the real samples was not present in the validation samples, a calibration curve resulting from a similar matrix in terms of lipid and protein content was used. This was the case for horse mackerel; the most similar matrix in the validation samples was sole.

Only contaminants with a satisfactory linearity ($r^2 > 0.995$) were selected for semi-quantitation.

2.10.2. Suspect screening

For the suspect screening analyses, data processing was performed using the open-source software MSDial (version 4.7), which allows for large-scale screening and annotation of compounds of interest against external MS/MS libraries, and for which the analytical standards are not available. In this work, MSDial software was linked to the MS/MS spectra contained in the Mass Bank of North America (MoNA). In total, 98,000 and 46,000 LC-MS/MS spectra in positive and negative mode, respectively, were used in this approach.

The suspect screening of potential contaminants was performed using the following criteria: (i) mass accuracy ± 5-ppm of precursor ion, (ii) spectral similarity >70% between the experimental and external reference MS/MS fragmentation spectra. The spectral comparison was performed using the reverse DOT algorithm, which works on the same principle as the FIT algorithm in MasterView™ software. All the contaminants reported that fulfilled these criteria were considered as putatively identified (confidence level 2a) according to Schymanski et al. (2014).

3. Results and discussion

3.1. Optimisation of the sample extraction and purification steps

Although presenting a simple experimental layout, the efficiency of the QuEChERS/QuPPe method depends on certain factors and, in general, the performance of the extraction method can be improved. These factors include sample amount, extraction solvent, pH, partition salt, clean-up and concentration/dilution of the extracts. Thus, selection of the experimental conditions is a crucial step and must be considered. A TOA approach was applied to find the best conditions for detection rates (%) for pesticides and veterinary drugs. Three parameters were optimised: extraction solvent, dSPE and the dilution of the extracts.

The values of the mean detection rates for all contaminants ranged from 49% to 83% (Tables S4, S5) for all experiments. Overall, the best performances were found with Experiment 1 and 6 for pesticides and veterinary drugs, respectively. According to the R values, the factor with the greatest impact on pesticide detection was dilution (R = 23), followed by extraction solvent (R = 14) and finally the dSPE (R = 3). For veterinary drug detection, the most influential factor was solvent extraction (R = 18), then dilution (R = 17), and finally dSPE (R = 8). The effects of the three studied factors on the pesticide and veterinary drug detection rates are also shown in Fig. 1. The detection rates are represented in bar charts; therefore, the greater the difference between the best and worst performing levels, the more significant the factor is. All factors were significant ($p < 0.05$) for the veterinary drug detection rates, and solvent extraction and dilution were significant for the pesticide detection rates (Tables S4, S5).

3.1.1. Extraction solvent

Three extraction solvents, namely, 10 mL of ACN, 10 mL of MeOH with 1% FA and 10 mL of ACN/MeOH (7:3, v/v), were assessed. ACN is the most used solvent in the QuEChERS

method for the extraction of medium-polar pesticides. MeOH with 1% FA is frequently used for the extraction of polar contaminants in the QuPPe method (Anastassiades et al., 2015). ACN/MeOH was also assessed based on previous studies that analysed pharmaceuticals in fishery products (Kim et al., 2017). As shown in Fig. 1, ACN was provided the best detection rate for pesticides, followed closely by ACN/MeOH and MeOH with 1% FA. For veterinary drugs (generally more polar than pesticides), the best detection rates were obtained with ACN/MeOH as the solvent, followed by ACN and MeOH with 1% FA. This result shows that pure ACN is most effective for the extraction of targeted pesticides. ACN/MeOH was not only suitable for the extraction of veterinary drugs, but also successfully extracted pesticides, making it a more versatile extraction solvent. This may be due to the fact that the resulting polarity of this mixture is a suitable compromise between that of targeted pesticides and veterinary drugs.

3.1.3. dSPE

As illustrated in Fig. 1, the best pesticide detection rates were obtained with a mixture of $MgSO_4$/PSA/C18 as dSPE reagent, closely followed by EMR-lipid. $MgSO_4$ is commonly used as a drying salt for ACN extraction because it effectively removes residual water. PSA has been shown to remove many polar organic acids from the extract, as well as polar pigments, sugars and fatty acids, whereas C18 can retain fats, vitamins and minerals (Kim et al., 2019). For veterinary drugs, the best detection rates were obtained with EMR-lipid, followed by a mixture of PSA/Na_2SO_4/C18EC. EMR-lipid, whose structure is a proprietary secret, removes lipids from sample matrices (Pang et al., 2021). This sorbent allows a highly selective and efficient interaction with lipids, providing excellent extraction efficiency, precision and matrix effect (Castilla-Fernández et al., 2021). Na_2SO_4 is also a drying agent, similar to $MgSO_4$. This salt performed better for veterinary drugs than $MgSO_4$, because the Mg^{2+} ions can also form complexes with some veterinary drugs, which reduces detection rates (Gros et al., 2019). Another difference is that Na_2SO_4 is a weak drying agent compared with $MgSO_4$, and when added to the organic extraction solvent, the amount of water is higher than when $MgSO_4$ is used, favouring the extraction of polar compounds, such as veterinary drugs (Munaretto et al., 2016). The C18EC products are based on reversed phase, bonded and end-capped octadecylsilane silica gel particles. The non-polar sorbent is end-capped (EC), which reduces polar secondary interactions associated with surface silanol groups (Sobczak et al., 2021).

3.1.4. Dilution

As observed in Fig. 1, non-dilution led to the best detection rates for both pesticides and veterinary drugs. Dilution combined with extraction and purification steps can decrease matrix effects, as shown in apple, tea and broccoli samples during analysis (Guo et al., 2019). However, sample dilution reduces the overall sensitivity of the method; thus, a compromise is needed to reduce matrix effects and nonetheless maintain high method sensitivity. In addition to the dilution of extracts, the concentration of final extracts can be important for the sensitivity of the target compounds and on matrix effects. To have a simple, reliable and time-effective method for application to a large number of seafood samples, the concentration of the sample was not considered in this study.

The conclusion based on the R values associated with the K1, K2, and K3 values and the main effects plot for detection is that the optimal extraction conditions for pesticides were obtained with pure ACN, $MgSO_4$/PSA/C18 for dSPE, and the non-dilution of extracts, which corresponds to a classical QuEChERS method, and consistent with previous results (Diallo et al., 2022). For the detection of veterinary drugs, the optimal extraction conditions were obtained with ACN/MeOH, EMR-lipid as the dSPE sorbent and the non-dilution of extracts, which corresponds to a modified QuPPe method.

3.2. Comparison of optimal conditions for the detection of pesticides and veterinary drugs

In this study, the objective was to optimise a sample preparation method for the simultaneous analysis of pesticides and veterinary drugs, as well as other organic contaminants. To do so, the optimal detection conditions for pesticides (QuEChERS) and veterinary drugs (QuPPe) were compared for all 364 combined contaminants studied for method optimisation. The mixture of the final QuEChERS and QuPPe extracts (QuEChERS + QuPPe in Fig. 2) was also evaluated as well as the sequential method of QuEChERS and QuPPe (QuEChUP). This sequential method consists of a QuEChERS extraction followed by a QuPPe extraction of the same sample and subsequent purification. The protocol for these four methods (QuEChERS, QuPPe, QuEChERS + QuPPe and QuEChUP) is summarised in Fig. 2.

As observed in Fig. 3, the QuEChERS method was more specific to pesticides, allowing a very high detection rate (97%) for pesticides, but low (54%) for veterinary drugs. The QuPPe method was more versatile, with a high detection rate for pesticides (84%) and veterinary drugs (86%). The best detection rates (90–91%) were obtained with the mixture of final

extracts (QuEChERS + QuPPe) and the sequential method (QuEChUP) for all 364 contaminants combined. In addition, both methods can cover a wide range of polarity (LogP from -4.2 to 7.2), as illustrated in Fig. S1. Indeed, these two methods combine the advantages of QuEChERS and QuPPe for the extraction of pesticides (generally medium-polar) and veterinary drugs (generally polar), respectively. The QuEChUP method was ultimately preferred to the QuEChERS + QuPPe method, because it is faster and allows the simultaneous analysis of a wide range of contaminants in small seafood samples (e.g. mussels) individually, which could be very useful in the case of a metabolomic approach, for example. For these reasons, the QuEChUP method followed by EMR lipid clean-up was chosen for the subsequent analyses (Fig. 2).

3.3. Validation of the screening method

Twelve different seafood matrices were tested in the validation of the method: oysters, mussels, scallops (*P. maximus* and *M. varia*), clams, cod, salmon, sole, anchovies, tuna, spiny lobster and crayfish. Two groups of each type were spiked with the mixture of 850 contaminants at three concentration levels (0.001, 0.01 and 0.1 $mg.kg^{-1}$) and analysed with their respective non-spiked samples for qualitative validation.

3.3.1. Selectivity of the screening method

In SANTE guidelines, no criteria have been set with respect to the occurrence of false positives. However, the selectivity of the method must reduce the false positive rate to a sufficiently low level to avoid manual verification or confirmatory analysis that may reduce the effectiveness of the screening method. The number of false positives was checked by analysing 24 non-spiked seafood samples. According to the results, a total of 42 ± 7 (standard deviation, SD) false positives (5% of the 850 target contaminants) were obtained across all non-spiked samples, applying the detection criteria, i.e. tolerances of ±5 ppm and ±0.1 min for mass accuracy and T_R, respectively. To reduce this false positive rate and to obtain a more reliable detection of contaminants, an additional criterion on the signal-to-noise (SN) ratio was added for detection. When the S/N threshold was set to S/N>10 instead of S/N>3 (as was originally the case), the number of false positives dropped drastically to 17 ± 4 contaminants, representing only 2% of the 850 targeted contaminants. The addition of this extra criterion had no impact on the detection rates of contaminants, which remained unchanged. Finally, when the identification criterion was considered by adding the MS/MS library score (Fit > 70%), the number of false positives dropped to 2 ± 1 contaminants (0.24% of the 850 targeted

contaminants). These false positives were due to misattributions during automatic MS/MS matching. False positive contaminants for 1,2-benzisothiazol-3(2H)-one (C7H5NOS) and pipenonyl butoxide ($C_{19}H_{30}O_5$) were each detected in five non-spiked seafood samples, whereas false positives for (E)-metominostrobin ($C_{16}H_{16}N_2O_3$) were observed in nine samples. The other false positives were only detected once each in the different samples. These results demonstrated the good selectivity of the method both in terms of detection (with S/N > 10) and identification.

3.3.2. Determination of SDL and LOI

The validation of the qualitative screening methodology included the determination of SDLs (European Commission, 2021). Although it is not required to satisfy SANTE guidelines, the LOI was also established. A summary of the SDLs and LOIs assessed in the 24 seafood samples is presented in Fig. 4 (see also Table S6 for individual values obtained for each contaminant). The SDLs were determined to be equal to or less than 0.001, 0.01 and 0.1 $mg.kg^{-1}$ for 86, 92 and 94% of pesticides, respectively (Fig. 4a). The SDL criteria were therefore not reached for 6% of contaminants. However, the proposed method was able to detect them in most of the samples at all three concentration levels. As can be seen in Fig. 4b, about 96–97% of the contaminants could be detected at 0.01 $mg.kg^{-1}$ and 0.1 $mg.kg^{-1}$, but the detection rate decreased to 91–95% at 0.001 $mg.kg^{-1}$. No significant differences were observed between the matrices studied. Ten contaminants (alpha-cypermethrin, benfluralin, bentazon-methyl, butocarboxim, chlorthiamide, diafenthiuron, dioxathion, fluorodifen, omethoate and tridiphane) were not detected in any of the spiked samples. These compounds may not be stable under the extraction conditions assayed or may be highly sensitive to matrix effects.

The LOI was determined to be equal to or less than 0.001, 0.01 and 0.1 $mg.kg^{-1}$ for 67, 78 and 85% of pesticides, respectively (Fig. 4c). Thus, 16% of the contaminants could not be validated for identification because the criteria of LOI were not met. For 82 contaminants (representing 10% of the selected contaminants), it was possible to establish the SDL at least at one of the three concentration levels, but not the LOI. For these compounds, validation was limited to detection (only the SDL could be set). Overall, the reliable identification was likely for 89% of contaminants at 0.1 $mg.kg^{-1}$ (Fig. 4d). This value decreased to 87% and 80% at 0.01 and 0.001 $mg.kg^{-1}$, respectively.

To check the applicability of the screening method, the resulting SDLs must be compared with the MRLs in food, established by the European Commission to ensure consumer safety. The MRL is the highest level of a contaminant or residue that is legally tolerated in food and can therefore be used. To date, no MRLs have been established for the targeted residues in seafood matrices. A general default MRL of 0.01 $mg.kg^{-1}$ applies where a contaminant is not specifically mentioned. Thus, the SDL and LOI obtained, in most cases less than or equal to 0.01 $mg.kg^{-1}$, can be considered satisfactory and the proposed methodology adequately sensitive for suspect and non-targeted screening purposes.

As shown in Table S7, as with the previous studies (Bai et al., 2022; Diallo et al., 2022; Munaretto et al., 2016), the present study also provided a thorough and complete validation of the qualitative method. The percentage of contaminants with SDLs equal to 0.01 $mg.kg^{-1}$ was higher than or equal to those of the previously reported methods in qualitative analysis (Bai et al., 2022; Diallo et al., 2022; Munaretto et al., 2016). Furthermore, none of these previous studies tested concentrations below 0.01 $mg.kg^{-1}$, but in the present study the lowest concentration level tested was 0.001 $mg.kg^{-1}$. It should be noted that most studies on multi-residue analysis of organic contaminants in seafood have been carried out using a quantitative method. In this case, SDLs have not been established and other criteria are used to assess the sensitivity of the method such as limits of quantification (LOQ). The percentage of contaminants with LOQs < 0.01 $mg.kg^{-1}$ in previous studies (Barbieri et al., 2019; Castilla-Fernández et al., 2021; Park et al., 2022) is also comparable to that of the SDLs < 0.01 $mg.kg^{-1}$ in this present study, signifying the good sensitivity of the sequential QuEChUP method followed by EMR lipid clean-up. Moreover, the addition of the S/N criterion (>10) can allow this method to be used for quantitative purposes.

3.4. Target screening in real seafood samples

Contaminants were identified using the criteria applied in this study (see sections 2.5 and 2.10.1). Fig. 5 showed an unequivocal identification of diuron and diclofenac in a mussel sample.

All samples analysed were positive for different mixtures of contaminants. The HRMS acting as a diagnostic system provides comprehensive and large-scale data on the occurrence of these mixtures. However, in an eco-exposure context, the concentration level of these contaminants must be at least estimated to ensure that the levels do not exceed the regulatory levels (e.g. provisional no-effect concentrations (PNECs)) (Nikolopoulou et al., 2023). Semi-

quantitation remains a relevant approach if the objective is to estimate the order of magnitude of the concentration level in a sample. However, to confirm the concentration levels, the subsequent use of a validated quantitative approach is necessary. Here, semi-quantitative approaches were used to estimate concentrations. To do so, three calibration curves were constructed. The aim was to evaluate a more general method (Calibration strategy A) for all seafood products as well as a more specific method (Calibration strategy C) for a given matrix (e.g. estimating the concentration of a contaminant in oysters with a calibration curve on an oyster matrix). As observed, the concentration values were similar for most contaminants in the same sample, regardless of the calibration strategy used, suggesting that matrix effects are equivalent (Table S8). However, in contrast, diclofenac and vedaprofen increased from 0.057 to 0.068 $mg.kg^{-1}$ in mussels and from 0.030 to 0.046 $mg.kg^{-1}$ in crayfish respectively, depending on the calibration strategy used.

As depicted in Fig. S2, the most frequent contaminants were pesticides and their TPs (59%), followed by veterinary drugs and their TPs (26%) and industrial chemicals (15%). The list of identified contaminants as well as their frequencies of appearance (FoA) and estimated mean concentration in target screening can be found in Table S8 and are discussed briefly in the following sections.

3.4.1. Pesticides and their transformation products (TPs)

For all the seafood samples, the most identified pesticides were herbicides and fungicides, most of them in the bivalve samples. The pesticides identified with 100% FoA in all seafood samples were *N*,*N*-diethyl-*m*-toluamide (DEET) and diphenylamine, with an estimated average concentration of 0.016 and 0.007 $mg.kg^{-1}$, respectively. Diuron and its TP 1-(3,4-dichlorophenyl)-3-methyl urea) were identified with a 63% FoA, with an estimated maximum concentration of 0.078 to 0.086 $mg.kg^{-1}$ for diuron in mussels. Butroxydim, diazinon, diflufenicen, prosulfocarb and spiroxamine were identified in oysters and mussels (50% FoA), with an estimated average concentration ranging from below the SDL for diazinon to 0.016 $mg.kg^{-1}$ for butroxidim. The pesticides with the lowest FoA (13%) were azimsulfuron, bupirimate, pyroxsulam, tebuconazole and thiabendiazole, which were only identified in crustacean samples (spiny lobsters or crayfish) with an estimated maximum concentration of 0.009 $mg.kg^{-1}$ for azimsulfuron in crayfish. These pesticides found in this study have also been identified in previous reports in seafood samples (Diallo et al., 2022; Slaby et al., 2022). The extraction procedure used in these previous works was QuEChERS, followed by LC-

HRMS and LC-MS/MS analysis in the case of Diallo et al. (2022) and Slaby et al. (2022), respectively.

3.4.2. Veterinary drugs

Generally, the categories of the seven identified veterinary drugs were antibiotics, NSAIDs and antihistamines. Of these, none had a FoA of 100%. Clarithromycin, dapsone and diclofenac were identified in oysters and mussels (50% FoA), with an estimated maximum concentration of 0.057 to 0.068 $mg.kg^{-1}$ for diclofenac in mussels. Vedaprofen was identified in crustacean and fish samples (50% FoA), with an estimated average concentration between 0.027 and 0.046 $mg.kg^{-1}$ in these samples. The veterinary drug with the lowest FoA (13%) was 4-dimethylaminoantipyrine, which was only identified in spiny lobster. Only diclofenac was previously detected in the bivalve using a QuEChERS-LC-HRMS method (Daniele et al., 2016), the other veterinary drugs were detected in environmental samples such as surface water using solid phase extraction (SPE), following by LC-MS/MS analysis (Ramírez-Morales et al., 2021).

3.4.3. Industrial chemicals

Two industrial chemicals were identified with a FoA of 100%. This is the case for tris(2-chloroethyl) phosphate (TRCP) and tri-*o*-cresyl phosphate (TCP). Two other industrial chemicals triphenyl phosphorothioate (TPPT) and 2-ethylhexyl diphenyl phosphate (EHDPP) were identified with FoAs of 75 and 63%, respectively. Most of these compounds are commonly detected in seafood and environmental samples (Diallo et al., 2022; Nikolopoulou et al., 2023; Peng et al., 2018).

3.5. Suspect screening analysis in real seafood samples

The method was also tested for the analysis of other organic contaminants such as pharmaceutical and personal care products (PCPs) to demonstrate its versatility by suspect screening.

The identification list contains various classes of emerging contaminants, especially pharmaceuticals (Table S9). For all the seafood samples, a total of 20 pharmaceuticals were identified, most of them in the bivalve samples. Generally, the categories identified were antiarrhythmic, anaesthetics, hormones, antibiotics, antihistamines and NSAIDs. Most of the pharmaceuticals identified in this study have previously been reported in previous work, such as ibuprofen (50% FoA), norethindrone (50% FoA), propafenone (50% FoA), progesterone

(25% FoA), fexofenadine (25% FoA) and methylprednisolone (13% FoA) (Dodder et al., 2014; Omar et al., 2019; Ramírez-Morales et al., 2021).

Tetrahydrocannabinol (THC), an illicit drug, was also identified in oyster and mussel samples (50% FoA). It has previously been found in fish from Argentina by suspect screening using four extraction methods (two involving SPE and two based on QuEChERS), follow by LC-HRMS analysis (Carrizo et al., 2022).

Two pesticide TPs (flufenacet-ethane sulfonic acid (ESA) and metamitron-desamino) were identified only in mussel samples (25% FoA). Flufenacet ESA has been reported in fish collected from north-eastern France (Slaby et al., 2022). Metamitron-desamino has been identified in environmental samples in Greece using SPE-LC-HRMS method (Nika et al., 2020).

A total of six PCPs (galaxolidone, dihydromuronic acid, 4-hydroxybenzoic acid, laurocapram, phenylacetaldehyde and Velvione®) were identified in all the seafood samples. Most of these PCPs have already been reported in seafood or environment samples in the literature (Gadelha et al., 2019; Nikolopoulou et al., 2023).

Four industrial chemicals (bisphenol S, triethylene glycol bis(2-ethylhexanoate) (TEG-EH), tri-isobutylphosphate (TiBP) and tris(1-chloro-2-propyl) phosphate (TCPP)) were also identified in the seafood samples, as previously observed (Nikolopoulou et al., 2023; Peng et al., 2018).

The contaminants mentioned in the target and suspect screening were mainly identified in positive ionisation mode (ESI^+). However, several other contaminants were identified in negative ionisation mode (ESI^-) in seafood samples. This is the case for allopurinol (antigout agent) and its TP oxypurinol, dinoterb (herbicide), gemfibrozil (fibrate), prostaglandin E1 (vasodilator), salicylic acid (NSAID). Chlordecone (organochloride insecticide) and its metabolite chlordecole were identified in crayfish and spiny lobster from the French West Indies. A perfluorooctane sulfonic acid (PFOS) precursor, N-ethylperfluorooctane sulfonamidoacetic acid (N-EtFOSAA), was also identified. This shows the importance of using both ionisation modes for wide-scope screening of multi-class contaminants.

4. Conclusion

The development and validation of an original QuEChUP-LC-HRMS method to screen 850 organic contaminants in seafood were carried out according to European Union

SANTE/11312/2021 guidelines. The list of target compounds included pesticides, veterinary drugs and industrial chemicals from different families with very distinct physicochemical properties. The use of L9 TOA for QuEChERS and QuPPe parameter optimisation greatly simplified the method development process. After obtaining an optimal method for each class of contaminants, their performance was evaluated on all contaminants. The QuEChUP (QuEChERS followed by QuPPe) procedure provided the best detection rates of the targeted contaminants. Moreover, this new method of extraction is very appropriate in an exposome context to extract the most diverse contaminants. QuEChUP is very suitable for metabolomic type studies where each individual is analysed separately and *a fortiori* when only small samples are available. Most of the target list compounds were detected and identified at all three concentration levels (0.001, 0.01 and 0.1 $mg.kg^{-1}$) with false positives averaging 0.24% on non-spiked matrices. The SDL and LOI were equal to or less than 0.01 $mg.kg^{-1}$ for 92% and 78% of targeted contaminants, respectively.

The applicability of this method for multi-class contaminants screening was demonstrated by analysing several samples of bivalves, fish and crustaceans. All samples analysed by target screening were exposed to mixtures of contaminants. Of these, 59% were pesticides, 26% veterinary drugs and 15% industrial chemicals. Diuron (herbicide) and diclofenac (NSAID) were the contaminants identified with the highest estimated average concentrations, especially in mussel samples with 0.076 and 0.068 $mg.kg^{-1}$, respectively. Vedaprofen (NSAID) was also found at concentrations well above the default MRL in fish and crustacean samples, and two antibiotics such as clarithromycin and dapsone were found at concentrations slightly greater than the MRL in bivalve samples. The rest of the contaminants were found at concentrations equal to or lower than the default MRL. These concentrations were estimated using different semi-quantitation strategies. However, the use of a validated quantitative method may be considered in future work to confirm and compare the concentration levels obtained with an MRL, if available. The method also demonstrated its versatility to identify other organic contaminants than those included in the method validation by suspect screening. This allowed the identification of other mixtures of contaminants, mainly pharmaceuticals, as well as illicit drugs and PCPs.

In this study, the combined results of targeted and suspect screening allow a better estimation of all contaminants likely to be present in the analysed samples, in a single analytical method based on an optimised extraction step and on the enhanced capabilities of HRMS detection. This innovative method will allow a better assessment of the combined actions of

contaminants (cocktail effects) in future studies and to better reflect the impact of environmental exposures.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

5. References

Anastassiades, M., Kolberg, D.I., Eichhorn, E., Benkenstein, A., Lukačević, S., Mack, D., Wildgrube, C., Sigalov, I., Dörk, D., Barth, A., 2015. Quick Method for the Analysis of numerous Highly Polar Pesticides in Foods of Plant Origin via LC-MS/MS involving Simultaneous Extraction with Methanol (QuPPe-Method).

Anses, 2020. Table de composition nutritionnelle Ciqual pour le calcul des apports nutritionnels CALNUT. Consulté le 02/11/2022. https://ciqual.anses.fr/.

Arroyo-Manzanares, N., Campillo, N., López-García, I., Hernández-Córdoba, M., Viñas, P., 2021. High-resolution mass spectrometry for the determination of mycotoxins in biological samples. A review. Microchem. J. 166, 106197. https://doi.org/10.1016/j.microc.2021.106197

Bai, M., Tang, R., Li, G., She, W., Chen, G., Shen, H., Zhu, S., Zhang, H., Wu, H., 2022. High-throughput screening of 756 chemical contaminants in aquaculture products using liquid chromatography/quadrupole time-of-flight mass spectrometry. Food Chem. X 15, 100380. https://doi.org/10.1016/j.fochx.2022.100380

Barbieri, M.V., Postigo, C., Guillem-Argiles, N., Monllor-Alcaraz, L.S., Simionato, J.I., Stella, E., Barceló, D., López de Alda, M., 2019. Analysis of 52 pesticides in fresh fish muscle by QuEChERS extraction followed by LC-MS/MS determination. Sci. Total Environ. 653, 958–967. https://doi.org/10.1016/j.scitotenv.2018.10.289

Breitwieser, M., Vigneau, E., Viricel, A., Becquet, V., Lacroix, C., Erb, M., Huet, V., Churlaud, C., Le Floch, S., Guillot, B., Graber, M., Thomas, H., 2018. What is the relationship between the bioaccumulation of chemical contaminants in the variegated scallop Mimachlamys varia and its health status? A study carried out on the French

688 Atlantic coast using the Path ComDim model. Sci. Total Environ. 640–641, 662–670.
689 https://doi.org/10.1016/j.scitotenv.2018.05.317
690 Carrizo, J.C., Vo Duy, S., Munoz, G., Marconi, G., Amé, M.V., Sauvé, S., 2022. Suspect
691 screening of pharmaceuticals, illicit drugs, pesticides, and other emerging
692 contaminants in Argentinean Piaractus mesopotamicus, a fish species used for local
693 consumption and export. Chemosphere 309, 136769.
694 https://doi.org/10.1016/j.chemosphere.2022.136769
695 Casado, J., Brigden, K., Santillo, D., Johnston, P., 2019. Screening of pesticides and
696 veterinary drugs in small streams in the European Union by liquid chromatography
697 high resolution mass spectrometry. Sci. Total Environ. 670, 1204–1225.
698 https://doi.org/10.1016/j.scitotenv.2019.03.207
699 Castilla-Fernández, D., Moreno-González, D., Bouza, M., Saez-Gómez, A., Ballesteros, E.,
700 García-Reyes, J.F., Molina-Díaz, A., 2021. Assessment of a specific sample cleanup
701 for the multiresidue determination of veterinary drugs and pesticides in salmon using
702 liquid chromatography/tandem mass spectrometry. Food Control 130, 108311.
703 https://doi.org/10.1016/j.foodcont.2021.108311
704 Daniele, G., Fieu, M., Joachim, S., James-Casas, A., Andres, S., Baudoin, P., Bonnard, M.,
705 Bonnard, I., Geffard, A., Vulliet, E., 2016. Development of a multi-residue analysis of
706 diclofenac and some transformation products in bivalves using QuEChERS extraction
707 and liquid chromatography-tandem mass spectrometry. Application to samples from
708 mesocosm studies. Talanta 155, 1–7. https://doi.org/10.1016/j.talanta.2016.04.016
709 Diallo, T., Leleu, J., Parinet, J., Guérin, T., Thomas, H., Lerebours, A., 2023. Approaches to
710 determine pesticides in marine bivalves. Anal. Bioanal. Chem.
711 https://doi.org/10.1007/s00216-023-04709-4
712 Diallo, T., Makni, Y., Lerebours, A., Thomas, H., Guérin, T., Parinet, J., 2022. Development
713 and validation according to the SANTE guidelines of a QuEChERS-UHPLC-QTOF-
714 MS method for the screening of 204 pesticides in bivalves. Food Chem. 386, 132871.
715 https://doi.org/10.1016/j.foodchem.2022.132871
716 Dodder, N.G., Maruya, K.A., Lee Ferguson, P., Grace, R., Klosterhaus, S., La Guardia, M.J.,
717 Lauenstein, G.G., Ramirez, J., 2014. Occurrence of contaminants of emerging concern
718 in mussels (Mytilus spp.) along the California coast and the influence of land use,
719 storm water discharge, and treated wastewater effluent. Mar. Pollut. Bull., U.S.
720 Coastal Monitoring: NOAA's Mussel Watch investigates Contaminants of Emerging
721 Concern 81, 340–346. https://doi.org/10.1016/j.marpolbul.2013.06.041
722 Douillet, C., Moloney, M., Di Rocco, M., Elliott, C., Danaher, M., 2022. Development and
723 validation of a quantitative method for 15 antiviral drugs in poultry muscle using
724 liquid chromatography coupled to tandem mass spectrometry. J. Chromatogr. A 1665,
725 462793. https://doi.org/10.1016/j.chroma.2021.462793
726 European Commission, 2021. SANTE/11312/2021. Analytical quality control and method
727 validation procedures for pesticide residues analysis in food and feed.
728 Gadelha, J.R., Rocha, A.C., Camacho, C., Eljarrat, E., Peris, A., Aminot, Y., Readman, J.W.,
729 Boti, V., Nannou, C., Kapsi, M., Albanis, T., Rocha, F., Machado, A., Bordalo, A.,
730 Valente, L.M.P., Nunes, M.L., Marques, A., Almeida, C.M.R., 2019. Persistent and
731 emerging pollutants assessment on aquaculture oysters (Crassostrea gigas) from NW
732 Portuguese coast (Ria De Aveiro). Sci. Total Environ. 666, 731–742.
733 https://doi.org/10.1016/j.scitotenv.2019.02.280
734 Gros, M., Mas-Pla, J., Boy-Roura, M., Geli, I., Domingo, F., Petrović, M., 2019. Veterinary
735 pharmaceuticals and antibiotics in manure and slurry and their fate in amended
736 agricultural soils: Findings from an experimental field site (Baix Empordà, NE

Catalonia). Sci. Total Environ. 654, 1337–1349. https://doi.org/10.1016/j.scitotenv.2018.11.061
Guo, J., Tong, M., Tang, J., Bian, H., Wan, X., He, L., Hou, R., 2019. Analysis of multiple pesticide residues in polyphenol-rich agricultural products by UPLC-MS/MS using a modified QuEChERS extraction and dilution method. Food Chem. 274, 452–459. https://doi.org/10.1016/j.foodchem.2018.08.134
Jansons, M., Pugajeva, I., Bartkevics, V., Karkee, H.B., 2021. LC-MS/MS characterisation and determination of dansyl chloride derivatised glyphosate, aminomethylphosphonic acid (AMPA), and glufosinate in foods of plant and animal origin. J. Chromatogr. B 1177, 122779. https://doi.org/10.1016/j.jchromb.2021.122779
Kim, H.-Y., Lee, I.-S., Oh, J.-E., 2017. Human and veterinary pharmaceuticals in the marine environment including fish farms in Korea. Sci. Total Environ. 579, 940–949. https://doi.org/10.1016/j.scitotenv.2016.10.039
Kim, L., Lee, D., Cho, H.-K., Choi, S.-D., 2019. Review of the QuEChERS method for the analysis of organic pollutants: Persistent organic pollutants, polycyclic aromatic hydrocarbons, and pharmaceuticals. Trends Environ. Anal. Chem. 22, e00063. https://doi.org/10.1016/j.teac.2019.e00063
Makni, Y., Diallo, T., Guérin, T., Parinet, J., 2022. Improving the monitoring of multi-class pesticides in baby foods using QuEChERS-UHPLC-Q-TOF with automated identification based on MS/MS similarity algorithms. Food Chem. 395, 133573. https://doi.org/10.1016/j.foodchem.2022.133573
Munaretto, J.S., May, M.M., Saibt, N., Zanella, R., 2016. Liquid chromatography with high resolution mass spectrometry for identification of organic contaminants in fish fillet: screening and quantification assessment using two scan modes for data acquisition. J. Chromatogr. A 1456, 205–216. https://doi.org/10.1016/j.chroma.2016.06.018
Narenderan, S.T., Meyyanathan, S.N., Karri, V.V.S.R., 2019. Experimental design in pesticide extraction methods: A review. Food Chem. 289, 384–395. https://doi.org/10.1016/j.foodchem.2019.03.045
Nika, M.C., Ntaiou, K., Elytis, K., Thomaidi, V.S., Gatidou, G., Kalantzi, O.I., Thomaidis, N.S., Stasinakis, A.S., 2020. Wide-scope target analysis of emerging contaminants in landfill leachates and risk assessment using Risk Quotient methodology. J. Hazard. Mater. 394, 122493. https://doi.org/10.1016/j.jhazmat.2020.122493
Nikolopoulou, V., Ajibola, A.S., Aalizadeh, R., Thomaidis, N.S., 2023. Wide-scope target and suspect screening of emerging contaminants in sewage sludge from Nigerian WWTPs by UPLC-qToF-MS. Sci. Total Environ. 857, 159529. https://doi.org/10.1016/j.scitotenv.2022.159529
Omar, T.F.T., Aris, A.Z., Yusoff, F.M., Mustafa, S., 2019. Occurrence and level of emerging organic contaminant in fish and mollusk from Klang River estuary, Malaysia and assessment on human health risk. Environ. Pollut. 248, 763–773. https://doi.org/10.1016/j.envpol.2019.02.060
Pang, X., Liu, X., Peng, L., Chen, Z., Qiu, J., Su, X., Yu, C., Zhang, J., Weng, R., 2021. Wide-scope multi-residue analysis of pesticides in beef by ultra-high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry. Food Chem. 351, 129345. https://doi.org/10.1016/j.foodchem.2021.129345
Park, H., Choi, S.Y., Kang, H.-S., Kwon, N. ji, 2022. Multi residue determination of 96 veterinary drug residues in domestic livestock and fishery products in South Korea. Aquaculture 553, 738064. https://doi.org/10.1016/j.aquaculture.2022.738064
Peng, Y., Fang, W., Krauss, M., Brack, W., Wang, Z., Li, F., Zhang, X., 2018. Screening hundreds of emerging organic pollutants (EOPs) in surface water from the Yangtze

River Delta (YRD): Occurrence, distribution, ecological risk. Environ. Pollut. 241, 484–493. https://doi.org/10.1016/j.envpol.2018.05.061
Rajski, Ł., Petromelidou, S., Díaz-Galiano, F.J., Ferrer, C., Fernández-Alba, A.R., 2021. Improving the simultaneous target and non-target analysis LC-amenable pesticide residues using high speed Orbitrap mass spectrometry with combined multiple acquisition modes. Talanta 228, 122241. https://doi.org/10.1016/j.talanta.2021.122241
Ramírez-Morales, D., Masís-Mora, M., Montiel-Mora, J.R., Cambronero-Heinrichs, J.C., Pérez-Rojas, G., Tormo-Budowski, R., Méndez-Rivera, M., Briceño-Guevara, S., Gutiérrez-Quirós, J.A., Arias-Mora, V., Brenes-Alfaro, L., Beita-Sandí, W., Rodríguez-Rodríguez, C.E., 2021. Multi-residue analysis of pharmaceuticals in water samples by liquid chromatography- mass spectrometry: Quality assessment and application to the risk assessment of urban-influenced surface waters in a metropolitan area of Central America. Process Saf. Environ. Prot. 153, 289–300. https://doi.org/10.1016/j.psep.2021.07.025
Schymanski, E.L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H.P., Hollender, J., 2014. Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence. Environ. Sci. Technol. 48, 2097–2098. https://doi.org/10.1021/es5002105
Slaby, S., Le Cor, F., Dufour, V., Auger, L., Pasquini, L., Cardoso, O., Curtet, L., Baudoin, J.-M., Wiest, L., Vulliet, E., Feidt, C., Dauchy, X., Banas, D., 2022. Distribution of pesticides and some of their transformation products in a small lentic waterbody: Fish, water, and sediment contamination in an agricultural watershed. Environ. Pollut. 292, 118403. https://doi.org/10.1016/j.envpol.2021.118403
Sobczak, Ł., Kołodziej, D., Goryński, K., 2021. Benefits of Innovative and Fully Water-Compatible Stationary Phases of Thin-Film Microextraction (TFME) Blades. Molecules 26, 4413. https://doi.org/10.3390/molecules26154413
Teysseire, R., Manangama, G., Baldi, I., Carles, C., Brochard, P., Bedos, C., Delva, F., 2021. Determinants of non-dietary exposure to agricultural pesticides in populations living close to fields: A systematic review. Sci. Total Environ. 761, 143294. https://doi.org/10.1016/j.scitotenv.2020.143294
Tudi, M., Daniel Ruan, H., Wang, L., Lyu, J., Sadler, R., Connell, D., Chu, C., Phung, D.T., 2021. Agriculture Development, Pesticide Application and Its Impact on the Environment. Int. J. Environ. Res. Public. Health 18, 1112. https://doi.org/10.3390/ijerph18031112
van der Oost, R., Beyer, J., Vermeulen, N.P.E., 2003. Fish bioaccumulation and biomarkers in environmental risk assessment: a review. Environ. Toxicol. Pharmacol. 13, 57–149. https://doi.org/10.1016/S1382-6689(02)00126-6

Figure captions

Fig. 1. Effects of extraction solvent (a), dispersive solid phase extraction (dSPE) sorbent (b) and dilution (c) on the detection rates of pesticides and veterinary drugs, with the significance of the ANOVA test p-value < 0.05 (*) and p-value < 0.01 (**). The error bars correspond to the standard deviation (SD) for the response measured (Mean ± SD, n = 3).

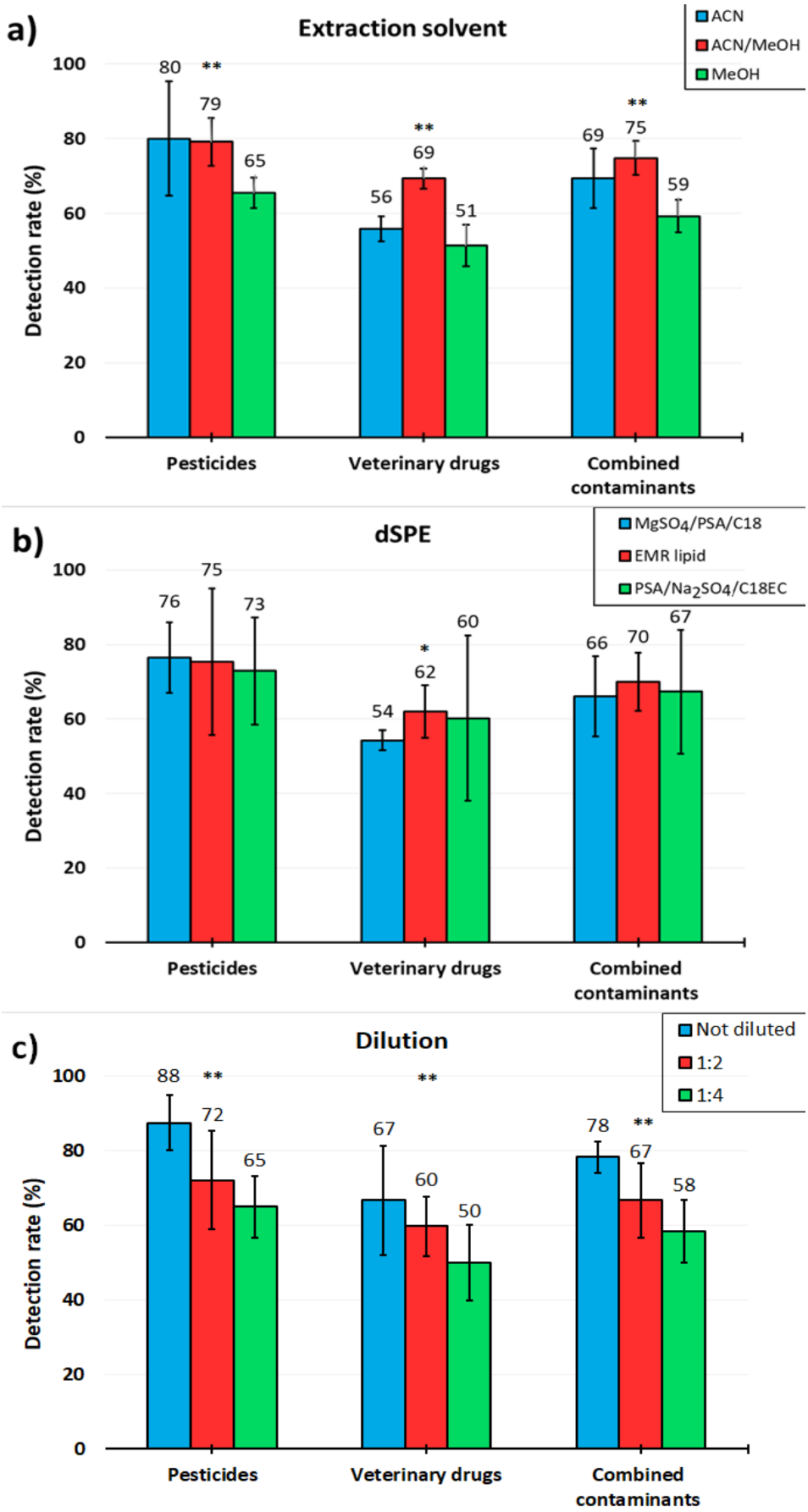
Fig. 2. Protocol of the four different sample preparation methods (QuEChERS, QuPPe, QuEChERS + QuPPe and QuEChUP, see text for method definitions) for the simultaneous analysis of 364 organic contaminants.

Fig. 3. Comparison of the QuEChERS, QuPPe, QuEChERS + QuPPe and QuEChUP sample preparation methods for detection of pesticides and veterinary drugs. The error bars correspond to the standard deviation (SD) (Mean ± SD, n = 3).

Fig. 4. Percentage of pesticides presenting screening detection limits (SDLs) (a) and limits of identification (LOIs) (b) at 0.001, 0.01, 0.1 and > 0.1 $mg.kg^{-1}$ under optimised conditions. Detection (c) and identification rates (d) across different seafood samples spiked at 0.001, 0.01 and 0.1 $mg.kg^{-1}$.

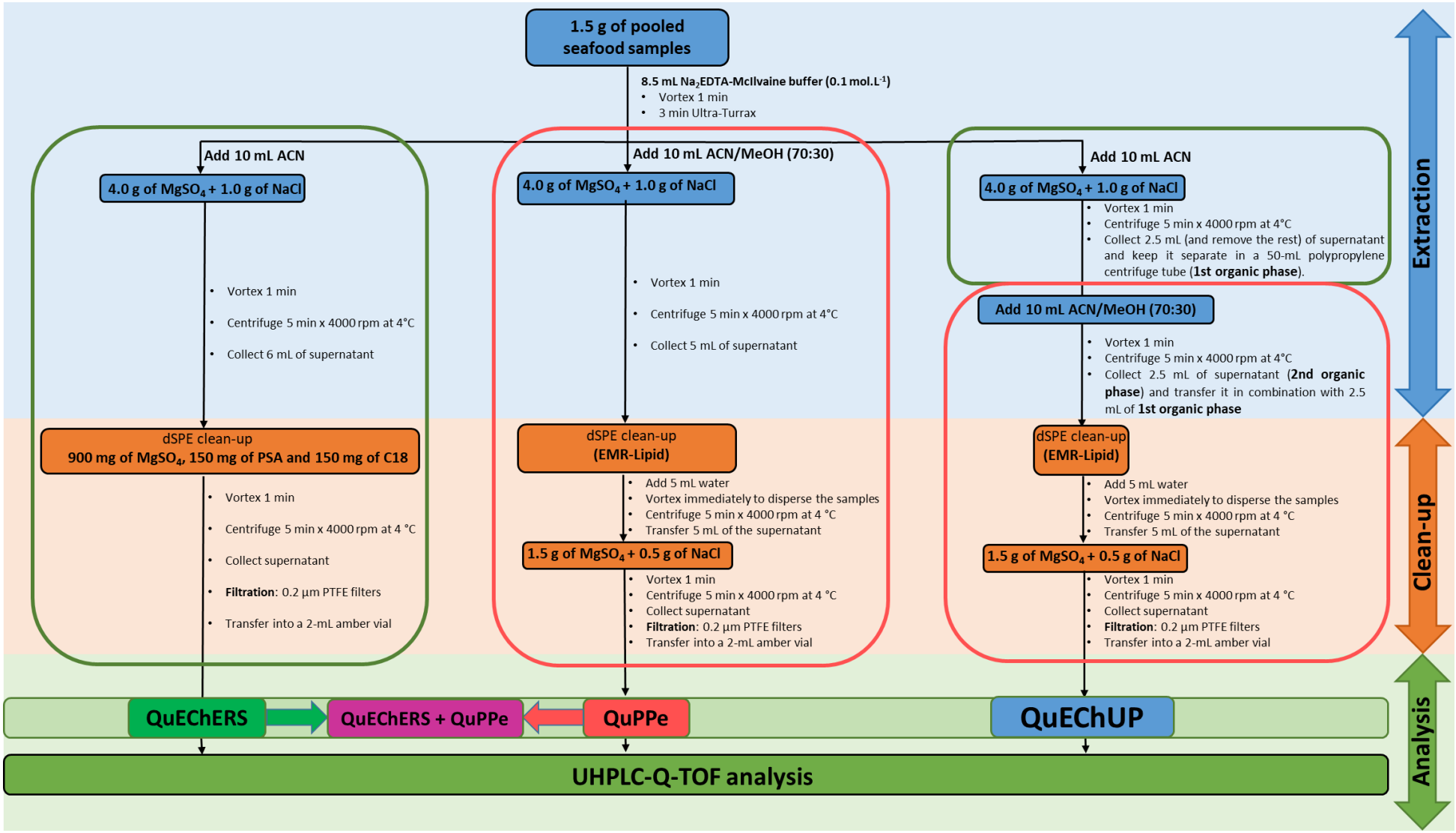
Fig. 5. Positive finding of diuron (a) and diclofenac (b) in a mussel sample, with corresponding extracted ion chromatogram (i); isotopic pattern (ii); experimental and reference MS/MS spectra comparison using the Fit algorithm (iii).

Fig. 1.


a)
Extraction solvent
ACN
ACN/MeOH
MeOH
Detection rate (%)
100
80
60
40
20
0
80
**
79
65
56
**
69
51
69
**
75
59
Pesticides
Veterinary drugs
Combined contaminants
b)
dSPE
MgSO4/PSA/C18
EMR lipid
PSA/Na2SO4/C18EC
Detection rate (%)
76
75
73
54
*
62
60
66
70
67
Pesticides
Veterinary drugs
Combined contaminants
c)
Dilution
Not diluted
1:2
1:4
Detection rate (%)
88
**
72
65
67
**
60
50
78
**
67
58
Pesticides
Veterinary drugs
Combined contaminants

848

849 **Fig. 2.**


1.5 g of pooled seafood samples
8.5 mL Na2EDTA-McIlvaine buffer (0.1 mol.L-1)
• Vortex 1 min
• 3 min Ultra-Turrax
Add 10 mL ACN
4.0 g of MgSO4 + 1.0 g of NaCl
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4°C
• Collect 6 mL of supernatant
dSPE clean-up
900 mg of MgSO4, 150 mg of PSA and 150 mg of C18
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4 °C
• Collect supernatant
• Filtration: 0.2 µm PTFE filters
• Transfer into a 2-mL amber vial
QuEChERS
Add 10 mL ACN/MeOH (70:30)
4.0 g of MgSO4 + 1.0 g of NaCl
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4°C
• Collect 5 mL of supernatant
dSPE clean-up
(EMR-Lipid)
• Add 5 mL water
• Vortex immediately to disperse the samples
• Centrifuge 5 min x 4000 rpm at 4 °C
• Transfer 5 mL of the supernatant
1.5 g of MgSO4 + 0.5 g of NaCl
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4 °C
• Collect supernatant
• Filtration: 0.2 µm PTFE filters
• Transfer into a 2-mL amber vial
QuPPe
QuEChERS + QuPPe
Add 10 mL ACN
4.0 g of MgSO4 + 1.0 g of NaCl
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4°C
• Collect 2.5 mL (and remove the rest) of supernatant and keep it separate in a 50-mL polypropylene centrifuge tube (1st organic phase).
Add 10 mL ACN/MeOH (70:30)
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4°C
• Collect 2.5 mL of supernatant (2nd organic phase) and transfer it in combination with 2.5 mL of 1st organic phase
dSPE clean-up
(EMR-Lipid)
• Add 5 mL water
• Vortex immediately to disperse the samples
• Centrifuge 5 min x 4000 rpm at 4 °C
• Transfer 5 mL of the supernatant
1.5 g of MgSO4 + 0.5 g of NaCl
• Vortex 1 min
• Centrifuge 5 min x 4000 rpm at 4 °C
• Collect supernatant
• Filtration: 0.2 µm PTFE filters
• Transfer into a 2-mL amber vial
QuEChUP
UHPLC-Q-TOF analysis
Extraction
Clean-up
Analysis

850

851

852 **Fig. 3.**

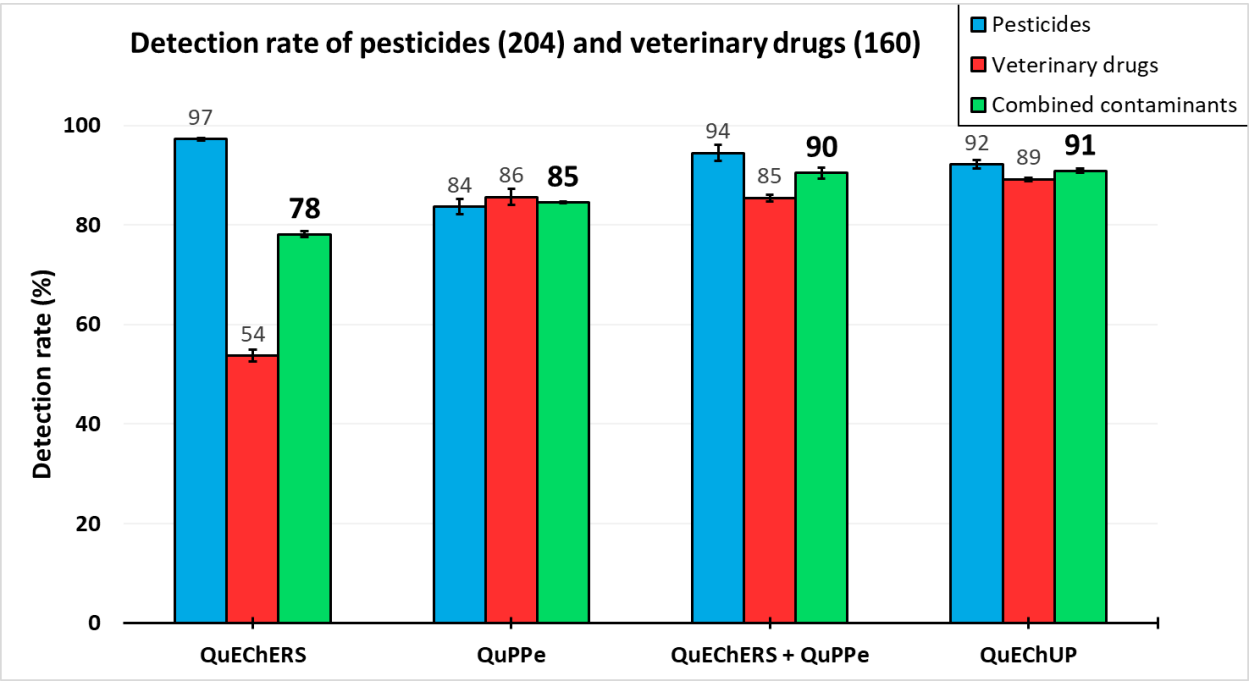

Detection rate of pesticides (204) and veterinary drugs (160)
Pesticides
Veterinary drugs
Combined contaminants
Detection rate (%)
100
80
60
40
20
0
97
54
78
84
86
85
94
85
90
92
89
91
QuEChERS
QuPPe
QuEChERS + QuPPe
QuEChUP

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Fig. 4.

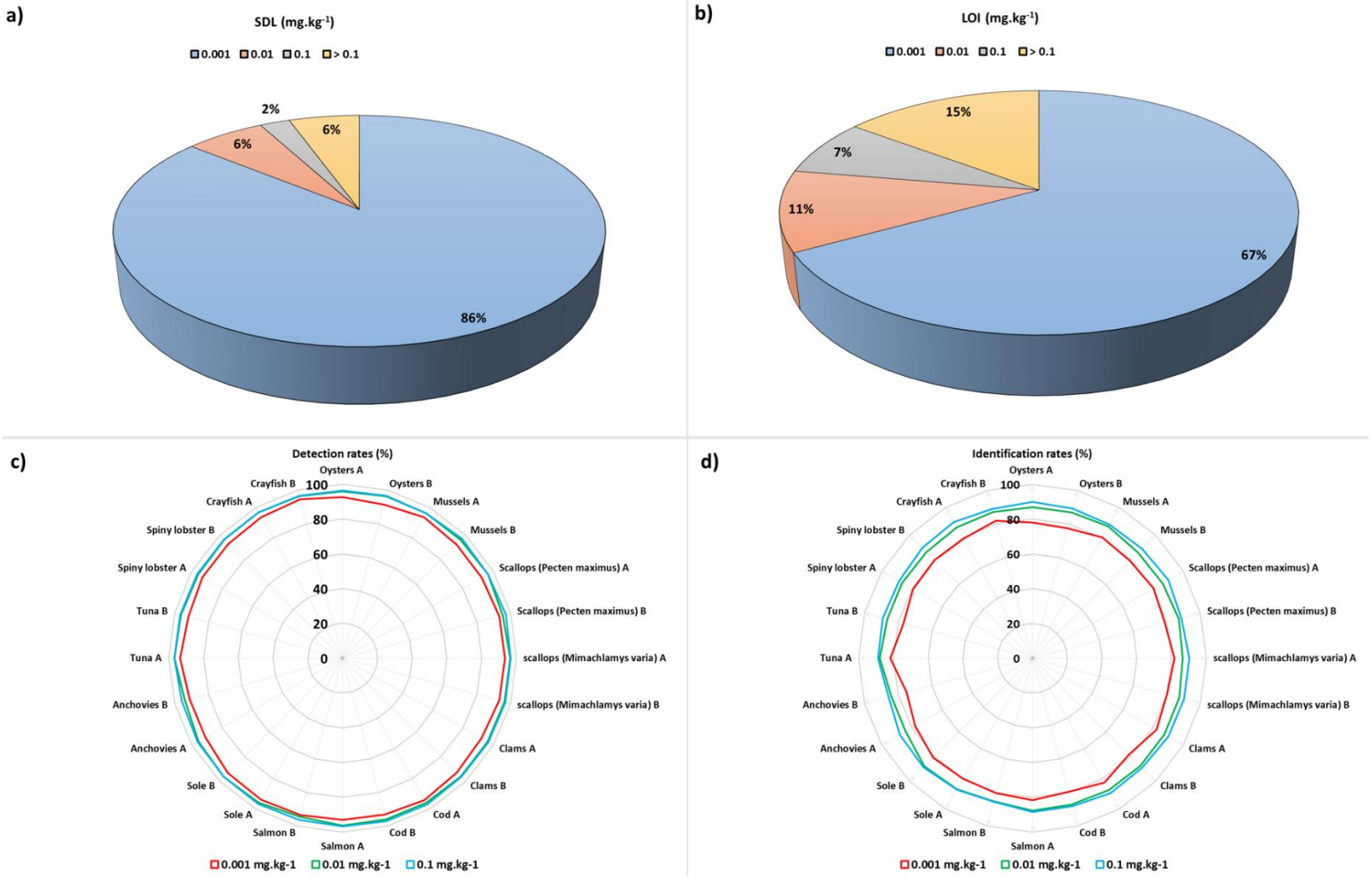
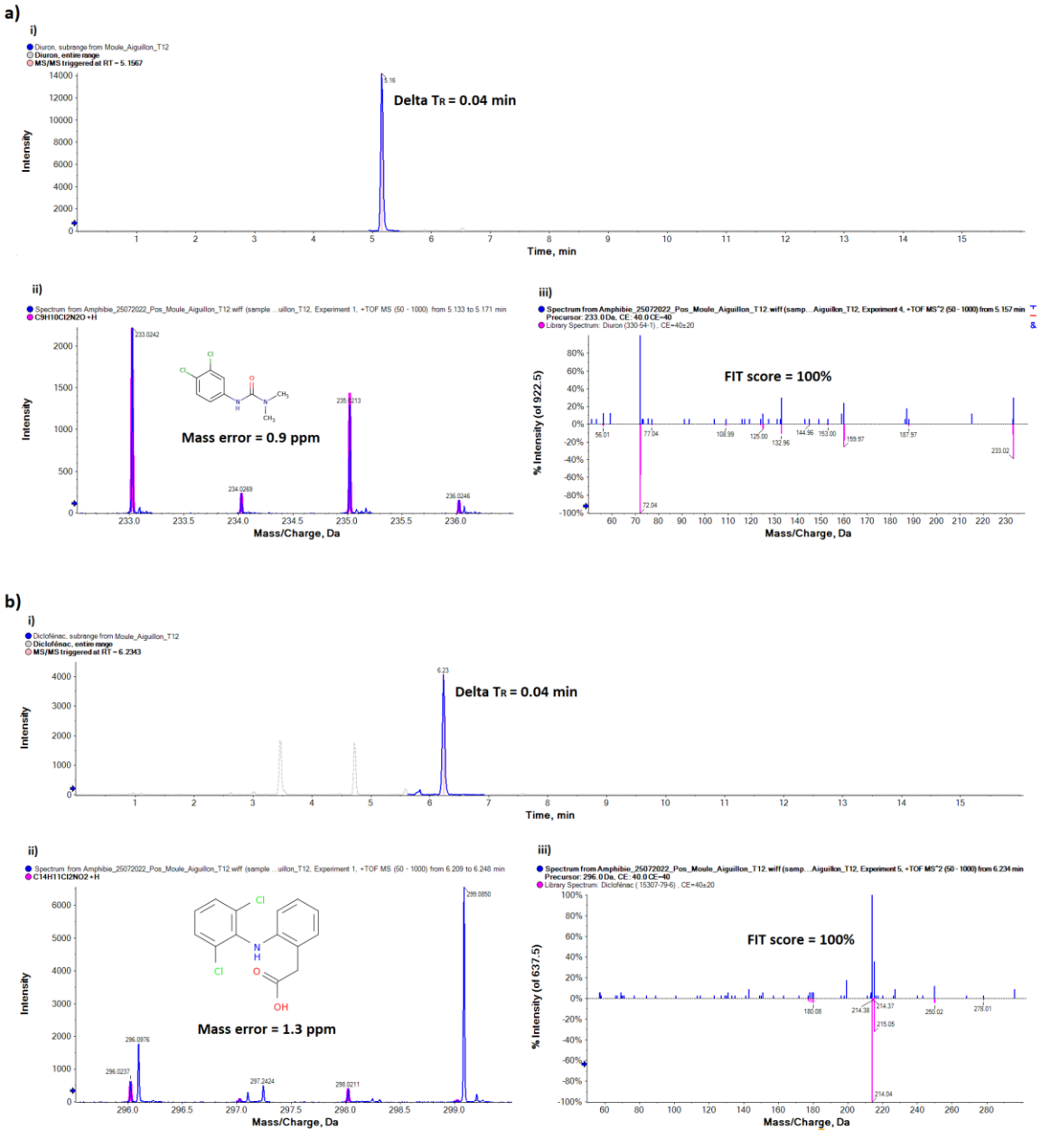

a)
SDL (mg.kg-1)
0.001 0.01 0.1 > 0.1
2%
6%
6%
86%
b)
LOI (mg.kg-1)
0.001 0.01 0.1 > 0.1
15%
7%
11%
67%
c)
Detection rates (%)
d)
Identification rates (%)
Oysters A
Oysters B
Mussels A
Mussels B
Scallops (Pecten maximus) A
Scallops (Pecten maximus) B
scallops (Mimachlamys varia) A
scallops (Mimachlamys varia) B
Clams A
Clams B
Cod A
Cod B
Salmon A
Salmon B
Sole A
Sole B
Anchovies A
Anchovies B
Tuna A
Tuna B
Spiny lobster A
Spiny lobster B
Crayfish A
Crayfish B
0 20 40 60 80 100
0.001 mg.kg-1
0.01 mg.kg-1
0.1 mg.kg-1

Fig. 5.


a)
i)
Diuron, subrange from Moule_Aiguillon_T12
Diuron, entire range
MS/MS triggered at RT = 5.1567
Intensity
Time, min
Delta TR = 0.04 min
ii)
Spectrum from Amphibie_25072022_Pos_Moule_Aiguillon_T12.wiff (sample ...uillon_T12, Experiment 1, +TOF MS (50 - 1000) from 5.133 to 5.171 min
C9H10Cl2N2O +H
Mass error = 0.9 ppm
Mass/Charge, Da
iii)
Spectrum from Amphibie_25072022_Pos_Moule_Aiguillon_T12.wiff (samp...Aiguillon_T12, Experiment 4, +TOF MS^2 (50 - 1000) from 5.157 min
Precursor: 233.0 Da, CE: 40.0 CE=40
Library Spectrum: Diuron (330-54-1) , CE=40±20
FIT score = 100%
% Intensity (of 922.5)
Mass/Charge, Da
b)
i)
Diclofénac, subrange from Moule_Aiguillon_T12
Diclofénac, entire range
MS/MS triggered at RT = 6.2343
Intensity
Time, min
Delta TR = 0.04 min
ii)
Spectrum from Amphibie_25072022_Pos_Moule_Aiguillon_T12.wiff (sample ...uillon_T12, Experiment 1, +TOF MS (50 - 1000) from 6.209 to 6.248 min
C14H11Cl2NO2 +H
Mass error = 1.3 ppm
Mass/Charge, Da
iii)
Spectrum from Amphibie_25072022_Pos_Moule_Aiguillon_T12.wiff (samp...Aiguillon_T12, Experiment 5, +TOF MS^2 (50 - 1000) from 6.234 min
Precursor: 296.0 Da, CE: 40.0 CE=40
Library Spectrum: Diclofénac (15307-79-6) , CE=40±20
FIT score = 100%
% Intensity (of 637.5)
Mass/Charge, Da

860

Table 1. Control factors and levels in the sample preparation process

Level	Factor		
	Extraction solvent	**dSPE sorbent**	**Dilution**
1	ACN	$MgSO_4$/PSA/C18	Not diluted
2	MeOH/ACN (7:3)	EMR-lipid	1:2
3	MeOH (1% FA)	PSA/Na_2SO_4/C18EC	1:4

ACN, acetonitrile; MeOH, methanol; EMR, Enhanced Matrix Removal; PSA, primary and secondary amines

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Supplementary Materials

Table S1. List of the target contaminants with their corresponding formulae, adduct or in-source fragments, theoretical m/z, retention times (T_R) and LogP values.

Compound	MRL ($mg.kg^{-1}$)*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
1-(3,4-Dichlorophenyl)-3-methylurea	0.01	$C_8H_8Cl_2N_2O$	$[M-H]^-$	219.00864	4.78	2.94
1-(4-Nitrophenyl)-3-propylure	0.01	$C_{10}H_{13}N_3O_3$	$[M-H]^-$	224.10297	4.69	2.4**
1,2-Benzisothiazol-3(*2H*)-one	0.01	C_7H_5NOS	$[M+H]^+$	152.01646	2.78	1.95
1,3-Diphenylurea	0.01	$C_{13}H_{12}N_2O$	$[M+H]^+$	213.10224	5.19	3
2,3,5-Trimethacarb	0.01	$C_{11}H_{15}NO_2$	$[M+H]^+$	194.11756	5.35	2.5
2,4-Dimethylaniline	0.01	$C_8H_{11}N$	$[M+H]^+$	122.09643	2.47	1.68
2,6-Dichlorobenzamide	0.01	$C_7H_5Cl_2NO$	$[M+H]^+$	189.9821	2.71	0.77
2,6-Diethylaniline	0.01	$C_{10}H_{15}N$	$[M+H]^+$	150.12773	5.75	2.7
2-Ethylhexyl diphenyl phosphate	0.01	$C_{20}H_{27}O_4P$	$[M+H]^+$	363.17197	8.64	6.3
2-N-Octyl-4-isothiazolin-3-one	0.01	$C_{11}H_{19}NOS$	$[M+H]^+$	214.12601	6.29	2.45
3,4-Dichloroaniline	0.01	$C_6H_5Cl_2N$	$[M+H]^+$	161.98718	5.32	2.7
3,4,5-Trimethacarb	0.01	$C_{11}H_{15}NO_2$	$[M+H]^+$	194.11756	5.28	2.7
3-Hydroxycarbofuran	0.01	$C_{12}H_{15}NO_4$	$C_{12}H_{14}NO_3^+$	220.09682	3.08	0.76
3-Ketocarbofuran	0.01	$C_{12}H_{13}NO_4$	$[M+H]^+$	236.09173	4.03	1.8
4-Acethylaminoantipyrine	0.01	$C_{13}H_{15}N_3O_2$	$[M+Na]^+$	246.12370	2.27	0
4-Aminoantipyrine	0.01	$C_{11}H_{13}N_3O$	$[M+H]^+$	204.11314	2.24	0.1
4-Bromo-3,5-dimethylphenyl-N-methylcarbamate	0.01	$C_{10}H_{12}BrNO_2$	$[M+H]^+$	258.01242	5.91	3.1
4-Dimethylaminoantipyrine	0.01	$C_{13}H_{17}N_3O$	$[M+H]^+$	232.14444	1.98	1

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
4-Formylaminoantipyrine	0.01	$C_{12}H_{13}N_3O_2$	$[M+H]^+$	232.10805	2.24	0
4-Methylaminoantipyrine	0.01	$C_{12}H_{15}N_3O$	$[M+H]^+$	218.12879	1.86	0
5-Hydroxy-flunixin	0.01	$C_{14}H_{11}F_3N_2O_3$	$[M+H]^+$	313.07945	5.10	3.7
8-Hydroxy-mutilin	0.01	$C_{20}H_{32}O_4$	$[M+H]^+$	337.23734	3.61	/
Abamectin	0.01	$C_{48}H_{72}O_{14}$	$[M+Na]^+$	895.48143	8.78	3.8
Abamectin B1a	0.01	$C_{48}H_{72}O_{14}$	$[M+Na]^+$	873.49948	8.86	3.8
Abamectin B1b	0.01	$C_{47}H_{70}O_{14}$	$[M+CH_3COO]^-$	876.51038	/	3.5
Abate® (temephos)	0.01	$C_{16}H_{20}O_6P_2S_3$	$[M+H]^+$	466.99701	8.03	6
Acephate	0.01	$C_4H_{10}NO_3PS$	$C_2H_8O_3PS^+$	142.99263	0.96	-0.8
Acetamiprid	0.01	$C_{10}H_{11}ClN_4$	$[M+H]^+$	223.0745	3.44	0.8
Acibenzolar-*S*-methyl	0.01	$C_8H_6N_2OS_2$	$[M+H]^+$	210.99943	6.07	3.1
Aclonifen	0.01	$C_{12}H_9ClN_2O_3$	$[M+H]^+$	265.03745	6.93	4.04
Aconitine	0.01	$C_{34}H_{47}NO_{11}$	$[M+H]^+$	646.32219	4.71	0.3**
Akton	0.01	$C_{12}H_{14}Cl_3O_3PS$	$[M+H]^+$	374.95396	8.3	4.8**
Alachlor	0.01	$C_{14}H_{20}ClNO_2$	$[M+H]^+$	270.12553	6.68	3.5
Albendazole	0.01	$C_{12}H_{15}N_3O_2S$	$[M+H]^+$	266.09578	4.80	2.7
Albendazole amino sulfone	0.01	$C_{10}H_{13}N_3O_2S$	$[M+H]^+$	240.08013	1.96	1.4
Albendazole sulfone	0.01	$C_{12}H_{15}N_3O_4S$	$[M+H]^+$	298.08560	3.44	1.6
Albendazole sulfoxide	0.01	$C_{12}H_{15}N_3O_3S$	$[M+H]^+$	282.09069	2.93	1.3
Aldicarb	0.01	$C_7H_{14}N_2O_2S$	$[M+Na]^+$	213.06682	3.8	1.13
Aldicarb sulfone	0.01	$C_7H_{14}N_2O_4S$	$[M+H]^+$	223.07471	3.44	0.79
Aldicarb sulfoxide	0.01	$C_7H_{14}N_2O_3S$	$[M+H]^+$	207.07979	0.94	-0.2
Allethrin	0.01	$C_{19}H_{26}O_3$	$[M+H]^+$	303.19547	8.08	4.78

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Allidochlor	0.01	$C_8H_{12}ClNO$	$[M+H]^+$	174.06802	4.23	1.83
Alloxydim sodium	0.01	$C_{17}H_{24}NNaO_5$	$[M+H]^+$	346.16249	7.12	/
Alpha-cypermethrin	0.01	$C_{22}H_{19}Cl_2NO_3$	$[M+H]^+$	433.10802	8.74	6.6
Ametoctradin	0.01	$C_{15}H_{25}N_5$	$[M+H]^-$	276.21827	6.57	4.6**
Ametryne	0.01	$C_9H_{17}N_5S$	$[M+H]^+$	228.12774	5.03	2.98
Amicarbazone	0.01	$C_{10}H_{19}N_5O_2$	$[M+H]^+$	242.16115	4.06	1.23
Amidosulfuron	0.01	$C_9H_{15}N_5O_7S_2$	$[M+H]^+$	370.04857	4.77	1.63
Amino flubendazole	0.01	$C_{14}H_{10}FN_3O$	$[M+H]^+$	256.08807	3.21	1.6
Amino mebendazole	0.01	$C_{14}H_{11}N_3O$	$[M+H]^+$	238.09749	3.02	2.6
Aminocarb	0.01	$C_{11}H_{16}N_2O_2$	$[M+H]^+$	209.12845	1.71	1.9
Amitraze	0.01	$C_{19}H_{23}N_3$	$[M+H]^+$	294.19647	8.58	5.5
Amoxicillin	0.01	$C_{16}H_{19}N_3O_5S$	$[M+H]^+$	366.11182	0.92	-2
Ampicillin +4	0.01	$C_{16}H_{19}N_3O_4S$	$[M+H]^+$	350.11690	0.95	-1.1
Ancymidol	0.01	$C_{15}H_{16}N_2O_2$	$[M+H]^+$	257.12845	4.26	1..91
Anilazine	0.01	$C_9H_5Cl_3N_4$	$[M+H]^+$	274.96526	6.26	3.88
Anilofos	0.01	$C_{13}H_{19}ClNO_3PS_2$	$[M+H]^+$	368.03053	7.12	3.81
Antipyrine phenazone	0.01	$C_{11}H_{12}N_2O$	$[M+H]^+$	189.10224	2.88	0.4
Aspon ™	0.01	$C_{12}H_{28}O_5P_2S_2$	$[M+H]^+$	379.09262	8.73	6
Asulam	0.01	$C_8H_{10}N_2O_4S$	$[M+H]^+$	231.04341	2.25	-0.27
Atraton	0.01	$C_9H_{17}N_5O$	$[M+H]^+$	212.15059	3.75	2.7
Atrazine	0.01	$C_8H_{14}ClN_5$	$[M+H]^+$	216.10105	5.12	2.6
Atrazine desisopropyl	0.01	$C_5H_8ClN_5$	$[M+H]^+$	174.0541	2.51	1.1**
Avilamycin	0.01	$C_{61}H_{88}Cl_2O_{32}$	$[M+H]^+$	1403.47085	/	/

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Azaconazole	0.01	$C_{12}H_{11}Cl_2N_3O_2$	$[M+H]^+$	300.03011	5.21	2.32
Azadirachtin	0.01	$C_{35}H_{44}O_{16}$	$[M+H]^+$	721.27021	5.01	1.09
Azamethiphos	0.01	$C_9H_{10}ClN_2O_5PS$	$[M+H]^+$	324.98094	4.44	1.05
Azimsulfuron	0.01	$C_{13}H_{16}N_{10}O_5S$	$[M+H]^+$	425.10986	5.03	0.65
Aziprotryne	0.01	$C_7H_{11}N_7S$	$[M+H]^+$	226.08694	6.15	3
Azoxystrobin	0.01	$C_{22}H_{17}N_3O_5$	$[M+H]^+$	404.1241	6.16	2.5
Bacitracin A	0.01	$C_{66}H_{103}N_{17}O_{16}S$	$[M+H]^+$	1422.75622	/	/
Baquiloprim	0.01	$C_{17}H_{20}N_6$	$[M+NH_4]^+$	326.20877	/	/
Barban	0.01	$C_{11}H_9Cl_2NO_2$	$[M+H]^+$	258.00831	6.25	3.47
Beflubutamid	0.01	$C_{18}H_{17}F_4NO_2$	$[M+H]^+$	356.12682	6.96	4.7
Benalaxyl	0.01	$C_{20}H_{23}NO_3$	$[M+H]^+$	326.17507	7.04	3.4
Benazolin	0.01	$C_9H_6ClNO_3S$	$[M+H]^+$	243.98297	3.88	2.5
Bendiocarb	0.01	$C_{11}H_{13}NO_4$	$[M+H]^+$	224.09173	4.7	1.7
Benfluralin (benefin)	0.01	$C_{13}H_{16}F_3N_3O_4$	$[M+H]^+$	336.11657	8.17	5.29
Benfuresate	0.01	$C_{12}H_{16}O_4S$	$[M+H]^+$	257.08421	6	2.41
Benodanil	0.01	$C_{13}H_{10}INO$	$[M+H]^+$	323.98799	5.67	2.85
Benomyl	0.01	$C_{14}H_{18}N_4O_3$	$[M+H]^+$	291.14517	6.1	2.12
Benoxacor	0.01	$C_{11}H_{11}Cl_2NO_2$	$[M+H]^+$	260.02396	6.06	2.7
Bensulfuron-methyl	0.01	$C_{16}H_{18}N_4O_7S$	$[M+H]^+$	411.0969	5.44	2.18
Bensulide	0.01	$C_{14}H_{24}NO_4PS_3$	$[M+H]^+$	398.06779	7.09	4.2
Bentazon	0.01	$C_{10}H_{12}N_2O_3S$	$[M+H]^+$	241.06414	4.48	2.34
Bentazon-methyl	0.01	$C_{11}H_{14}N_2O_3S$	$[M+H]^+$	255.07979	5.32	2.31
Benthiavalicarb-isopropyl	0.01	$C_{18}H_{24}FN_3O_3S$	$[M+H]^+$	382.15952	5.93	2.52

Compound	MRL ($mg.kg^{-1}$)*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Benzoximate	0.01	$C_{18}H_{18}ClNO_5$	$C_9H_8ClO_3^+$	199.01565	7.53	3.73
Benzoylprop ethyl	0.01	$C_{18}H_{17}Cl_2NO_3$	$[M+H]^+$	366.06583	7.28	4.1**
Benzthiazuron	0.01	$C_9H_9N_3OS$	$[M+H]^-$	208.05391	3.88	1.6**
Bifenthrin	0.01	$C_{23}H_{22}ClF_3O_2$	$[M+H]^+$	423.13332	/	6
Bioresmethrin	0.01	$C_{22}H_{26}O_3$	$[M+H]^+$	339.19547	8.89	4.7
Bitertanole (mixture of isomers)	0.01	$C_{20}H_{23}N_3O_2$	$[M+H]^+$	338.1863	6.65	4.16
Bixafen	0.01	$C_{18}H_{12}Cl_2F_3N_3O$	$[M+H]^-$	414.03823	6.69	4.7**
Bladex	0.01	$C_9H_{13}ClN_6$	$[M+H]^+$	241.0963	4.4	2.22
Boscalid	0.01	$C_{18}H_{12}Cl_2N_2O$	$[M+H]^+$	343.03995	6.32	2.96
Bromacil	0.01	$C_9H_{13}BrN_2O_2$	$[M+H]^-$	261.02332	4.18	2.11
Bromofenvinphos-ethyl	0.01	$C_{12}H_{14}BrCl_2O_4P$	$[M+H]^+$	404.92397	7.03	3.2**
Bromophos-methyl	0.01	$C_8H_8BrCl_2O_3PS$	$[M+H]^+$	366.85409	8.06	5.21
Bromuconazole (mixture of isomers)	0.01	$C_{13}H_{12}BrCl_2N_3O$	$[M+H]^+$	377.95902	6.12	3.24
Bufencarb	0.01	$C_{26}H_{38}N_2O_4$	$[M+H]^+$	443.29043	/	/
Bupirimate	0.01	$C_{13}H_{24}N_4O_3S$	$[M+H]^+$	317.16419	6.49	2.7
Buprofezin	0.01	$C_{16}H_{23}N_3OS$	$[M+H]^+$	306.16346	7.96	4.3
Butachlor	0.01	$C_{17}H_{26}ClNO_2$	$[M+H]^+$	312.17248	8.11	4.5
Butafenacil	0.01	$C_{20}H_{18}ClF_3N_2O_6$	$[M+NH_4]^+$	492.11437	6.72	3.2
Butocarboxim	0.01	$C_7H_{14}N_2O_2S$	$[M+H]^+$	191.08488	4	1.1
Butocarboxim sulfoxide	0.01	$C_7H_{14}N_2O_3S$	$[M+Na]^+$	229.06174	0.96	-1.02
Butoxycarboxim	0.01	$C_7H_{14}N_2O_4S$	$[M+H]^+$	223.07471	3.44	-0.1
Butroxydim	0.01	$C_{24}H_{33}NO_4$	$[M+H]^+$	400.24824	8.14	1.9
Buturon	0.01	$C_{12}H_{13}ClN_2O$	$[M+H]^+$	237.07892	5.57	3**

Compound	MRL ($mg.kg^{-1}$)*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Butylate	0.01	$C_{11}H_{23}NOS$	$[M+H]^+$	218.15731	7.97	4.15
Cadusafos	0.01	$C_{10}H_{23}O_2PS_2$	$[M+H]^+$	271.09499	7.33	3.9
Cafenstrole	0.01	$C_{16}H_{22}N_4O_3S$	$[M+H]^+$	351.14854	6.62	3.21
Carbaryl	0.01	$C_{12}H_{11}NO_2$	$C_{10}H_9O^+$	145.06479	4.89	2.36
Carbendazim	0.01	$C_9H_9N_3O_2$	$[M+H]^+$	192.07675	2.19	1.52
Carbetamide	0.01	$C_{12}H_{16}N_2O_3$	$[M+H]^+$	237.12337	4.04	1,75
Carbofuran	0.01	$C_{12}H_{15}NO_3$	$[M+H]^+$	222.11247	4.75	2.32
Carbophenothion	0.01	$C_{11}H_{16}ClO_2PS_3$	$[M+H]^+$	342.98114	8.39	5.33
Carboxine	0.01	$C_{12}H_{13}NO_2S$	$[M+H]^+$	236.07398	5.07	2.14
Carfentrazone-ethyl	0.01	$C_{15}H_{14}Cl_2F_3N_3O_3$	$[M+H]^+$	412.04371	6.93	3.36
Carprofen	0.01	$C_{15}H_{12}ClNO_2$	$[M+H]^+$	274.06293	6.01	4
Carpropamid	0.01	$C_{15}H_{18}Cl_3NO$	$[M+H]^+$	334.05267	7.1	4.23
Cefacetrile	0.01	$C_{13}H_{13}N_3O_6S$	$[M+H]^+$	357.08633	/	/
Cefalexine	0.01	$C_{16}H_{17}N_3O_4S$	$[M+H]^+$	348.10125	0.95	0.6
Cefapirine	0.01	$C_{17}H_{17}N_3O_6S_2$	$[M-H]^+$	424.06316	0.95	-1.1
Cefazolin	0.01	$C_{14}H_{14}N_8O_4S_3$	$[M+H]^+$	455.03729	2.41	-0.6
Cefoperazone	0.01	$C_{25}H_{27}N_9O_8S_2$	$[M+H]^+$	646.14968	2.90	-0.7
Ceftiofur +4	0.01	$C_{19}H_{17}N_5O_7S_3$	$[M+H]^+$	524.03629	3.58	0.2
Ceftriaxone (CAS)	0.01	$C_{18}H_{18}N_8O_7S_3$	$[M+H]^+$	555.05334	/	/
Cefuroxim	0.01	$C_{16}H_{16}N_4O_8S$	$[M-H]^-$	442.10271	2.58	-0.2
Cephradine	0.01	$C_{16}H_{19}N_3O_4S$	$[M+H]^+$	350.11690	0.95	/
Chinomethionate	0.01	$C_{10}H_6N_2OS_2$	$[M+H]^+$	234.99943	7.38	3.78
Chlorantraniliprole	0.01	$C_{18}H_{14}BrCl_2N_5O_2$	$[M+H]^+$	483.97579	5.68	2.76

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Chlorbromuron	0.01	$C_9H_{10}BrClN_2O_2$	$[M+H]^+$	294.96648	6.1	3.09
Chlorbufam	0.01	$C_{11}H_{10}ClNO_2$	$[M+H]^+$	224.04728	4.95	3.59
Chlordimeform	0.01	$C_{10}H_{13}ClN_2$	$[M+H]^+$	197.084	2.64	2.89
Chlorfenapyr	0.01	$C_{15}H_{11}BrClF_3N_2O$	$[M+H]^+$	408.97465	7.93	4.83
Chlorfenvinphos (mixture of Z and E)	0.01	$C_{12}H_{14}Cl_3O_4P$	$[M+H]^+$	358.97681	6.93	3.81
Chlorfluazuron	0.01	$C_{20}H_9Cl_3F_5N_3O_3$	$[M-H]^-$	539.97024	8.3	5.8
Chloridazon	0.01	$C_{10}H_8ClN_3O$	$[M+H]^+$	222.04287	3.19	1.14
Chlorimuron-ethyl	0.01	$C_{15}H_{15}ClN_4O_6S$	$[M+H]^+$	415.04736	6.06	2.5
Chlormephos	0.01	$C_5H_{12}ClO_2PS_2$	$[M+H]^+$	234.97777	/	3
Chlormequat chloride	0.01	$C_5H_{13}Cl_2N$	$[M+H]^+$	158.04978	/	/
Chlorobenzuron	0.01	$C_{14}H_{10}Cl_2N_2O_2$	$[M+H]^+$	309.01921	6.64	5**
Chlorosulfuron	0.01	$C_{12}H_{12}ClN_5O_4S$	$[M+H]^+$	358.03713	4.8	/
Chlorotoluron	0.01	$C_{10}H_{13}ClN_2O$	$[M+H]^+$	213.07892	4.93	2.41
Chloroxuron	0.01	$C_{15}H_{15}ClN_2O_2$	$[M+H]^+$	291.08948	6.07	3.7
Chlorpyrifos	0.01	$C_9H_{11}Cl_3NO_3PS$	$[M+H]^+$	349.93356	8.21	4.96
Chlorpyrifos-methyl	0.01	$C_7H_7Cl_3NO_3PS$	$[M+H]^+$	321.90226	7.49	4.31
Chlorpyrifos-oxon	0.01	$C_9H_{11}Cl_3NO_4P$	$[M+H]^+$	333.95641	6.48	3.5**
Chlortetracycline	0.01	$C_{22}H_{23}ClN_2O_8$	$[M+H]^+$	479.12157	/	/
Chlorthiamid	0.01	$C_7H_5Cl_2NS$	$[M+H]^+$	205.95925	4.16	1.4**
Chlorthiophos	0.01	$C_{11}H_{15}Cl_2O_3PS_2$	$[M+H]^+$	360.96501	8.36	6**
Chromafenozide	0.01	$C_{24}H_{30}N_2O_3$	$[M-H]^-$	395.23292	6.65	5**
Cinidon-ethyl	0.01	$C_{19}H_{17}Cl_2NO_4$	$[M+H]^+$	394.06074	7.85	4.51
Cinmethylin	0.01	$C_{18}H_{26}O_2$	$[M+NH_4]^+$	292.22711	8.08	4.62

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Cinosulfuron	0.01	$C_{15}H_{19}N_5O_7S$	$[M+H]^+$	414.1078	4.57	2.04
Cinoxacin	0.01	$C_{12}H_{10}N_2O_5$	$[M+H]^+$	263.06625	3.58	1.5
Ciprofloxacin	0.01	$C_{17}H_{18}FN_3O_3$	$[M+H]^+$	332.14050	2.46	-1.1
Clarithromycin	0.01	$C_{38}H_{69}NO_{13}$	$[M+H]^+$	748.48417	4.89	3.16
Clarithromycin	0.01	$C_{38}H_{69}NO_{13}$	$[M+H]^+$	748.48417	5.17	3.2
Clethodim	0.01	$C_{17}H_{26}ClNO_3S$	$[M+H]^+$	360.13947	7.86	4.21
Climbazol	0.01	$C_{15}H_{17}ClN_2O_2$	$[M+H]^+$	293.10513	5.02	3.76
Clindamycin	0.01	$C_{18}H_{33}ClN_2O_5S$	$[M+H]^+$	425.18715	3.30	2.2
Clodinafop (acid-free)	0.01	$C_{14}H_{11}ClFNO_4$	$[M+H]^+$	312.04334	5.76	3.4**
Clodinafop-propargyl	0.01	$C_{17}H_{13}ClFNO_4$	$[M+H]^+$	350.05899	7.11	3.9
Clofentezine	0.01	$C_{14}H_8Cl_2N_4$	$[M+H]^+$	303.01988	7.39	3.1
Clomeprop	0.01	$C_{16}H_{15}Cl_2NO_2$	$[M-H]^-$	324.05526	7.76	4.8
Cloquintocet-mexyl	0.01	$C_{18}H_{22}ClNO_3$	$[M+H]^+$	336.1361	7.9	5.03
Cloransulam-methyl	0.01	$C_{15}H_{13}ClFN_5O_5S$	$[M+H]^+$	430.03827	5.41	-0.365
Clorsulon	0.01	$C_8H_8Cl_3N_3O_4S_2$	$[M-H]^-$	401.89140	/	1.2
Closantel	0.01	$C_{22}H_{14}Cl_2I_2N_2O_2$	$[M+H]^+$	662.85946	9.00	7.2
Clothianidin	0.01	$C_6H_8ClN_5O_2S$	$[M+H]^+$	250.016	3.03	0.7
Cloxacillin	0.01	$C_{12}H_{10}N_2O_5$	$[M+H]^+$	263.06625	3.58	2.4
Command (clomazone)	0.01	$C_{12}H_{14}ClNO_2$	$[M+H]^+$	240.07858	5.69	2.5
Coumaphos	0.01	$C_{14}H_{16}ClO_5PS$	$[M+H]^+$	363.02174	7.33	4.13
Coumaphos-oxon	0.01	$C_{14}H_{16}ClO_6P$	$[M+H]^+$	347.04458	5.69	2.78
Crimidine	0.01	$C_7H_{10}ClN_3$	$[M+H]^+$	172.0636	3.73	1.31
Crotoxyphos	0.01	$C_{14}H_{19}O_6P$	$[M+NH_4]^+$	332.12575	5.89	3.3

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Crufomate	0.01	$C_{12}H_{19}ClNO_3P$	$[M+H]^+$	292.08639	6.23	3.42
Cumyluron	0.01	$C_{17}H_{19}ClN_2O$	$[M+H]^+$	303.12587	6.15	3.7
Cyanofenphos	0.01	$C_{15}H_{14}NO_2PS$	$[M+H]^+$	304.05557	7.17	4.29
Cyanophos	0.01	$C_9H_{10}NO_3PS$	$[M+H]^+$	244.01918	5.85	2.71
Cyantraniliprole	0.01	$C_{19}H_{14}BrClN_6O_2$	$[M+H]^+$	475.0102	5.17	3.9**
Cyazofamid	0.01	$C_{13}H_{13}ClN_4O_2S$	$[M+H]^+$	325.05205	6.92	3.2
Cyclanilide	0.01	$C_{11}H_9Cl_2NO_3$	$[M+H]^+$	274.00323	5.71	3.25
Cycloate	0.01	$C_{11}H_{21}NOS$	$[M+H]^+$	216.14166	7.62	3.88
Cyclohexamide	0.01	$C_{15}H_{23}NO_4$	$[M+H]^+$	282.16998	3.79	0.55
Cycloprothrin	0.01	$C_{26}H_{21}Cl_2NO_4$	$[M+H]^+$	482.09204	8.52	6.2**
Cyclosulfamuron	0.01	$C_{17}H_{19}N_5O_6S$	$[M+H]^+$	422.11288	6.36	2.05
Cycloxidim	0.01	$C_{17}H_{27}NO_3S$	$[M+H]^+$	326.17844	7.78	3.23
Cycluron	0.01	$C_{11}H_{22}N_2O$	$[M+H]^+$	199.18049	5.12	2.4**
Cyflufenamid	0.01	$C_{20}H_{17}F_5N_2O_2$	$[M+H]^+$	413.1283	7.55	4.7
Cyhalofop-butyl	0.01	$C_{20}H_{20}FNO_4$	$[M+H]^+$	358.14491	7.75	3.31
Cymiazole	0.01	$C_{12}H_{14}N_2S$	$[M+H]^+$	219.09505	3.19	3**
Cymoxanil	0.01	$C_7H_{10}N_4O_3$	$C_4H_6N_3O_2^+$	128.04545	3.66	0.59
Cypermethrin (mixture of isomers)	0.01	$C_{22}H_{19}Cl_2NO_3$	$[M+H]^+$	416.08148	8.78	6.6
Cyphenothrin	0.01	$C_{24}H_{25}NO_3$	$[M+H]^+$	376.19072	8.89	6.29
Cyprazine	0.01	$C_9H_{14}ClN_5$	$[M+H]^+$	228.10105	5.13	3.06
Cyproconazole (mixture of isomers)	0.01	$C_{15}H_{18}ClN_3O$	$[M+H]^+$	292.12112	6.17	2.9
Cyprodinil	0.01	$C_{14}H_{15}N_3$	$[M+H]^+$	226.13387	6.48	4
Cyprofuram	0.01	$C_{14}H_{14}ClNO_3$	$[M+H]^+$	280.0735	5.23	2.5**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Cyprosulfamide	0.01	$C_{18}H_{18}N_2O_5S$	$[M+H]^+$	375.10092	4.73	2.1**
Cyromazine	0.01	$C_6H_{10}N_6$	$[M+H]^+$	167.10397	0.94	-0.06
Cythioate	0.01	$C_8H_{12}NO_5PS_2$	$[M+H]^+$	297.99673	4.41	1.6**
Daimuron	0.01	$C_{17}H_{20}N_2O$	$[M+H]^+$	269.16484	6.22	2.7
Daminozide	0.01	$C_6H_{12}N_2O_3$	$[M+H]^+$	161.09207	0.9	-1.5
Danitol	0.01	$C_{22}H_{23}NO_3$	$[M+H]^+$	350.17507	8.59	5.7
Danofloxacin	0.01	$C_{19}H_{20}FN_3O_3$	$[M+H]^+$	358.15615	2.60	-0.3
Dapsone	0.01	$C_{12}H_{12}N_2O_2S$	$[M+H]^+$	249.06923	3.02	1
Dazomet	0.01	$C_5H_{10}N_2S_2$	$[M+H]^+$	163.03582	2.51	0.63
Dementon-*S*-methyl sulfone	0.01	$C_6H_{15}O_5PS_2$	$[M+H]^+$	263.01713	2.55	-0.3
Demeton O	0.01	$C_8H_{19}O_3PS_2$	$[M+H]^+$	259.0586	/	3.21
Demeton S	0.01	$C_8H_{19}O_3PS_2$	$[M+H]^+$	259.0586	5.51	2.09
Demeton-*S*-methyl	0.01	$C_6H_{15}O_3PS_2$	$[M+H]^+$	231.0273	4.48	1.02
Deoxynivalenol	0.01	$C_{15}H_{20}O_6$	$[M+H]^+$	297.13327	0.93	-0.71
Desethyl atrazine	0.01	$C_6H_{10}ClN_5$	$[M+H]^+$	188.06975	3.28	1.51
Desfuroylceftiofur cysteine disulfide (DCCD)	0.01	$C_{17}H_{20}N_6O_7S_4$	$[M+H]^+$	549.03491	/	-4.2
Desmedipham	0.01	$C_{16}H_{16}N_2O_4$	$[M+H]^+$	301.11828	5.78	3.39
Desmethyl norflurazon	0.01	$C_{11}H_7ClF_3N_3O$	$[M+H]^-$	290.03025	4.82	1.6**
Desmethyl-formamido-pirimicarb	0.01	$C_{11}H_{16}N_4O_3$	$[M+H]^+$	253.12952	4.36	0.9**
Desmetryn	0.01	$C_8H_{15}N_5S$	$[M+H]^+$	214.11209	4.36	2.38
Diafenthiuron	0.01	$C_{23}H_{32}N_2OS$	$[M+H]^+$	385.23081	8.52	6
Dialifos	0.01	$C_{14}H_{17}ClNO_4PS_2$	$[M+H]^+$	394.00979	7.6	4.69
Diazinon	0.01	$C_{12}H_{21}N_2O_3PS$	$[M+H]^+$	305.10833	7.39	3.81

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Diazinon-O-analog	0.01	$C_{12}H_{21}N_2O_4P$	$[M+H]^+$	289.13117	5.37	2.07
Dibrom	0.01	$C_4H_7Br_2Cl_2O_4P$	$[M+H]^+$	380.7876	5.46	1.38
Dichlofenthion	0.01	$C_{10}H_{13}Cl_2O_3PS$	$[M+H]^+$	314.97729	8.17	5.14
Dichlormid	0.01	$C_8H_{11}Cl_2NO$	$[M+H]^+$	208.02905	5.21	1.84
Dichlorvos	0.01	$C_4H_7Cl_2O_4P$	$[M+H]^+$	220.95318	4.4	1.43
Diclazuril	0.01	$C_{17}H_9Cl_3N_4O_2$	$[M-H]^-$	406.98639	6.46	4.1
Diclobutrazol	0.01	$C_{15}H_{19}Cl_2N_3O$	$[M+H]^+$	328.09779	6.49	3.8
Diclocymet	0.01	$C_{15}H_{18}Cl_2N_2O$	$[M+H]^+$	313.0869	6.74	4.3**
Diclofénac	0.01	$C_{14}H_{11}Cl_2NO_2$	$[M+H]^+$	296.02396	6.26	4
Diclosulam	0.01	$C_{13}H_{10}Cl_2FN_5O_3S$	$[M+H]^+$	405.99382	5.5	0.85
Dicrotophos	0.01	$C_8H_{16}NO_5P$	$[M+H]^+$	238.08389	2.57	0
Diethatyl-ethyl	0.01	$C_{16}H_{22}ClNO_3$	$[M+H]^+$	312.1361	6.96	3.6
Diethofencarb	0.01	$C_{14}H_{21}NO_4$	$[M+H]^+$	268.15433	6.01	2.91
Difenoconazole (mixture of isomers)	0.01	$C_{19}H_{17}Cl_2N_3O_3$	$[M+H]^+$	406.07197	7.18	4.3
Difenoxurone	0.01	$C_{16}H_{18}N_2O_3$	$[M+H]^+$	287.13902	5.28	2.54
Difloxacin	0.01	$C_{21}H_{19}F_2N_3O_3$	$[M+H]^+$	400.14672	3.04	1.6
Diflubenzuron	0.01	$C_{14}H_9ClF_2N_2O_2$	$[M+H]^+$	311.03934	6.43	3.88
Diflufenicen	0.01	$C_{19}H_{11}F_5N_2O_2$	$[M-H]^-$	395.08135	7.56	4.6**
Dimefox	0.01	$C_4H_{12}FN_2OP$	$[M+H]^+$	155.07441	2.66	-0.43
Dimefuron	0.01	$C_{15}H_{19}ClN_4O_3$	$[M+H]^+$	339.12184	5.64	2.51
Dimepiperate	0.01	$C_{15}H_{21}NOS$	$[M+H]^+$	264.14166	7.7	4.02
Dimethachlor	0.01	$C_{13}H_{18}ClNO_2$	$[M+H]^+$	256.10988	5.58	2.17
Dimethametryn	0.01	$C_{11}H_{21}N_5S$	$[M+H]^+$	256.15904	6.36	3.9

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Dimethenamid	0.01	$C_{12}H_{18}ClNO_2S$	$[M+H]^+$	276.08195	6.11	2.15
Dimethirimol	0.01	$C_{11}H_{19}N_3O$	$[M+H]^+$	210.16009	3.01	1.5**
Dimethoate	0.01	$C_5H_{12}NO_3PS_2$	$[M+H]^+$	230.0069	3.33	0.78
Dimethomorph	0.01	$C_{21}H_{22}ClNO_4$	$[M+H]^+$	388.13101	5.85	2.68
Dimethylvinphos	0.01	$C_{10}H_{10}Cl_3O_4P$	$[M+H]^+$	330.94551	6.19	3.13
Dimetilan	0.01	$C_{10}H_{16}N_4O_3$	$[M+H]^+$	241.12952	3.41	0.27
Dimetridazole	0.01	$C_5H_7N_3O_2$	$[M+H]^+$	142.06110	2.36	0.1
Dimoxystrobin	0.01	$C_{19}H_{22}N_2O_3$	$[M+H]^+$	327.17032	6.75	3.9**
Diniconazole (E isomer)	0.01	$C_{15}H_{17}Cl_2N_3O$	$[M+H]^+$	326.08214	6.82	4.3
Diniconazole (Z isomer)	0.01	$C_{15}H_{17}Cl_2N_3O$	$[M-H]^+$	326.08214	6.82	4.3
Dinitramine	0.01	$C_{11}H_{13}F_3N_4O_4$	$[M+H]^-$	323.09617	7.18	4.3
Dinotefuran	0.01	$C_7H_{14}N_4O_3$	$[M+H]^+$	203.11387	1.83	-0.55
Dioxacarb	0.01	$C_{11}H_{13}NO_4$	$[M+H]^+$	224.09173	3.37	0.67
Dioxathion (mixture of isomers)	0.01	$C_{12}H_{26}O_6P_2S_4$	$[M+H]^+$	457.01603	6.02	3
Diphenamid	0.01	$C_{16}H_{17}NO$	$[M+H]^+$	240.13829	5.62	2.17
Diphenyl phosphate	0.01	$C_{12}H_{11}O_4P$	$[M+H]^+$	251.04677	8.52	1.4**
Diphenylamine	0.01	$C_{12}H_{11}N$	$[M+H]^+$	170.09643	6.57	3.5
Dipropetryn	0.01	$C_{11}H_{21}N_5S$	$[M+H]^+$	256.15904	6.37	3.81
Disosultap	0.01	$C_5H_{11}NNa_2O_6S4$	$[M+H]^+$	355.93374	/	/
Disulfoton sulfone	0.01	$C_8H_{19}O_4PS_3$	$[M+H]^+$	307.02559	5.65	1.87
Disulfoton sulfoxide	0.01	$C_8H_{19}O_3PS_3$	$[M+H]^+$	291.03067	5	1.73
Ditalimfos	0.01	$C_{12}H_{14}NO_4PS$	$[M+H]^+$	300.04539	6.63	3.48
Dithianon	0.01	$C_{14}H_4N_2O_2S_2$	$[M+H]^+$	296.9787	6.45	2.84

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Dithiopyr	0.01	$C_{15}H_{16}F_5NO_2S_2$	$[M+H]^+$	402.06154	7.82	4.75
Diuron	0.01	$C_9H_{10}Cl_2N_2O$	$[M+H]^+$	233.02429	5.2	2.68
DMA	0.01	$C_8H_{11}N$	$[M+H]^+$	122.09643	2.55	1.8
DMF	0.01	$C_9H_{11}NO$	$[M+H]^+$	150.09134	3.98	1.5
DMPF	0.01	$C_{10}H_{14}N_2$	$[M+H]^+$	163.12298	2.43	1.7
DMST	0.01	$C_9H_{14}N_2O_2S$	$[M+H]^+$	215.08488	4.46	1.2**
Dodemorph	0.01	$C_{18}H_{35}NO$	$[M+H]^+$	282.27914	5.1	5.8**
Dodine	0.01	$C_{15}H_{33}N_3O_2$	$[M+H]^+$	288.26455	/	1.15
Doramectin	0.01	$C_{50}H_{74}O_{14}$	$[M+Na]^+$	921.49708	9.18	4.4
Doxycycline	0.01	$C_{22}H_{24}N_2O_8$	$[M+H]^+$	445.16054	/	/
Dyfonate ™	0.01	$C_{10}H_{15}OPS_2$	$[M+H]^+$	247.03747	7.39	3.94
Edifenphos	0.01	$C_{14}H_{15}O_2PS_2$	$[M+H]^+$	311.03239	6.91	3.48
Emamectin	0.01	$C_{49}H_{75}NO_{13}$	$[M+H]^+$	886.53112	6.92	5
Emamectin B1a	0.01	$C_{49}H_{75}NO_{13}$	$[M+H]^+$	886.53112	8.12	4.1
Empenthrin	0.01	$C_{18}H_{26}O_2$	$[M+H]^+$	275.20056	8.82	/
Enrofloxacin	0.01	$C_{19}H_{22}FN_3O_3$	$[M+H]^+$	360.17180	2.71	-0.2
Epi CTC	0.01	$C_{22}H_{23}ClN_2O_8$	$[M+H]^+$	479.12157	/	/
Epi OTC	0.01	$C_{22}H_{24}N_2O_9$	$[M+H]^+$	461.15546	/	/
Epi tetra	0.01	$C_{22}H_{24}N_2O_8$	$[M+H]^+$	445.16054	/	/
Epn	0.01	$C_{14}H_{14}NO_4PS$	$[M+H]^+$	324.04539	7.56	4.78
Epoxiconazole (iso)	0.01	$C_{17}H_{13}ClFN_3O$	$[M+H]^+$	330.08039	6.29	3.44
Eprinomectin	0.01	$C_{50}H_{75}NO_{14}$	$[M+H]^+$	914.52603	8.46	5.7
Eprinomectin B1a	0.01	$C_{50}H_{75}NO_{14}$	$[M+H]^+$	914.52603	8.48	3.8

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
EPTC (S-ethyl dipropylthiocarbamate)	0.01	$C_9H_{19}NOS$	$[M+H]^+$	190.12601	6.91	3.21
Erythromycin	0.01	$C_{37}H_{67}NO_{13}$	$[M+H]^+$	734.46852	4.15	3.06
Erythromycin	0.01	$C_{37}H_{67}NO_{13}$	$[M+H]^+$	734.46852	4.30	2.7
Esbiol	0.01	$C_{19}H_{26}O_3$	$[M+H]^+$	303.19547	8.07	/
Esprocarb	0.01	$C_{15}H_{23}NOS$	$[M+H]^+$	266.15731	8.06	4.6
Etaconazole	0.01	$C_{14}H_{15}Cl_2N_3O_2$	$[M+H]^+$	328.06141	6.34	3.1
Ethaboxam	0.01	$C_{14}H_{16}N_4OS_2$	$[M+H]^+$	321.08383	5.1	/
Ethametsulfuron-methyl	0.01	$C_{15}H_{18}N_6O_6S$	$[M+H]^+$	411.10813	4.93	1.59
Ethephone	0.01	$C_2H_6ClO_3P$	$[M+H]^+$	144.98159	/	/
Ethidimuron	0.01	$C_7H_{12}N_4O_3S_2$	$[M+H]^+$	265.04236	3.07	/
Ethiofencarb	0.01	$C_{11}H_{15}NO_2S$	$[M+H]^+$	226.08963	5.05	2.04
Ethiofencarb sulfone	0.01	$C_{11}H_{15}NO_4S$	$[M+H]^+$	258.07946	3.03	/
Ethiofencarb sulfoxide	0.01	$C_{11}H_{15}NO_3S$	$[M+H]^+$	242.08454	2.95	/
Ethion	0.01	$C_9H_{22}O_4P_2S_4$	$[M+H]^+$	384.9949	8.22	5.07
Ethiozin	0.01	$C_9H_{16}N_4OS$	$[M+H]^+$	229.11176	5.19	2.08
Ethiprole	0.01	$C_{13}H_9Cl_2F_3N_4OS$	$[M-H]^-$	396.9899	5.85	2.9
Ethirimol	0.01	$C_{11}H_{19}N_3O$	$[M+H]^+$	210.16009	3.07	2.22
Ethofenprox	0.01	$C_{25}H_{28}O_3$	$[M+H]^+$	377.21112	/	7.05
Ethofumesate	0.01	$C_{13}H_{18}O_5S$	$[M+H]^+$	287.09477	6.28	2.7
Ethoprophos (prophos)	0.01	$C_8H_{19}O_2PS_2$	$[M+H]^+$	243.06369	6.38	3.59
Ethoxyquin	0.01	$C_{14}H_{19}NO$	$[M+H]^+$	218.15394	6.19	4.05
Ethoxysulfuron	0.01	$C_{15}H_{18}N_4O_7S$	$[M+H]^+$	399.0969	6.07	/
Ethyclozate	0.01	$C_{11}H_{11}ClN_2O_2$	$[M+H]^+$	239.05818	5.28	/

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Etobenzanid	0.01	$C_{16}H_{15}Cl_2NO_3$	$[M+H]^+$	340.05018	7.25	/
Etoxazole	0.01	$C_{21}H_{23}F_2NO_2$	$[M+H]^+$	360.17696	8.46	5.59
Etrimfos	0.01	$C_{10}H_{17}N_2O_4PS$	$[M+H]^+$	293.07194	7.21	/
Famoxadone	0.01	$C_{22}H_{18}N_2O_4$	$[M+H]^+$	375.13393	7.21	4.65
Famphur	0.01	$C_{10}H_{16}NO_5PS_2$	$[M+H]^+$	326.02803	5.8	2.2
Fenamidone	0.01	$C_{17}H_{17}N_3OS$	$[M+H]^+$	312.11651	6.19	2.8
Fenamiphos	0.01	$C_{13}H_{22}NO_3PS$	$[M+H]^+$	304.11308	6.17	3.23
Fenamiphos sulfone	0.01	$C_{13}H_{22}NO_5PS$	$[M+H]^+$	336.10291	4.58	/
Fenamiphos sulfoxide	0.01	$C_{13}H_{22}NO_4PS$	$[M+H]^+$	320.108	4.04	/
Fenarimol	0.01	$C_{17}H_{12}Cl_2N_2O$	$[M+H]^+$	331.03995	6.17	3.6
Fenazaflor	0.01	$C_{15}H_7Cl_2F_3N_2O_2$	$[M+H]^+$	374.99094	/	/
Fenazaquin	0.01	$C_{20}H_{22}N_2O$	$[M+H]^+$	307.18049	8.51	5.51
Fenazox	0.01	$C_{12}H_{10}N_2O$	$[M+H]^+$	199.08659	7.02	#N/A
Fenbendazole	0.01	$C_{15}H_{13}N_3O_2S$	$[M+H]^+$	300.08013	5.45	3.6
Fenbuconazole	0.01	$C_{19}H_{17}ClN_4$	$[M+H]^+$	337.12145	6.5	3.23
Fenchlorazol-ethyl	0.01	$C_{12}H_8Cl_5N_3O_2$	$[M+H]^+$	403.91031	7.51	/
Fenchlorphos-oxon	0.01	$C_8H_8Cl_3O_4P$	$[M+H]^+$	304.92986	6.17	/
Fenclorim	0.01	$C_{10}H_6Cl_2N_2$	$[M+H]^+$	224.99808	/	4.2**
Fenfuram	0.01	$C_{12}H_{11}NO_2$	$[M+H]^+$	202.08626	5.14	2.2**
Fenhexamid	0.01	$C_{14}H_{17}Cl_2NO_2$	$[M+H]^+$	302.07091	6.31	3.51
Fenitrothion	0.01	$C_9H_{12}NO_5PS$	$[M+H]^+$	278.02466	6.58	3.3
Fenobucarb	0.01	$C_{12}H_{17}NO_2$	$[M+H]^+$	208.13321	5.87	2.78
Fenothiocarb	0.01	$C_{13}H_{19}NO_2S$	$[M+H]^+$	254.12093	6.76	3.3

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Fenoxanil	0.01	$C_{15}H_{18}Cl_2N_2O_2$	$[M+H]^+$	329.08181	6.89	4.5
Fenoxaprop	0.01	$C_{16}H_{12}ClNO_5$	$[M+H]^+$	334.04768	6.22	3.4**
Fenoxaprop-P-ethyl	0.01	$C_{18}H_{16}ClNO_5$	$[M+H]^+$	362.07898	7.7	4.1**
Fenoxycarb	0.01	$C_{17}H_{19}NO_4$	$[M+H]^+$	302.13868	5.94	4.3
Fenpiclonil	0.01	$C_{11}H_6Cl_2N_2$	$[M+H]^+$	236.99808	5.72	4.3**
Fenpropathrin	0.01	$C_{22}H_{23}NO_3$	$[M+H]^+$	350.17507	8.6	6
Fenpropidin	0.01	$C_{19}H_{31}N$	$[M+H]^+$	274.25293	5.25	5.5
Fenpropimorph	0.01	$C_{20}H_{33}NO$	$[M+H]^+$	304.26349	5.34	4.93
Fenpyroximate	0.01	$C_{24}H_{27}N_3O_4$	$[M+H]^+$	422.20743	8.46	5.01
Fensulfothion	0.01	$C_{11}H_{17}O_4PS_2$	$[M+H]^+$	309.03787	5.37	2.23
Fensulfothion-oxon	0.01	$C_{11}H_{17}O_5PS$	$[M+H]^+$	293.06071	3.56	1.4**
Fensulfothion-oxon sulfone	0.01	$C_{11}H_{17}O_6PS$	$[M+H]^+$	309.05563	4.11	1.5**
Fensulfothion sulfone	0.01	$C_{11}H_{17}O_5PS_2$	$[M+H]^+$	325.03278	5.94	2.6**
Fenthion	0.01	$C_{10}H_{15}O_3PS_2$	$[M+H]^+$	279.0273	7.14	4.1
Fenthion-oxon	0.01	$C_{10}H_{15}O_4PS$	$[M+H]^+$	263.05015	5.37	2.4**
Fenthion-oxon sulfoxide	0.01	$C_{10}H_{15}O_5PS$	$[M+H]^+$	279.04506	3.03	1**
Fenthion sulfoxide	0.01	$C_{10}H_{15}O_4PS_2$	$[M+H]^+$	295.02222	4.76	2.7**
Fenthion-ethyl	0.01	$C_{12}H_{19}O_3PS_2$	$[M+H]^+$	307.0586	7.86	5**
Fenthion sulfone	0.01	$C_{10}H_{15}O_5PS_2$	$[M+H]^+$	311.01713	5.41	2.8**
Fenthoxon sulfone	0.01	$C_{10}H_{15}O_6PS$	$[M+H]^+$	295.03998	3.57	1.1**
Fentin acetate as Fentin	0.01	$C_{20}H_{18}O_2Sn$	$[M+H]^+$	411.04016	/	3.43
Fenuron	0.01	$C_9H_{12}N_2O$	$[M+H]^+$	165.10224	3.19	0.98
Ferimzone	0.01	$C_{15}H_{18}N_4$	$[M+H]^+$	255.16042	4.37	3.5**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Fipronil	0.01	$C_{12}H_4Cl_2F_6N_4OS$	$[M+H]^-$	436.94598	6.87	4
Fipronil sulfide	0.01	$C_{12}H_4Cl_2F_6N_4S$	$[M-H]^-$	420.95107	7.3	5.5**
Fipronil-desulfinyl	0.01	$C_{12}H_4Cl_2F_6N_4$	$[M+H]^-$	388.979	7.05	4.6**
Flamprop-isopropyl	0.01	$C_{19}H_{19}ClFNO_3$	$[M+H]^+$	364.11103	7.25	4**
Flamprop-methyl (Metaven)	0.01	$C_{17}H_{15}ClFNO_3$	$[M+H]^+$	336.07973	6.47	3.2**
Flamprop-M-isopropyl	0.01	$C_{19}H_{19}ClFNO_3$	$[M+H]^+$	364.11103	7.25	4**
Flazasulfuron	0.01	$C_{13}H_{12}F_3N_5O_5S$	$[M+H]^+$	408.0584	5.48	1.08
Fleroxacin	0.01	$C_{17}H_{18}F_3N_3O_3$	$[M+H]^+$	370.13730	2.43	-0.1
Flonicamid	0.01	$C_9H_6F_3N_3O$	$[M+H]^+$	230.05357	2.71	0.3
Florasulam	0.01	$C_{12}H_8F_3N_5O_3S$	$[M+H]^+$	360.03727	4.63	1.22
Florfénicol	0.01	$C_{12}H_{14}Cl_2FNO_4S$	$[M+H]^+$	375.03429	3.33	0.8
Florfenicol amine	0.01	$C_{10}H_{14}FNO_3S$	$[M+H]^+$	270.05706	/	/
Fluacrypyrim	0.01	$C_{20}H_{21}F_3N_2O_5$	$[M+H]^+$	427.14753	7.64	4.1**
Fluazifop	0.01	$C_{15}H_{12}F_3NO_4$	$[M+H]^+$	328.07912	5.77	2.9**
Fluazifop-butyl	0.01	$C_{19}H_{20}F_3NO_4$	$[M+H]^+$	384.14172	8.04	4.5
Fluazifop-P-butyl	0.01	$C_{19}H_{20}F_3NO_4$	$[M+H]^+$	384.14172	8.03	4.5**
Fluazinam	0.01	$C_{13}H_4Cl_2F_6N_4O_4$	$[M-H]^-$	464.95866	7.9	4.01
Fluazuron	0.01	$C_{20}H_{10}Cl_2F_5N_3O_3$	$[M+H]^+$	506.00921	7.89	6.1**
Flubendazole	0.01	$C_{16}H_{12}FN_3O_3$	$[M+H]^+$	314.09355	4.68	2.9
Flubendiamide	0.01	$C_{23}H_{22}F_7IN_2O_4S$	$[M+H]^+$	683.03061	6.88	4.2
Flucarbazone sodium	0.01	$C_{12}H_{10}F_3N_4NaO_6S$	$[M+H]^+$	419.02436	4.21	-1.85
Fluchloralin	0.01	$C_{12}H_{13}ClF_3N_3O_4$	$[M+H]^+$	356.06195	7.69	5.07
Flucycloxuron	0.01	$C_{25}H_{20}ClF_2N_3O_3$	$[M+H]^+$	484.1234	8.11	6.1**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Flucythrinate	0.01	$C_{26}H_{23}F_2NO_4$	$[M+H]^+$	452.16679	/	6.2
Fludioxonil	0.01	$C_{12}H_6F_2N_2O_2$	$[M-H]^-$	249.04701	8.21	4.12
Flufenacet	0.01	$C_{14}H_{13}F_4N_3O_2S$	$[M+H]^+$	364.07374	6.7	3.2
Flufenoxuron	0.01	$C_{21}H_{11}ClF_6N_2O_3$	$[M+H]^+$	489.04352	8.09	6.16
Flumequine	0.01	$C_{14}H_{12}FNO_3$	$[M+H]^+$	262.08740	4.73	2.9
Flumestulam	0.01	$C_{12}H_9F_2N_5O_2S$	$[M-H]^-$	326.05178	7.76	0.21
Flumetralin	0.01	$C_{16}H_{12}ClF_4N_3O_4$	$[M+H]^+$	422.05252	8.23	5.2**
Flumiclorac-pentyl	0.01	$C_{21}H_{23}ClFNO_5$	$[M+NH_4]^+$	441.1587	7.88	4.8**
Flumioxazin	0.01	$C_{19}H_{15}FN_2O_4$	$[M+H]^+$	355.10886	5.84	2.55
Flumorph	0.01	$C_{21}H_{22}FNO_4$	$[M+H]^+$	372.16056	5.3	3.4**
Flunixin	0.01	$C_{14}H_{11}F_3N_2O_2$	$[M+H]^+$	297.08454	5.71	4.1
Fluoglycofene-ethyl	0.01	$C_{18}H_{13}ClF_3NO_7$	$[M+NH_4]^+$	465.06709	7.69	3.6**
Fluometuron	0.01	$C_{10}H_{11}F_3N_2O$	$[M-H]^-$	233.08962	5	2.42
Fluopicolide	0.01	$C_{14}H_8Cl_3F_3N_2O$	$[M+H]^+$	382.97271	6.41	3.26
Fluopyram	0.01	$C_{16}H_{11}ClF_6N_2O$	$[M+H]^+$	397.05369	6.46	4.5**
Fluorodifen	0.01	$C_{13}H_7F_3N_2O_5$	$[M+H]^+$	329.03798	7.01	3.7**
Fluotrimazol	0.01	$C_{22}H_{16}F_3N_3$	$[M+H]^+$	380.13691	/	5.7**
Fluoxastrobin	0.01	$C_{21}H_{16}ClFN_4O_5$	$[M+H]^+$	459.0866	6.69	2.86
Flupyradifurone	0.01	$C_{12}H_{11}ClF_2N_2O_2$	$[M+H]^+$	289.05499	3.72	2.3**
Flupyrsulfuron-methyl sodium	0.01	$C_{15}H_{13}F_3N_5NaO_7S$	$[M+H]^+$	488.04583	5.79	/
Fluquinconazole	0.01	$C_{16}H_8Cl_2FN_5O$	$[M+H]^+$	376.01627	6.34	3.24
Fluralaner	0.01	$C_{22}H_{17}Cl_2F_6N_3O_3$	$[M+H]^+$	556.06239	7.39	5.6
Flurenol-butyl	0.01	$C_{18}H_{18}O_3$	$[M+H]^+$	283.13287	/	3.6**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Flurenol-methyl	0.01	$C_{15}H_{12}O_3$	$[M+H]^+$	241.08592	4.36	2.3**
Fluridone	0.01	$C_{19}H_{14}F_3NO$	$[M+H]^+$	330.11003	5.86	1.87
Flurilazole	0.01	$C_{11}H_{13}Cl_2NO_3$	$[M+H]^+$	278.03453	3.66	2**
Flurochloridon (ISO)	0.01	$C_{12}H_{10}Cl_2F_3NO$	$[M+H]^+$	312.01643	6.56	3.4**
Fluroxypyr	0.01	$C_7H_5Cl_2FN_2O_3$	$[M+H]^+$	254.9734	4.03	2.2
Fluroxypyr-meptyl	0.01	$C_{15}H_{21}Cl_2FN_2O_3$	$[M+H]^+$	367.0986	8.43	5.4**
Flurprimidol	0.01	$C_{15}H_{15}F_3N_2O_2$	$[M+H]^+$	313.11584	5.92	3.3**
Flurtamone	0.01	$C_{18}H_{14}F_3NO_2$	$[M+H]^-$	334.10494	5.95	4.5**
Flusilazole	0.01	$C_{16}H_{15}F_2N_3Si$	$[M+H]^+$	316.10761	6.51	3.7
Fluthiacet-methyl	0.01	$C_{15}H_{15}ClFN_3O_3S_2$	$[M+H]^+$	404.03002	6.92	3.77
Flutolanil	0.01	$C_{17}H_{16}F_3NO_2$	$[M+H]^-$	324.12059	6.56	3.7
Flutriafol	0.01	$C_{16}H_{13}F_2N_3O$	$[M+H]^+$	302.10995	4.98	2.29
Fomesafen	0.01	$C_{15}H_{10}ClF_3N_2O_6S$	$[M-H]^-$	456.02385	6.13	2.4**
Foramsulfuron	0.01	$C_{17}H_{20}N_6O_7S$	$[M+H]^+$	453.1187	4.2	0.17
Forchlorfenuron	0.01	$C_{12}H_{10}ClN_3O$	$[M-H]^-$	248.05852	4.95	3.2
Formetanate HCl	0.01	$C_{11}H_{15}N_3O_2$	$[M+H]^+$	222.1237	0.95	/
Fosthiazate	0.01	$C_9H_{18}NO_3PS_2$	$[M+H]^+$	284.05385	5.05	1.68
Fuberidazole	0.01	$C_{11}H_8N_2O$	$[M+H]^+$	185.07094	2.55	2.67
Furalaxyl	0.01	$C_{17}H_{19}NO_4$	$[M+H]^+$	302.13868	5.94	2.61
Furathiocarb	0.01	$C_{18}H_{26}N_2O_5S$	$[M+H]^+$	383.16352	7.97	4.7
Furmecyclox	0.01	$C_{14}H_{21}NO_3$	$[M+H]^+$	252.15942	6.94	3.1**
Fusidic acid	0.01	$C_{31}H_{48}O_6$	$[M+H]^-$	534.37892	7.46	5.5
Gamithromycin	0.01	$C_{40}H_{76}N_2O_{12}$	$[M+H]^+$	777.54710	3.89	4.9

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Guthion-ethyl	0.01	$C_{12}H_{16}N_3O_3PS_2$	$[M+H]^+$	346.04435	6.67	3.4**
Guthion®	0.01	$C_{10}H_{12}N_3O_3PS_2$	$[M+H]^+$	318.01305	5.92	2.75
Halofenozide	0.01	$C_{18}H_{19}ClN_2O_2$	$[M+H]^+$	331.12078	5.99	3.22
Halofuginone	0.01	$C_{16}H_{17}BrClN_3O_3$	$[M+H]^+$	414.02146	3.40	1.4
Halosulfuron-methyl	0.01	$C_{13}H_{15}ClN_6O_7S$	$[M+H]^+$	435.04842	6.05	1.3**
Haloxyfop	0.01	$C_{15}H_{11}ClF_3NO_4$	$[M+H]^+$	362.04015	6.47	4.2**
Haloxyfop-2-ethoxyethyl	0.01	$C_{19}H_{19}ClF_3NO_5$	$[M+H]^+$	434.09766	7.81	4.7**
Haloxyfop-methyl	0.01	$C_{16}H_{13}ClF_3NO_4$	$[M+H]^+$	376.0558	7.51	4.5**
Haloxyfop-P-methyl	0.01	$C_{16}H_{13}ClF_3NO_4$	$[M+H]^+$	376.0558	7.52	4.5**
Heptenophos	0.01	$C_9H_{12}ClO_4P$	$[M+H]^+$	251.02345	5.31	2.32
Hexaconazole	0.01	$C_{14}H_{17}Cl_2N_3O$	$[M+H]^+$	314.08214	6.52	3.9
Hexaflumuron	0.01	$C_{16}H_8Cl_2F_6N_2O_3$	$[M+H]^-$	460.98889	7.37	5.68
Hexazinone	0.01	$C_{12}H_{20}N_4O_2$	$[M+H]^+$	253.1659	4.13	1.85
Hexythiazox	0.01	$C_{17}H_{21}ClN_2O_2S$	$[M+H]^+$	353.1085	8.23	5.57
HMMNI	0.01	$C_5H_7N_3O_3$	$[M+H]^+$	175.08257	1.81	-0.4
Hydroxy-flubendazole	0.01	$C_{16}H_{14}FN_3O_3$	$[M+H]^+$	316.10920	3.56	1.9
Hydroxy-mebendazole	0.01	$C_{16}H_{15}N_3O_3$	$[M+H]^+$	298.11862	3.30	2.3
Hydroxy-thiabendazole	0.01	$C_{10}H_7N_3OS$	$[M+H]^+$	218.03826	1.84	2.1
Hymexazole	0.01	$C_4H_5NO_2$	$[M+H]^+$	100.0393	1.73	0.1**
Imazalil	0.01	$C_{14}H_{14}Cl_2N_2O$	$[M+H]^+$	297.0556	4.47	3.82
Imazamethabenz-methyl	0.01	$C_{16}H_{20}N_2O_3$	$[M+H]^+$	289.15467	4.14	2.6**
Imazamox	0.01	$C_{15}H_{19}N_3O_4$	$[M+H]^+$	306.14483	3.19	0.73
Imazapic	0.01	$C_{14}H_{17}N_3O_3$	$[M+H]^+$	276.13427	3.3	0.39

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Imazaquin	0.01	$C_{17}H_{17}N_3O_3$	$[M+H]^+$	312.13427	4.45	2.5**
Imazethapyr	0.01	$C_{15}H_{19}N_3O_3$	$[M+H]^+$	290.14992	3.95	1
Imazosulfuron	0.01	$C_{14}H_{13}ClN_6O_5S$	$[M+H]^+$	413.04294	5.53	1.49
Imibenconazole	0.01	$C_{17}H_{13}Cl_3N_4S$	$[M+H]^-$	410.99993	7.69	5.8**
Imidacloprid	0.01	$C_9H_{10}ClN_5O_2$	$[M+H]^+$	256.05958	3.19	0.57
Imidacloprid-olefin	0.01	$C_9H_8ClN_5O_2$	$[M+H]^+$	254.04393	2.6	2**
Imidocarb dipropionate	0.01	$C_{25}H_{32}N_6O_5$	$[M+H]^+$	497.25069	/	/
Imiprothrin (mixture of isomers)	0.01	$C_{17}H_{22}N_2O_4$	$[M+H]^+$	319.16523	6.51	2.9
Inabenfide	0.01	$C_{19}H_{15}ClN_2O_2$	$[M+H]^+$	339.08948	5.55	3.7**
Indanofan	0.01	$C_{20}H_{17}ClO_3$	$[M+H]^+$	341.0939	5.47	4.1**
Indaziflam	0.01	$C_{16}H_{20}FN_5$	$[M+H]^+$	302.17755	5.78	3.2**
Indoxacarb	0.01	$C_{22}H_{17}ClF_3N_3O_7$	$[M+H]^+$	528.07799	7.52	4.65
Iodofenphos	0.01	$C_8H_8Cl_2IO_3PS$	$[M+H]^+$	412.84264	8.14	5.51
Iodosulfuron-methyl sodium	0.01	$C_{14}H_{13}IN_5NaO_6S$	$[M+H]^+$	529.96018	5.57	/
Ipconazole	0.01	$C_{18}H_{28}N_2O_3$	$[M+H]^+$	321.21727	6.08	4.1**
Iprobenfos	0.01	$C_{13}H_{21}O_3PS$	$[M+H]^+$	289.10218	6.61	3
Iprodione	0.01	$C_{13}H_{13}Cl_2N_3O_3$	$[M+H]^+$	330.04067	6.49	3.34
Ipronidazole	0.01	$C_7H_{11}N_3O_2$	$[M+H]^+$	170.09240	3.79	1.1
Ipronidazole OH	0.01	$C_7H_{11}N_3O_3$	$[M+H]^+$	186.08732	2.79	-0.5
Iprovalicarb	0.01	$C_{18}H_{28}N_2O_3$	$[M+H]^+$	321.21727	6.14	3.37**
Irgarol (cybutryne)	0.01	$C_{11}H_{19}N_5S$	$[M+H]^+$	254.14339	5.99	3.95
Isazophos	0.01	$C_9H_{17}ClN_3O_3PS$	$[M+H]^+$	314.04896	6.89	3.82
Isocarbamide	0.01	$C_8H_{15}N_3O_2$	$[M+H]^+$	186.1237	3.14	0.8**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Isofenphos	0.01	$C_{15}H_{24}NO_4PS$	$[M+H]^+$	346.12365	7.64	4.12
Isofenphos-methyl	0.01	$C_{14}H_{22}NO_4PS$	$[M+H]^+$	332.108	7.27	3.8**
Isofenphos-oxon	0.01	$C_{15}H_{24}NO_5P$	$[M+H]^+$	330.14649	6.02	2.4**
Isomethiozin	0.01	$C_{12}H_{20}N_4OS$	$[M+H]^+$	269.14306	6.2	3.5**
Isonoruron	0.01	$C_{13}H_{22}N_2O$	$[M+H]^+$	223.18049	5.46	2.3**
Isoprocarb	0.01	$C_{11}H_{15}NO_2$	$[M+H]^+$	194.11756	5.34	2.31
Isopropalin	0.01	$C_{15}H_{23}N_3O_4$	$[M+H]^+$	310.17613	8.73	5.6**
Isoprothiolane	0.01	$C_{12}H_{18}O_4S_2$	$[M+H]^+$	291.07193	6.59	2.88
Isoproturon	0.01	$C_{12}H_{18}N_2O$	$[M+H]^+$	207.14919	5.19	2.87
Isouron	0.01	$C_{10}H_{17}N_3O_2$	$[M+H]^+$	212.13935	4.34	1.6**
Isoxaben	0.01	$C_{18}H_{24}N_2O_4$	$[M+H]^+$	333.18088	6.4	3.94
Isoxadifen-ethyl	0.01	$C_{18}H_{17}NO_3$	$[M+H]^+$	296.12812	7.03	3.5
Isoxaflutole	0.01	$C_{15}H_{12}F_3NO_4S$	$[M+H]^+$	360.05119	6	2.32
Isoxathion	0.01	$C_{13}H_{16}NO_4PS$	$[M+H]^+$	314.06104	7.53	3.73
Ivermectin	0.01	$C_{48}H_{74}O_{14}$	$[M+Na]^+$	897.49708	9.69	5.83
Ivermectin B1a	0.01	$C_{48}H_{74}O_{14}$	$[M+Na]^+$	875.51513	9.74	3.8
Josamycin	0.01	$C_{42}H_{69}NO_{15}$	$[M+H]^+$	828.47400	5.49	2.9
Karbutilate	0.01	$C_{14}H_{21}N_3O_3$	$[M+H]^+$	280.16557	4.62	1.7**
Ketoprofen	0.01	$C_{16}H_{14}O_3$	$[M+H]^+$	255.10157	5.26	3.12
Ketotriclabendazole	0.01	$C_{13}H_7Cl_3N_2O_2$	$[M+H]^+$	328.96459	5.90	4
Kresoxim-methyl	0.01	$C_{18}H_{19}NO_4$	$[M+H]^+$	314.13868	6.86	3.4
Lactofen	0.01	$C_{19}H_{15}ClF_3NO_7$	$[M+NH_4]^+$	479.08274	7.97	4.81
Lambda cyhalothrin	0.01	$C_{23}H_{19}ClF_3NO_3$	$[M+H]^+$	450.10783	/	7

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Lasalocid A	0.01	$C_{34}H_{54}O_8$	$[M+NH_4]^+$	608.41569	9.37	6.4
Lenacil	0.01	$C_{13}H_{18}N_2O_2$	$[M-H]^-$	235.1441	4.59	1.7**
Leptophos	0.01	$C_{13}H_{10}BrCl_2O_2PS$	$[M+H]^+$	412.87485	8.86	6.3**
Levamisole	0.01	$C_{11}H_{12}N_2S$	$[M+H]^+$	205.07940	2.07	1.8
Levofloxacin	0.01	$C_{18}H_{20}FN_3O_4$	$[M+H]^+$	362.15106	2.32	-0.39
Lincomycin	0.01	$C_{18}H_{34}N_2O_6S$	$[M+H]^+$	407.22104	0.95	0.2
Linuron	0.01	$C_9H_{10}Cl_2N_2O_2$	$[M+H]^+$	249.01921	5.96	3.2
Lomefloxacin	0.01	$C_{17}H_{19}F_2N_3O_3$	$[M+H]^+$	352.14672	2.58	-0.8
Lontrel (clopyralid)	0.01	$C_6H_3Cl_2NO_2$	$[M+H]^+$	191.96136	/	1.06
Lufenuron	0.01	$C_{17}H_8Cl_2F_8N_2O_3$	$[M+H]^+$	510.9857	7.89	5.12
Maduramicin	0.01	$C_{47}H_{83}NO_{17}$	$[M+H]^+$	934.57338	10.58	4.3
Magnamycin A	0.01	$C_{42}H_{67}NO_{16}$	$[M+H]^+$	842.45326	/	/
Malaoxon	0.01	$C_{10}H_{19}O_7PS$	$[M+H]^+$	315.06619	4.68	0.6**
Malathion	0.01	$C_{10}H_{19}O_6PS_2$	$[M+H]^+$	331.04335	6.53	2.36
Mandipropamid	0.01	$C_{23}H_{22}ClNO_4$	$[M+H]^+$	412.13101	6.23	3.2
Marbofloxacin	0.01	$C_{17}H_{19}FN_4O_4$	$[M+H]^+$	363.14631	2.31	-0.5
Mebendazole	0.01	$C_{16}H_{13}N_3O_3$	$[M+H]^+$	296.10297	4.48	2.8
Mecarbam	0.01	$C_{10}H_{20}NO_5PS_2$	$[M+H]^+$	330.05933	6.84	2.29
Mefenacet	0.01	$C_{16}H_{14}N_2O_2S$	$[M+H]^+$	299.08488	6.26	3.23
Mefenamic acid	0.01	$C_{15}H_{15}NO_2$	$[M-H]^-$	242.11756	6.83	5.1
Mefenpyr-diethyl	0.01	$C_{16}H_{18}Cl_2N_2O_4$	$[M+H]^+$	373.07164	7.41	3.9**
Mefluidide	0.01	$C_{11}H_{13}F_3N_2O_3S$	$[M+H]^+$	311.06718	4.61	2.02
Meloxicam	0.01	$C_{14}H_{13}N_3O_4S_2$	$[M+H]^+$	352.04203	5.49	3

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Mepanipyrim	0.01	$C_{14}H_{13}N_3$	$[M+H]^+$	224.11822	6.46	3.28
Mephosfolan	0.01	$C_8H_{16}NO_3PS_2$	$[M+H]^+$	270.0382	4.27	1**
Mepiquat chloride	0.01	$C_7H_{16}ClN$	$[M+H]^+$	150.1044	/	-2.82
Mepronil	0.01	$C_{17}H_{19}NO_2$	$[M+H]^+$	270.14886	6.49	3.66
Mesosulfuron-methyl	0.01	$C_{17}H_{21}N_5O_9S_2$	$[M+H]^+$	504.08535	4.96	-0.48
Mesotrione	0.01	$C_{14}H_{13}NO_7S$	$[M+H]^+$	340.04855	4.34	0.9
Metaflumizone	0.01	$C_{24}H_{16}F_6N_4O_2$	$[M-H]^-$	507.12502	7.8	6.2**
Metalaxyl	0.01	$C_{15}H_{21}NO_4$	$[M+H]^+$	280.15433	5.21	1.65
Metalaxyl-M	0.01	$C_{15}H_{21}NO_4$	$[M+H]^+$	280.15433	5.21	1.6**
Metamitron	0.01	$C_{10}H_{10}N_4O$	$[M+H]^+$	203.09274	3.03	0.83
Metazachlor	0.01	$C_{14}H_{16}ClN_3O$	$[M+H]^+$	278.10547	5.48	2.7**
Metconazole	0.01	$C_{17}H_{22}ClN_3O$	$[M+H]^+$	320.15242	6.75	3.85
Methabenzthiazuron	0.01	$C_{10}H_{11}N_3OS$	$[M+H]^+$	222.06956	4.89	2.64
Methacrifos	0.01	$C_7H_{13}O_5PS$	$[M+H]^+$	241.02941	5.91	1.9**
Methamidophos	0.01	$C_2H_8NO_2PS$	$[M+H]^+$	142.00862	0.92	-0.8
Methazine	0.01	$C_{11}H_{19}N_7$	$[M+H]^+$	250.17747	/	/
Methfuroxam	0.01	$C_{14}H_{15}NO_2$	$[M+H]^+$	230.11756	5.91	3**
Methidathion	0.01	$C_6H_{11}N_2O_4PS_3$	$[M+H]^+$	302.96914	5.87	2.2
Methiocarb	0.01	$C_{11}H_{15}NO_2S$	$C_9H_{13}OS^+$	169.06816	5.82	2.92
Methiocarb sulfone	0.01	$C_{11}H_{15}NO_4S$	$[M+H]^+$	258.07946	3.67	1.6**
Methiocarb sulfoxide	0.01	$C_{11}H_{15}NO_3S$	$[M+H]^+$	242.08454	2.96	1.5**
Methomyl	0.01	$C_5H_{10}N_2O_2S$	$[M+H]^+$	163.05358	/	0.6
Methomyl oxime	0.01	C_3H_7NOS	$[M+H]^+$	106.03211	/	0.2**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Methoprotryne	0.01	$C_{11}H_{21}N_5OS$	$[M+H]^+$	272.15396	5.09	2.82
Methoxyfenozide	0.01	$C_{22}H_{28}N_2O_3$	$[M+H]^-$	313.15467	6.43	3.7
Methyl paraoxon	0.01	$C_8H_{10}NO_6P$	$[M+H]^+$	248.03185	4.27	1.3**
Methyl parathion	0.01	$C_8H_{10}NO_5PS$	$[M+H]^+$	264.00901	6.25	2.86
Metobromuron	0.01	$C_9H_{11}BrN_2O_2$	$[M+H]^+$	259.00767	5.34	2.38
Metolachlor	0.01	$C_{15}H_{22}ClNO_2$	$[M+H]^+$	284.14118	6.71	3.13
Metolcarb	0.01	$C_9H_{11}NO_2$	$[M+H]^+$	166.08626	4.32	1.7
(E)-Metominostrobin	0.01	$C_{16}H_{16}N_2O_3$	$[M+H]^+$	285.12337	5.52	3.2**
(Z)-Metominostrobin	0.01	$C_{16}H_{16}N_2O_3$	$[M+H]^+$	285.12337	5.58	3.2**
Metosulam	0.01	$C_{14}H_{13}Cl_2N_5O_4S$	$[M+H]^+$	418.01381	5.02	3.08
Metoxuron	0.01	$C_{10}H_{13}ClN_2O_2$	$[M+H]^+$	229.07383	3.99	1.6**
Metrafenone	0.01	$C_{19}H_{21}BrO_5$	$[M+H]^+$	409.06451	7.65	4.6**
Metribuzin	0.01	$C_8H_{14}N_4OS$	$[M+H]^+$	215.09611	4.49	1.7
Metronidazole	0.01	$C_6H_9N_3O_3$	$[M+H]^+$	172.07167	1.86	0
Metronidazole OH	0.01	$C_6H_9N_3O_4$	$[M+H]^+$	188.06658	0.95	/
Metsulfuron-methyl	0.01	$C_{14}H_{15}N_5O_6S$	$[M+H]^+$	382.08158	4.55	2.2
Mevinphos	0.01	$C_7H_{13}O_6P$	$C_6H_{10}O_5P^+$	193.02604	3.54	0.13
Mexacarbate	0.01	$C_{12}H_{18}N_2O_2$	$[M+H]^+$	223.1441	3.48	2.56
MGK-264 (mixture of isomers)	0.01	$C_{17}H_{25}NO_2$	$[M+H]^+$	276.19581	7.42	3.7
Molinate	0.01	$C_9H_{17}NOS$	$[M+H]^+$	188.11036	6.31	3.21
Monensin	0.01	$C_{36}H_{62}O_{11}$	$[M+NH_4]^+$	688.46304	9.94	4.2
Monepantel	0.01	$C_{20}H_{13}F_6N_3O_2S$	$[M+H]^+$	474.07054	7.23	5.2
Monepantel sulfone	0.01	$C_{20}H_{13}F_6N_3O_4S$	$[M-H]^-$	506.06037	6.85	3.9

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Monocrotophos	0.01	$C_7H_{14}NO_5P$	$[M+H]^+$	224.06824	2.29	-0.2
Monolinuron	0.01	$C_9H_{11}ClN_2O_2$	$[M+H]^+$	215.05818	5.14	2.3
Monuron	0.01	$C_9H_{11}ClN_2O$	$[M+H]^+$	199.06327	4.31	1.94
Morantel	0.01	$C_{12}H_{16}N_2S$	$[M+H]^+$	221.11070	3.07	1.9
Morpholine	0.01	C_4H_9NO	$[M+H]^+$	88.07569	/	-0.86
Moxidectin	0.01	$C_{37}H_{53}NO_8$	$[M+H]^+$	640.38439	9.31	4.3
N,N-Diethyl-*m*-toluamide (DEET)	0.01	$C_{12}H_{17}NO$	$[M+H]^+$	192.13829	5.23	2.02
N,N'-Ethylenethiourea	0.01	$C_3H_6N_2S$	$[M+H]^+$	103.03245	0.9	-0.5
Nafcillin	0.01	$C_{21}H_{22}N_2O_5S$	$[M-H]^-$	415.13222	5.22	2.9
Nalidixic acid	0.01	$C_{12}H_{12}N_2O_3$	$[M+H]^+$	233.09207	4.68	/
Naphthalophos (naftalofos)	0.01	$C_{16}H_{16}NO_6P$	$[M+H]^+$	350.0788	5.76	2.4**
Napropamide	0.01	$C_{17}H_{21}NO_2$	$[M+H]^+$	272.16451	6.49	3.36
Naproxen	0.01	$C_{14}H_{14}O_3$	$[M+H]^+$	231.10157	5.35	3.3
Naptalam	0.01	$C_{18}H_{13}NO_3$	$[M+H]^+$	292.09682	4.49	3.5**
Narasin	0.01	$C_{43}H_{72}O_{11}$	$[M+NH_4]^+$	782.54129	10.37	6.2
Neburon	0.01	$C_{12}H_{16}Cl_2N_2O$	$[M+H]^+$	275.07125	6.8	4.1
Neospiramycin	0.01	$C_{36}H_{62}N_2O_{11}$	$[M+H]^+$	716.46919	/	/
Nereistoxin oxalate	0.01	$C_7H_{13}NO_4S_2$	$[M+H]^+$	240.03588	/	/
Nicarbazin (DNC)	0.01	$C_{19}H_{18}N_6O_6$	$[M+H]^+$	444.16261	/	/
Nicosulfuron	0.01	$C_{15}H_{18}N_6O_6S$	$[M+H]^+$	411.10813	4.05	/
Nigericin	0.01	$C_{40}H_{68}O_{11}$	$[M+NH_4]^+$	742.50999	10.84	4.3
Nitenpyram (ISO)	0.01	$C_{11}H_{15}ClN_4O_2$	$[M+H]^+$	271.09563	2.25	-0.66
Nitralin	0.01	$C_{13}H_{19}N_3O_6S$	$[M+H]^+$	346.10673	6.84	3.7**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Nitrapyrin (2-chloro-6-(trichloromethyl)pyridine)	0.01	$C_6H_3Cl_4N$	$[M+H]^+$	231.9063	/	3.4
Nitroguanidine	0.01	$CH_4N_4O_2$	$[M+H]^+$	105.0407	/	-0.89
Nitroxinil	0.01	$C_7H_3IN_2O_3$	$[M+H]^+$	290.92612	4.37	2.3
Norfloxacin	0.01	$C_{16}H_{18}FN_3O_3$	$[M+H]^+$	320.14050	2.36	-1
Norflurazon	0.01	$C_{12}H_9ClF_3N_3O$	$[M+H]^+$	304.0459	5.34	2.3
Noruron	0.01	$C_{13}H_{22}N_2O$	$[M+H]^+$	223.18049	5.52	2.3**
Novaluron	0.01	$C_{17}H_9ClF_8N_2O_4$	$[M+H]^-$	493.01959	7.54	5.27
Novobiocin	0.01	$C_{31}H_{36}N_2O_{11}$	$[M-H]^-$	613.23919	6.88	3.3
Nuarimol	0.01	$C_{17}H_{12}ClFN_2O$	$[M+H]^+$	315.0695	5.62	3.18
O-Acetyltylosin	0.01	$C_{48}H_{79}NO_{18}$	$[M+H]^+$	958.53699	4.79	1.6
Ofloxacin	0.01	$C_{18}H_{20}FN_3O_4$	$[M+H]^+$	362.15106	2.43	-0.4
Ofurace	0.01	$C_{14}H_{16}ClNO_3$	$[M+H]^+$	282.08915	5.09	2.7**
Oleandomycin	0.01	$C_{35}H_{61}NO_{12}$	$[M+H]^+$	688.42665	4.29	1.7
Omethoate	0.01	$C_5H_{12}NO_4PS$	$[M+H]^+$	214.02974	0.92	-0.74
Orbencarb	0.01	$C_{12}H_{16}ClNOS$	$[M+H]^+$	258.07139	7.36	3.4**
Orbifloxacin	0.01	$C_{19}H_{20}F_3N_3O_3$	$[M+H]^+$	396.15295	2.74	0.9
Ormetoprim	0.01	$C_{14}H_{18}N_4O_2$	$[M+H]^+$	275.15025	2.41	1.2
Orysastrobin	0.01	$C_{18}H_{25}N_5O_5$	$[M+H]^+$	392.19285	6.23	2.5**
Oryzalin	0.01	$C_{12}H_{18}N_4O_6S$	$[M-H]^-$	347.10198	6.47	3.73
Oxacillin	0.01	$C_{19}H_{19}N_3O_5S$	$[M-H]^-$	402.11182	4.72	2.4
Oxadiargyl	0.01	$C_{15}H_{14}Cl_2N_2O_3$	$[M+H]^+$	341.04542	7.35	4.1**
Oxadiazon	0.01	$C_{15}H_{18}Cl_2N_2O_3$	$[M+H]^+$	345.07672	8.15	4.8
Oxadixyl	0.01	$C_{14}H_{18}N_2O_4$	$[M+H]^+$	279.13393	4.24	0.8

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Oxamyl	0.01	$C_7H_{13}N_3O_3S$	$[M+H]^+$	242.05698	2.93	-0.47
Oxasulfuron	0.01	$C_{17}H_{18}N_4O_6S$	$[M+H]^+$	407.10198	4.4	1.6**
Oxaziclomefone	0.01	$C_{20}H_{19}Cl_2NO_2$	$[M+H]^+$	376.08656	7.98	5.2**
Oxfendazole (fenbendazole sulfoxide)	0.01	$C_{15}H_{13}N_3O_3S$	$[M+H]^+$	316.07504	3.49	2.3
Oxfendazole sulfone (fenbendazole sulfone)	0.01	$C_{15}H_{13}N_3O_4S$	$[M+H]^+$	332.06995	4.15	2.3
Oxibendazole	0.01	$C_{12}H_{15}N_3O_3$	$[M+H]^+$	250.11862	3.79	2.4
Oximino oxamyl	0.01	$C_5H_{10}N_2O_2S$	$[M+H]^+$	163.05358	/	1.2**
Oxolinic acid	0.01	$C_{13}H_{11}NO_5$	$[M+H]^+$	262.07100	3.82	-0.2
Oxycarboxin	0.01	$C_{12}H_{13}NO_4S$	$[M+H]^+$	268.06381	3.84	0.77
Oxyclozanide	0.01	$C_{13}H_6Cl_5NO_3$	$[M-H]^-$	399.88631	6.83	5.7
Oxydemeton-methyl (demeton-*S*-)	0.01	$C_6H_{15}O_4PS_2$	$[M+H]^+$	247.02222	/	-0.74
Oxyfluorfen	0.01	$C_{15}H_{11}ClF_3NO_4$	$[M+H]^+$	362.04015	7.98	4.73
Oxyphenbutazone	0.01	$C_{19}H_{20}N_2O_3$	$[M-H]^-$	325.15467	5.36	2.7
Oxytetracycline	0.01	$C_{22}H_{24}N_2O_9$	$[M+H]^+$	461.15546	/	/
Paclobutrazol	0.01	$C_{15}H_{20}ClN_3O$	$[M+H]^+$	294.13677	5.83	3.2
Paraoxon-ethyl	0.01	$C_{10}H_{14}NO_6P$	$[M+H]^+$	276.06315	5.28	1.98
Parathion	0.01	$C_{10}H_{14}NO_5PS$	$[M+H]^+$	292.04031	7.1	3.83
Pebulate	0.01	$C_{10}H_{21}NOS$	$[M+H]^+$	204.14166	7.57	3.83
Penconazol	0.01	$C_{13}H_{15}Cl_2N_3$	$[M-H]^+$	284.07158	6.7	3.72
Pencycuron	0.01	$C_{19}H_{21}ClN_2O$	$[M+H]^-$	329.14152	7.42	4.8**
Pendimethalin	0.01	$C_{13}H_{19}N_3O_4$	$[M+H]^+$	282.14483	8.22	5.2
Penfluron	0.01	$C_{15}H_9F_5N_2O_2$	$[M+H]^-$	345.0657	6.73	4**
Penicillin-G	0.01	$C_{16}H_{18}N_2O_4S$	$[M-H]^-$	335.10601	4.07	1.8

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Penicilllin-V^{+4}	0.01	$C_{16}H_{18}N_2O_5S$	$[M-H]^-$	351.10092	4.43	2.1
Penoxsulam	0.01	$C_{16}H_{14}F_5N_5O_5S$	$[M-H]^-$	484.07086	5.37	-0.354
Pentachlorocyanobenzene	0.01	C_7Cl_5N	$[M+H]^+$	275.85168	/	/
Pentanochlor	0.01	$C_{13}H_{18}ClNO$	$[M+H]^+$	240.11497	6.89	4.3**
Penthiopyrad	0.01	$C_{16}H_{20}F_3N_3OS$	$[M-H]^-$	360.1352	7.03	4**
Pethoxamid	0.01	$C_{16}H_{22}ClNO_2$	$[M+H]^+$	296.14118	6.66	3.5**
Phenmedipham	0.01	$C_{16}H_{16}N_2O_4$	$[M+H]^+$	301.11828	5.78	3.6**
Phenothrin	0.01	$C_{23}H_{26}O_3$	$[M+H]^+$	351.19547	9.11	7.54
Phenthoate	0.01	$C_{12}H_{17}O_4PS_2$	$[M+H]^+$	321.03787	7.15	3.7**
Phénylbutazone	0.01	$C_{19}H_{20}N_2O_2$	$[M+H]^+$	309.15975	6.64	3.2
Phenylurea	0.01	$C_7H_8N_2O$	$[M+H]^+$	137.07094	2.34	0.8**
Phorate	0.01	$C_7H_{17}O_2PS_3$	$[M+H]^+$	261.02011	/	3.56
Phorate-oxon sulfoxide	0.01	$C_7H_{17}O_4PS_2$	$[M+H]^+$	261.03787	3.03	1.8**
Phorate sulfoxide	0.01	$C_7H_{17}O_3PS_3$	$[M+H]^+$	277.01502	5	3.5**
Phorate-oxon	0.01	$C_7H_{17}O_3PS$	$[M+H]^+$	213.07088	/	2.1**
Phorate-oxon sulfone	0.01	$C_7H_{17}O_5PS_2$	$[M+H]^+$	277.03278	3.66	2**
Phorat sulfone	0.01	$C_7H_{17}O_4PS_3$	$[M+H]^+$	293.00994	5.71	3.7**
Phosalone	0.01	$C_{12}H_{15}ClNO_4PS_2$	$[M+H]^+$	367.99414	7.45	4.38
Phosfolan	0.01	$C_7H_{14}NO_3PS_2$	$[M+H]^+$	256.02255	3.72	0.6**
Phosmet	0.01	$C_{11}H_{12}NO_4PS_2$	$[M+H]^+$	318.00182	6.03	2.95
Phosmet-oxon	0.01	$C_{11}H_{12}NO_5PS$	$[M+H]^+$	302.02466	4.07	1.1**
Phosphamidon	0.01	$C_{10}H_{19}ClNO_5P$	$[M+H]^+$	300.07622	4.11	0.8
Phospholan-methyl	0.01	$C_5H_{10}NO_3PS_2$	$[M+H]^+$	227.99125	2.58	1.1**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Phoxim	0.01	$C_{12}H_{15}N_2O_3PS$	$[M+H]^+$	299.06138	7.04	4.4**
Phthalylsulfathiazole (CAS)	0.01	$C_{17}H_{13}N_3O_5S_2$	$[M-H]^-$	404.03694	3.16	1.1
Picolinafen	0.01	$C_{19}H_{12}F_4N_2O_2$	$[M+H]^+$	377.09077	7.85	4.9**
Picoxystrobin	0.01	$C_{18}H_{16}F_3NO_4$	$[M+H]^+$	368.11042	7.03	3.6
Piperalin	0.01	$C_{16}H_{21}Cl_2NO_2$	$[M+H]^+$	330.10221	4.56	4.31
Piperonyl butoxide	0.01	$C_{19}H_{30}O_5$	$[M+NH_4]^+$	356.24315	7.92	4.75
Piperophos	0.01	$C_{14}H_{28}NO_3PS_2$	$[M+H]^+$	354.1321	7.59	4.2**
Pirimicarb	0.01	$C_{11}H_{18}N_4O_2$	$[M+H]^+$	239.15025	3.91	1.7
Pirimicarb-desmethyl	0.01	$C_{10}H_{16}N_4O_2$	$[M+H]^+$	225.1346	2.68	1.6**
Pirimiphos-methyl	0.01	$C_{11}H_{20}N_3O_3PS$	$[M+H]^+$	306.10358	7.47	4.12
Pirimiphos-ethyl	0.01	$C_{13}H_{24}N_3O_3PS$	$[M+H]^+$	334.13488	8.17	5
Pirimiphos-methyl-N-desethyl	0.01	$C_9H_{16}N_3O_3PS$	$[M+H]^+$	278.07228	5.36	3.7**
Pirlymycin	0.01	$C_{17}H_{31}ClN_2O_5S$	$[M+H]^+$	411.17150	3.09	1.7
Prallethrin	0.01	$C_{19}H_{24}O_3$	$[M+H]^+$	301.17982	7.58	4.49
Pretilachlor	0.01	$C_{17}H_{26}ClNO_2$	$[M+H]^+$	312.17248	7.69	4.1**
Primisulfuron-methyl	0.01	$C_{15}H_{12}F_4N_4O_7S$	$[M+H]^-$	469.04356	6.19	/
Probenazole	0.01	$C_{10}H_9NO_3S$	$[M+H]^+$	224.03759	4.96	1.4**
Prochloraz	0.01	$C_{15}H_{16}Cl_3N_3O_2$	$[M+H]^+$	376.03809	6.62	4.1
Procyazine	0.01	$C_{10}H_{13}ClN_6$	$[M+H]^+$	253.0963	4.55	2.4**
Procymidone	0.01	$C_{13}H_{11}Cl_2NO_2$	$[M+H]^+$	284.02396	6.64	3**
Profenofos	0.01	$C_{11}H_{15}BrClO_3PS$	$[M+H]^+$	374.94017	7.68	4.68
Profoxydim lithium	0.01	$C_{24}H_{32}ClNO_4S$	$[M+H]^+$	466.18133	8.88	/
Prohydrojasmon	0.01	$C_{15}H_{26}O_3$	$[M+H]^+$	255.19547	7.5	3.6**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Promecarb	0.01	$C_{12}H_{17}NO_2$	$[M+H]^+$	208.13321	5.87	3.1
Prometon	0.01	$C_{10}H_{19}N_5O$	$[M+H]^+$	226.16624	4.41	2.99
Prometryn	0.01	$C_{10}H_{19}N_5S$	$[M+H]^+$	242.14339	5.88	3.51
Propachlor	0.01	$C_{11}H_{14}ClNO$	$[M+H]^+$	212.08367	5.49	2.18
Propamocarb	0.01	$C_9H_{20}N_2O_2$	$[M+H]^+$	189.15975	0.96	1.12
Propamocarb HCl	0.01	$C_9H_{21}ClN_2O_2$	$[M+H]^+$	225.13643	2.64	/
Propanil	0.01	$C_9H_9Cl_2NO$	$[M+H]^-$	218.0134	5.69	3.07
Propaphos	0.01	$C_{13}H_{21}O_4PS$	$[M+H]^+$	305.0971	6.75	3.67
Propaquizafop	0.01	$C_{22}H_{22}ClN_3O_5$	$[M+H]^+$	444.13208	7.84	4.6
Propargite	0.01	$C_{19}H_{26}O_4S$	$[M+NH_4]^+$	368.18901	8.36	5
Propazine	0.01	$C_9H_{16}ClN_5$	$[M+H]^+$	230.1167	6.53	2.93
Propazine-2-hydroxy	0.01	$C_9H_{17}N_5O$	$[M+H]^+$	212.15059	3.71	0.6**
Propetamphos	0.01	$C_{10}H_{20}NO_4PS$	$[M+H]^+$	282.09235	6.5	3.82
Propham	0.01	$C_{10}H_{13}NO_2$	$C_7H_8NO_2^+$	138.05496	5.41	2.6
Propiconazol (mixture of isomers)	0.01	$C_{15}H_{17}Cl_2N_3O_2$	$[M+H]^+$	342.07706	6.87	3.72
Propisochlor	0.01	$C_{15}H_{22}ClNO_2$	$[M+H]^+$	284.14118	6.71	3.9**
Propoxur	0.01	$C_{11}H_{15}NO_3$	$C_8H_{10}NO_3^+$	168.06552	4.65	1.52
Propyzamide (pronamide)	0.01	$C_{12}H_{11}Cl_2NO$	$[M+H]^+$	256.02905	6.31	3.43
Proquinazid	0.01	$C_{14}H_{17}IN_2O_2$	$[M+H]^+$	373.04076	8.68	3.7**
Prosulfocarb	0.01	$C_{14}H_{21}NOS$	$[M+H]^+$	252.14166	7.8	3.9**
Prosulfuron	0.01	$C_{15}H_{16}F_3N_5O_4S$	$[M+H]^+$	420.09479	5.87	-0.21
Prothioconazole	0.01	$C_{14}H_{15}Cl_2N_3OS$	$[M+H]^+$	344.03857	6.8	3.82
Prothioconazole-desthio	0.01	$C_{14}H_{15}Cl_2N_3O$	$[M+H]^+$	312.06649	6.24	2.7**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Pymetrozine	0.01	$C_{10}H_{11}N_5O$	$[M+H]^+$	218.10364	1.62	-0.18
Pyracarbolid	0.01	$C_{13}H_{15}NO_2$	$[M+H]^+$	218.11756	4.88	2.1**
Pyraclofos	0.01	$C_{14}H_{18}ClN_2O_3PS$	$[M+H]^+$	361.05371	7.16	3.8**
Pyraclostrobin	0.01	$C_{19}H_{18}ClN_3O_4$	$[M+H]^+$	388.10586	7.3	3.99
Pyraflufen-ethyl	0.01	$C_{15}H_{13}Cl_2F_3N_2O_4$	$[M+H]^+$	413.02772	7.12	3.49
Pyrantel	0.01	$C_{11}H_{14}N_2S$	$[M+H]^+$	207.09505	2.50	1.6
Pyrazolynate	0.01	$C_{19}H_{16}Cl_2N_2O_4S$	$[M+H]^+$	439.02806	7.48	3.8**
Pyrazophos	0.01	$C_{14}H_{20}N_3O_5PS$	$[M+H]^+$	374.09341	7.27	3.1**
Pyrazosulfuron-ethyl	0.01	$C_{14}H_{18}N_6O_7S$	$[M+H]^+$	415.10305	5.93	0.7**
Pyrazoxyfen	0.01	$C_{20}H_{16}Cl_2N_2O_3$	$[M+H]^+$	403.06107	6.96	3.7**
Pyrethrin (mixture of isomers)	0.01	$C_{22}H_{28}O_5$	$[M+H]^+$	373.20095	7.57	4.3
Pyributicarb	0.01	$C_{18}H_{22}N_2O_2S$	$[M+H]^+$	331.14748	8.21	5.2**
Pyridaben	0.01	$C_{19}H_{25}ClN_2OS$	$[M+H]^+$	365.14489	8.82	6.37
Pyridafol	0.01	$C_{10}H_7ClN_2O$	$[M+H]^+$	207.03197	3.48	2.4**
Pyridalyl	0.01	$C_{18}H_{14}Cl_4F_3NO_3$	$[M+H]^+$	491.9725	9.59	7.59
Pyridaphenthion	0.01	$C_{14}H_{17}N_2O_4PS$	$[M+H]^+$	341.07194	6.32	3.3**
Pyridate	0.01	$C_{19}H_{23}ClN_2O_2S$	$[M+H]^+$	379.12415	9.25	6.6**
Pyrifenox (mixture of isomers)	0.01	$C_{14}H_{12}Cl_2N_2O$	$[M+H]^+$	295.03995	5.56	2.5**
Pyrimethanil	0.01	$C_{12}H_{13}N_3$	$[M+H]^+$	200.11822	5.49	2.84
Pyriproxyfen	0.01	$C_{20}H_{19}NO_3$	$[M+H]^+$	322.14377	8.11	5.37
Pyroquilon	0.01	$C_{11}H_{11}NO$	$[M+H]^+$	174.09134	4.07	1.57
Pyroxsulam	0.01	$C_{14}H_{13}F_3N_6O_5S$	$[M+H]^+$	435.0693	4.66	1.7**
Quinalphos	0.01	$C_{12}H_{15}N_2O_3PS$	$[M+H]^+$	299.06138	7.04	4.4**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Quinclorac	0.01	$C_{10}H_5Cl_2NO_2$	$[M+H]^+$	241.97701	3.81	2.97
Quinine	0.01	$C_{20}H_{24}N_2O_2$	$[M+H]^+$	325.19105	2.91	/
Quinine sulfate	0.01	$C_{40}H_{54}N_4O_{10}S$	$[M+H]^+$	783.36334	/	/
Quinmerac	0.01	$C_{11}H_8ClNO_2$	$[M+H]^+$	222.03163	3.21	2.7**
Quinoclamine	0.01	$C_{10}H_6ClNO_2$	$[M+H]^+$	208.01598	4.36	2.1**
Quinoline	0.01	C_9H_7N	$[M+H]^+$	130.06513	2.1	2.03
Quinoxyfen	0.01	$C_{15}H_8Cl_2FNO$	$[M+H]^+$	308.00397	8	4.66
Quizalofop	0.01	$C_{17}H_{13}ClN_2O_4$	$[M+H]^+$	345.06366	6.27	3.6**
Quizalofop-ethyl	0.01	$C_{19}H_{17}ClN_2O_4$	$[M+H]^+$	373.09496	7.75	4.28
Quizalofop-P-ethyl	0.01	$C_{19}H_{17}ClN_2O_4$	$[M+H]^+$	373.09496	7.74	4.3
Rafoxanide	0.01	$C_{19}H_{11}Cl_2I_2NO_3$	$[M+H]^+$	625.82783	/	7
Reserpine	0.01	$C_{33}H_{40}N_2O_9$	$[M+H]^+$	609.28066	4.84	3.2
Resmethrin	0.01	$C_{22}H_{26}O_3$	$[M+H]^+$	339.19547	8.89	5.43
Rifampicin	0.01	$C_{43}H_{58}N_4O_{12}$	$[M+H]^+$	823.41240	5.94	2.7
Rifamycin	0.01	$C_{37}H_{47}NO_{12}$	$[M+H]^+$	698.31710	/	/
Rifaximin	0.01	$C_{43}H_{51}N_3O_{11}$	$[M+H]^+$	786.35964	6.24	3.2
Rimsulfuron	0.01	$C_{14}H_{17}N_5O_7S_2$	$[M+H]^+$	432.06422	4.77	-1.47
Robenidine	0.01	$C_{15}H_{13}Cl_2N_5$	$[M+H]^+$	334.06208	5.57	3.8
Ronidazole	0.01	$C_6H_8N_4O_4$	$[M+H]^+$	201.06183	/	/
Rotenone	0.01	$C_{23}H_{22}O_6$	$[M+H]^+$	395.14892	6.72	4.1
Roxithromycin	0.01	$C_{41}H_{76}N_2O_{15}$	$[M+H]^+$	837.53185	4.99	1.7
Saflufenacil	0.01	$C_{17}H_{17}ClF_4N_4O_5S$	$[M+H]^+$	501.06171	5.99	2.1**
Salinomycin	0.01	$C_{42}H_{70}O_{11}$	$[M+NH_4]^+$	768.52564	9.98	5.7

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Sarafloxacin	0.01	$C_{20}H_{17}F_2N_3O_3$	$[M+H]^+$	386.13107	2.98	0.3
Schradan (DMPA)	0.01	$C_8H_{24}N_4O_3P_2$	$[M+H]^+$	287.13964	3.05	-0.3
Sebuthylazin	0.01	$C_9H_{16}ClN_5$	$[M+H]^+$	230.1167	5.9	3.1**
Sebuthylazin-desethyl	0.01	$C_7H_{12}ClN_5$	$[M+H]^+$	202.0854	3.98	2.2**
Secbumeton	0.01	$C_{10}H_{19}N_5O$	$[M+H]^+$	226.16624	4.45	3.2**
Selamectin impurity B	0.01	$C_{43}H_{63}NO_{11}$	$[M+H]^+$	770.44739	9.65	5.4**
Semduramicin	0.01	$C_{45}H_{76}O_{16}$	$[M+H]^+$	873.52061	7.59	/
Sethoxydim	0.01	$C_{17}H_{29}NO_3S$	$[M+H]^+$	328.19409	8.09	/
S-Hydroprene	0.01	$C_{17}H_{30}O_2$	$[M+H]^+$	267.23186	/	6.5
Siduron	0.01	$C_{14}H_{20}N_2O$	$[M+H]^+$	233.16484	5.77	3.8
Silthiofam	0.01	$C_{13}H_{21}NOSSi$	$[M+H]^+$	268.11859	/	/
Simazine	0.01	$C_7H_{12}ClN_5$	$[M+H]^+$	202.0854	4.4	2.18
Simeconazole	0.01	$C_{14}H_{20}FN_3OSi$	$[M+H]^+$	294.14325	6.16	/
Simeton	0.01	$C_8H_{15}N_5O$	$[M+H]^+$	198.13494	3.36	1.8
Simetryn	0.01	$C_8H_{15}N_5S$	$[M+H]^+$	214.11209	4.41	2.8
S-Metolachlor	0.01	$C_{15}H_{22}ClNO_2$	$[M+H]^+$	284.14118	6.72	3.1
Spinetoram (mixture of isomers)	0.01	$C_{42}H_{69}NO_{10}$	$[M+H]^+$	748.49942	6.94	5.9**
Spinosad (mixure of spinosyn A and D)	0.01	$C_{41}H_{65}NO_{10}$	$[M+H]^+$	732.46812	6.34	4.9**
Spiramycin	0.01	$C_{43}H_{74}N_2O_{14}$	$[M+H]^+$	843.52128	3.33	2.1
Spirodiclofen	0.01	$C_{21}H_{24}Cl_2O_4$	$[M+H]^+$	411.11244	8.81	5.1
Spiromesifen	0.01	$C_{23}H_{30}O_4$	$[M+H]^+$	371.22169	8.7	4.55
Spirotetramat	0.01	$C_{21}H_{27}NO_5$	$[M+H]^+$	374.1962	6.04	3.2**
Spirotetramat-enol	0.01	$C_{18}H_{23}NO_3$	$[M+H]^+$	302.17507	4.45	2.4**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Spirotetramat-enol-glucoside	0.01	$C_{24}H_{33}NO_8$	$[M+H]^+$	464.22789	2.38	0.5**
Spirotetramat-mono-hydroxy	0.01	$C_{21}H_{27}NO_5$	$[M+H]^+$	374.1962	6.04	2.1**
Spiroxamine (mixture of isomers)	0.01	$C_{18}H_{35}NO_2$	$[M+H]^+$	298.27406	5.39	4.2**
Sulbactam	0.01	$C_8H_{11}NO_5S$	$[M+NH_4]^+$	256.02502	/	/
Sulcotrione	0.01	$C_{14}H_{13}ClO_5S$	$[M+H]^+$	329.0245	4.61	1.5**
Sulfacetamide	0.01	$C_8H_{10}N_2O_3S$	$[M+H]^+$	215.04849	/	-1
Sulfachloropyridazine	0.01	$C_{10}H_9ClN_4O_2S$	$[M+H]^+$	285.02075	3.12	1
Sulfaclozine	0.01	$C_{10}H_9ClN_4O_2S$	$[M+H]^+$	285.02075	3.79	0.9
Sulfadiazine	0.01	$C_{10}H_{10}N_4O_2S$	$[M+H]^+$	251.05972	2.07	-0.1
Sulfadimerazine	0.01	$C_{12}H_{14}N_4O_2S$	$[M+H]^+$	279.09102	2.79	0.1
Sulfadimethoxine	0.01	$C_{12}H_{14}N_4O_4S$	$[M+H]^+$	311.08085	3.86	1.6
Sulfadoxine	0.01	$C_{12}H_{14}N_4O_4S$	$[M+H]^+$	311.08085	3.35	0.7
Sulfaguanidine	0.01	$C_7H_{10}N_4O_2S$	$[M+H]^+$	215.05972	0.95	-0.7
Sulfallate	0.01	$C_8H_{14}ClNS_2$	$[M+H]^+$	224.0329	7.25	3.15
Sulfamerazine	0.01	$C_{11}H_{12}N_4O_2S$	$[M+H]^+$	265.07537	2.46	0.14
Sulfamerazine	0.01	$C_{11}H_{12}N_4O_2S$	$[M+H]^+$	265.07537	2.46	0.1
Sulfamethizole	0.01	$C_9H_{10}N_4O_2S_2$	$[M+H]^+$	271.03180	2.64	2.9
Sulfamethoxazole	0.01	$C_{10}H_{11}N_3O_3S$	$[M+H]^+$	254.05939	3.25	0.9
Sulfamethoxypyridazine	0.01	$C_{11}H_{12}N_4O_3S$	$[M+H]^+$	281.07029	2.98	0.3
Sulfamonomethoxine	0.01	$C_{11}H_{12}N_4O_3S$	$[M+H]^+$	281.07029	3	0.8
Sulfamonomethoxine	0.01	$C_{11}H_{12}N_4O_3S$	$[M+H]^+$	281.07029	2.72	0.7
Sulfanilamide	0.01	$C_6H_8N_2O_2S$	$[M+H]^+$	173.03793	/	-0.6
Sulfaphenazole	0.01	$C_{15}H_{14}N_4O_2S$	$[M+H]^+$	315.09102	3.93	1.5

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Sulfaquinoxaline	0.01	$C_{14}H_{12}N_4O_2S$	$[M+H]^+$	301.07537	3.89	1.7
Sulfathiazole	0.01	$C_9H_9N_3O_2S_2$	$[M+H]^+$	256.02090	2.13	0.1
Sulfentrazone	0.01	$C_{11}H_{10}Cl_2F_2N_4O_3S$	$[M+H]^+$	386.98915	4.91	0.99
Sulfisoxazole	0.01	$C_{11}H_{13}N_3O_3S$	$[M+H]^+$	268.07504	3.44	1
Sulfometuron-methyl	0.01	$C_{15}H_{16}N_4O_5S$	$[M+H]^+$	365.09142	4.73	1.2
Sulfosulfuron	0.01	$C_{16}H_{18}N_6O_7S_2$	$[M+H]^+$	471.07512	5.3	-0.77
Sulfoxaflor	0.01	$C_{10}H_{10}F_3N_3OS$	$[M+H]^+$	278.05695	3.91	0.8
Sulfluramid	0.01	$C_{10}H_6F_{17}NO_2S$	$[M-H]^-$	527.99206	8.32	5.6**
Sulprofos sulfoxide	0.01	$C_{12}H_{19}O_3PS_3$	$[M+H]^+$	339.03067	6.37	3.5**
Systhane™	0.01	$C_{15}H_{17}ClN_4$	$[M+H]^+$	289.12145	6.16	2.94
Tau-fluvalinate	0.01	$C_{26}H_{22}ClF_3N_2O_3$	$[M+H]^+$	503.13438	9.02	7.7**
TDCPP	0.01	$C_9H_{15}Cl_6O_4P$	$[M+H]^+$	430.88829	6.89	3.65
Tebuconazole (Folicur®)	0.01	$C_{16}H_{22}ClN_3O$	$[M+H]^+$	308.15242	6.49	3.7
Tebufenozide	0.01	$C_{22}H_{28}N_2O_2$	$C_{18}H_{21}N_2O_2^+$	297.15975	6.82	4.25
Tebufenpyrad	0.01	$C_{18}H_{24}ClN_3O$	$[M+H]^+$	334.16807	7.86	4.61
Tebupirimfos	0.01	$C_{13}H_{23}N_2O_3PS$	$[M+H]^+$	319.12398	8.21	4.2
Tebutam	0.01	$C_{15}H_{23}NO$	$[M+H]^+$	234.18524	6.72	3.4**
Tebuthiuron	0.01	$C_9H_{16}N_4OS$	$[M+H]^+$	229.11176	4.06	1.79
Teflubenzuron	0.01	$C_{14}H_6Cl_2F_4N_2O_2$	$[M+H]^+$	380.98152	7.46	4.56
Telithromycin	0.01	$C_{43}H_{65}N_5O_{10}$	$[M+H]^+$	812.48042	3.89	4.2
Tembotrione	0.01	$C_{17}H_{16}ClF_3O_6S$	$[M+NH_4]^+$	458.06465	5.97	-1.09
Tepraloxydim	0.01	$C_{17}H_{24}ClNO_4$	$[M+H]^-$	342.14666	6.44	2.6**
Terbufos	0.01	$C_9H_{21}O_2PS_3$	$[M+H]^+$	289.05141	8.09	4.48

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Terbufos sulfone	0.01	$C_9H_{21}O_4PS_3$	$[M+H]^+$	321.04124	6.33	2.5**
Terbufos sulfoxide	0.01	$C_9H_{21}O_3PS_3$	$[M+H]^+$	305.04633	5.74	2.2**
Terbumeton	0.01	$C_{10}H_{19}N_5O$	$[M+H]^+$	226.16624	4.41	3.1**
Terbumeton-desethyl	0.01	$C_8H_{15}N_5O$	$[M+H]^+$	198.13494	3.27	2.1**
Terbutaline sulfate	0.01	$C_{24}H_{40}N_2O_{10}S$	$[M+H]^+$	549.24764	/	/
Terbuthylazine	0.01	$C_9H_{16}ClN_5$	$[M+H]^+$	230.1167	5.96	3.4
Terbuthylazine-desethyl	0.01	$C_7H_{12}ClN_5$	$[M+H]^+$	202.0854	4.4	2**
Terbutol (terbucarb)	0.01	$C_{17}H_{27}NO_2$	$[M+H]^+$	278.21146	7.52	5.2**
Terbutryn	0.01	$C_{10}H_{19}N_5S$	$[M+H]^+$	242.14339	5.88	3.74
Terbutylazine-2-hydroxy	0.01	$C_9H_{17}N_5O$	$[M+H]^+$	212.15059	2.69	0.3**
Tetrachlorvinphos (ISO)	0.01	$C_{10}H_9C_{l4}O_4P$	$[M+H]^+$	366.90367	6.65	3.53
Tetraconazole	0.01	$C_{13}H_{11}Cl_2F_4N_3O$	$[M+H]^+$	372.02881	6.33	3.56
Tetracycline	0.01	$C_{22}H_{24}N_2O_8$	$[M+H]^+$	445.16054	/	/
Tetraethyl dithiopyrophosphate	0.01	$C_8H_{20}O_5P_2S_2$	$[M+H]^+$	323.03002	7.36	3.99
Tetraethyl pyrophosphate	0.01	$C_8H_{20}O_7P_2$	$[M+H]^+$	291.07571	4.04	/
Tetramethrin	0.01	$C_{19}H_{25}NO_4$	$[M+H]^+$	332.18564	7.96	4.73
Thenylchlor	0.01	$C_{16}H_{18}ClNO_2S$	$[M+H]^+$	324.08195	6.69	3.8**
Thiabendazole	0.01	$C_{10}H_7N_3S$	$[M+H]^+$	202.04335	2.43	2.47
Thiacloprid	0.01	$C_{10}H_9ClN_4S$	$[M+H]^+$	253.03092	3.9	1.26
Thiamethoxam	0.01	$C_8H_{10}ClN_5O_3S$	$[M+H]^+$	292.02657	2.63	-0.13
Thiamphenicol	0.01	$C_{12}H_{15}Cl_2NO_5S$	$[M+H]^+$	373.03863	2.48	-0.3
Thiazafluron	0.01	$C_6H_7F_3N_4OS$	$[M+H]^+$	241.03654	4.41	0.8**
Thiazopyr	0.01	$C_{16}H_{17}F_5N_2O_2S$	$[M+H]^+$	397.10037	7.3	3.89

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Thidiazuron	0.01	$C_9H_8N_4OS$	$[M+H]^-$	221.04916	4.09	1.77
Thiencarbazone-methyl	0.01	$C_{12}H_{14}N_4O_7S_2$	$[M+H]^+$	391.03767	4.54	1.2**
Thifensulfuron-methyl	0.01	$C_{12}H_{13}N_5O_6S_2$	$[M+H]^+$	388.038	4.41	/
Thifluzamide	0.01	$C_{13}H_6Br_2F_6N_2O_2S$	$[M+H]^+$	528.84733	6.91	6**
Thiobencarb	0.01	$C_{12}H_{16}ClNOS$	$[M+H]^+$	258.07139	7.36	3.4
Thiocarbazyl	0.01	$C_{16}H_{25}NOS$	$[M+H]^+$	280.17296	8.55	/
Thiocyclam hydrogen oxalate	0.01	$C_7H_{13}NO_4S_3$	$[M+H]^+$	272.00795	/	/
Thiodicarb	0.01	$C_{10}H_{18}N_4O_4S_3$	$[M+H]^+$	355.0563	4.71	1.62
Thiofanox	0.01	$C_9H_{18}N_2O_2S$	$[M+Na]^+$	241.09812	5.02	2.2**
Thiofanox sulfone	0.01	$C_9H_{18}N_2O_4S$	$[M+H]^+$	251.10601	3.38	0.9**
Thiofanox sulfoxide	0.01	$C_9H_{18}N_2O_3S$	$[M+H]^+$	235.11109	2.8	0.8**
Thionazin (Zinophos^{TM})	0.01	$C_8H_{13}N_2O_3PS$	$[M+H]^+$	249.04573	5.66	2**
Thiophanate-methyl	0.01	$C_{12}H_{14}N_4O_4S_2$	$[M+H]^+$	343.05293	4.48	2.6**
Thiophanate-ethyl	0.01	$C_{14}H_{18}N_4O_4S_2$	$[M+H]^+$	371.08423	5.49	3.3**
Tiadinil	0.01	$C_{11}H_{10}ClN_3OS$	$[M+H]^-$	268.03059	6.13	3**
Tiamulin	0.01	$C_{28}H_{47}NO_4S$	$[M+H]^+$	494.32986	4.86	4.5
Tiamulin fumarate	0.01	$C_{32}H_{51}NO_8S$	$[M+H]^+$	610.34082	/	/
Ticarcillin	0.01	$C_{15}H_{16}N_2O_6S_2$	$[M+H]^+$	385.05226	/	/
Tildipirosin	0.01	$C_{41}H_{71}N_3O_8$	$[M+H]^+$	751.55794	/	/
Tilmicosin	0.01	$C_{46}H_{80}N_2O_{13}$	$[M+Na]^+$	891.55526	9.33	/
Tokuthion®	0.01	$C_{11}H_{15}Cl_2O_2PS_2$	$[M+H]^+$	344.97009	8.96	4.9**
Tolclofos-methyl	0.01	$C_9H_{11}Cl_2O_3PS$	$[M+H]^+$	300.96164	7.47	4.56
Tolfenamic acid	0.01	$C_{14}H_{12}ClNO_2$	$[M-H]^-$	262.06293	7.02	5.2

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Tolfenpyrade	0.01	$C_{21}H_{22}ClN_3O_2$	$[M+H]^+$	384.14733	7.84	4.7**
Toltrazuril	0.01	$C_{18}H_{14}F_3N_3O_4S$	$[M+H]^+$	426.07299	6.76	2.9
Toltrazuril sulfone	0.01	$C_{18}H_{14}F_3N_3O_6S$	$[M+H]^+$	458.06282	6.09	2.7
Tolylfluanid	0.01	$C_{10}H_{13}Cl_2FN_2O_2S_2$	$[M+H]^+$	346.98523	7.35	3.9
Topramezone	0.01	$C_{16}H_{17}N_3O_5S$	$[M+H]^+$	364.09617	3.57	1.44
Tralkoxydim	0.01	$C_{20}H_{27}NO_3$	$[M+H]^+$	330.20637	8.24	4.1**
Triadimefon	0.01	$C_{14}H_{16}ClN_3O_2$	$[M+H]^+$	294.10038	6.27	2.77
Triadimenol (Baytan®)	0.01	$C_{14}H_{18}ClN_3O_2$	$[M+H]^+$	296.11603	5.78	3.56
Triallate	0.01	$C_{10}H_{16}Cl_3NOS$	$[M+H]^+$	304.0091	8.5	4.6
Triasulfuron	0.01	$C_{14}H_{16}ClN_5O_5S$	$[M+H]^+$	402.06334	4.75	-0.59
Triazamate	0.01	$C_{13}H_{22}N_4O_3S$	$[M+H]^+$	315.14854	6.69	2.7**
Triaziflam	0.01	$C_{17}H_{24}FN_5O$	$[M+H]^+$	334.20377	6.12	3.5**
Triazophos	0.01	$C_{12}H_{16}N_3O_3PS$	$[M+H]^+$	314.07228	6.58	3.34
Triazoxid	0.01	$C_{10}H_6ClN_5O$	$[M+H]^+$	248.03336	4.56	0.9**
Tribenuron-methyl	0.01	$C_{15}H_{17}N_5O_6S$	$[M+H]^+$	396.09723	5.55	0.78
Tribufos (defiolant)	0.01	$C_{12}H_{27}OPS_3$	$[M+H]^+$	315.10345	8.89	3.2**
Trichlorfon	0.01	$C_4H_8Cl_3O_4P$	$[M+H]^+$	256.92986	2.9	0.51
Triclabendazole	0.01	$C_{14}H_9Cl_3N_2OS$	$[M+H]^+$	358.95739	6.97	5.5
Triclabendazole sulfone	0.01	$C_{14}H_9Cl_3N_2O_3S$	$[M+H]^+$	390.94722	6.50	4.5
Triclabendazole sulfoxide	0.01	$C_{14}H_9Cl_3N_2O_2S$	$[M+H]^+$	374.95231	6.16	4.4
Tricyclazole	0.01	$C_9H_7N_3S$	$[M+H]^+$	190.04335	3.57	1.7
Tridemorph (mixture of isomers)	0.01	$C_{19}H_{39}NO$	$[M+H]^+$	298.31044	6.43	6.9**
Tridiphane	0.01	$C_{10}H_7Cl_5O$	$[M+H]^+$	320.89832	/	4.7**

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Trietazine	0.01	$C_9H_{16}ClN_5$	$[M+H]^+$	230.1167	6.58	3.34
Trifloxystrobin	0.01	$C_{20}H_{19}F_3N_2O_4$	$[M+H]^+$	409.13697	7.64	4.5
Trifloxystrobin metabolite	0.01	$C_{19}H_{17}F_3N_2O_4$	$[M+H]^+$	395.12132	6.71	4.3**
Trifloxysulfuron sodium	0.01	$C_{14}H_{13}F_3N_5NaO_6S$	$[M+H]^+$	460.05091	5.07	/
Triflumizole	0.01	$C_{15}H_{15}ClF_3N_3O$	$[M+H]^+$	346.09285	7.12	2.9
Triflumuron	0.01	$C_{15}H_{10}ClF_3N_2O_3$	$[M+H]^+$	359.04048	7	4.91
Trifluralin	0.01	$C_{13}H_{16}F_3N_3O_4$	$[M+H]^+$	336.11657	8.17	5.34
Triflusulfuron-methyl	0.01	$C_{17}H_{19}F_3N_6O_6S$	$[M+H]^+$	493.11117	6.22	3.1**
Triforine	0.01	$C_{10}H_{14}Cl_6N_4O_2$	$[M+H]^+$	434.92917	5.3	2.2
Trimethoprim	0.01	$C_{14}H_{18}N_4O_3$	$[M+H]^+$	291.14517	2.20	0.4
Trinexapac-ethyl	0.01	$C_{13}H_{16}O_5$	$[M+H]^+$	253.10705	5.52	0.9**
Triphenyl phosphorothionate	0.01	$C_{18}H_{15}O_3PS$	$[M+H]^+$	343.05523	8.21	6.3**
Tris(2-chloroethyl) phosphate (TRCP)	0.01	$C_6H_{12}Cl_3O_4P$	$[M+H]^+$	284.96116	4.71	1.78
Tri-*o*-cresyl phosphate (TCP)	0.01	$C_{21}H_{21}O_4P$	$[M+H]^+$	369.12502	8.28	6.34
Triticonazole	0.01	$C_{17}H_{20}ClN_3O$	$[M+H]^+$	318.13677	6.03	3.29
Tritosulfuron	0.01	$C_{13}H_9F_6N_5O_4S$	$[M-H]^-$	446.03522	5.93	3.1**
Trovafloxacin	0.01	$C_{20}H_{15}F_3N_4O_3$	$[M+H]^+$	417.11690	3.33	0.3
Tulathromycin	0.01	$C_{41}H_{79}N_3O_{12}$	$[M+H]^+$	806.57365	/	/
Tylosin	0.01	$C_{46}H_{77}NO_{17}$	$[M+H]^+$	916.52643	4.55	1
Tylvalosin	0.01	$C_{53}H_{87}NO_{19}$	$[M+H]^+$	1042.59451	/	/
Uniconazole	0.01	$C_{15}H_{18}ClN_3O$	$[M+H]^+$	292.12112	6.22	3.6**
Valnemulin	0.01	$C_{31}H_{52}N_2O_5S$	$[M+H]^+$	565.36697	5.17	5.3
Vamidothion	0.01	$C_8H_{18}NO_4PS_2$	$[M+H]^+$	288.04877	2.92	0.16

Compound	MRL (mg.kg^{-1})*	Formula [M]	Ion	Theoretical m/z	T_R (min)	LogP
Vamidothion sulfoxide	0.01	$C_8H_{18}NO_5PS_2$	$[M+H]^+$	304.04368	0.93	-1.1
Vedaprofen	0.01	$C_{19}H_{22}O_2$	$[M+H]^+$	300.19581	7.62	5.7
Vernolate	0.01	$C_{10}H_{21}NOS$	$[M+H]^+$	204.14166	7.57	/
Virginiamycin M1	0.01	$C_{28}H_{35}N_3O_7$	$[M+H]^+$	526.25478	5.1	2.5
XMC (3,5-xylyl methylcarbamate)	0.01	$C_{10}H_{13}NO_2$	$[M+H]^+$	180.10191	4.97	2.23
Z-mevinphos	0.01	$C_7H_{13}O_6P$	$[M+H]^+$	193.02604	3.06	1.2**
Zoxamide	0.01	$C_{14}H_{16}Cl_3NO_2$	$[M+H]^+$	336.03194	7.2	3.76

867 ***** General default maximum residue limit (MRL) value in seafood matrices
868 ****** LogP predicted by XLogP3 (PubChem)

Table S2. Taguchi L9 orthogonal array (TOA) used for optimization of sample preparation (3 factors, 3 levels).

Experiment	Factor		
	Extraction solvent	dSPE sorbent	Dilution
1	1	1	1
2	1	2	3
3	1	3	2
4	2	1	3
5	2	2	2
6	2	3	1
7	3	1	2
8	3	2	1
9	3	3	3

Table S3. Ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry (UHPLC-Q-TOF-MS) conditions.

Instrument	Parameter	Condition		
UHPLC	Column temperature	50°C		
	Injection volume	10 µL		
	Flow rate	0.5 mL.min^{-1}		
	Mobile phase	A: H_2O containing 0.01% formic acid		
		B: ACN containing 0.01% formic acid		
		Time (min)	% A	% B
		0	90	10
		9	0	100
		12	0	100
		12.1	90	10
		16	90	10
Q-TOF-MS	Ion source type	ESI		
	Ion spray voltage floating (ISVF)	(+) 5500 V, (-) 4500 V		
	Source temperature (TEM)	500 °C		
	Curtain gas (CUR)	30 psi		
	Nebulising gas (GS1)	40 psi		
	Heater gas (GS2)	45 psi		

ACN, acetonitrile

Table S4. Pesticide detection rates observed in the L9 orthogonal array used for the optimisation of sample preparation.

Experiment	Factor			Mean detection rate (%)	SD
	Extraction solvent	dSPE sorbent	Dilution		
1	1	1	1	96.08	0.85
2	1	2	3	65.52	0.75
3	1	3	2	78.43	8.36
4	2	1	3	72.88	5.93
5	2	2	2	80.88	3.21
6	2	3	1	83.66	1.50
7	3	1	2	57.03	3.44
8	3	2	1	82.84	2.98
9	3	3	3	56.54	2.21
K1*	80.01	76.42	87.53		
K2	79.14	75.33	72.11		
K3	65.47	72.88	64.98		
R**	14.54	3.54	22.55		
***F*-value**	15.01	0.74	29.97		
p*-value**	< 0.05	> 0.05	< 0.05		

* The average detection rate for each level (Ki), used to select the best level for each factor.

** The range of detection rates, used to rank factors by their impact on the detection rate. The higher this value, the greater the impact of the given parameter on the response.

*** One-way ANOVA test

878 **Table S5.** Veterinary drug detection rates of L9 orthogonal array (TOA) for the optimisation of sample preparation.

Experiment	Factor			Mean detection rate (%)	SD
	Extraction solvent	dSPE sorbent	Dilution		
1	1	1	1	53.75	1.25
2	1	2	3	54.17	1.57
3	1	3	2	59.58	4.52
4	2	1	3	57.29	4.25
5	2	2	2	67.92	2.82
6	2	3	1	82.71	0.72
7	3	1	2	51.88	6.53
8	3	2	1	63.75	3.31
9	3	3	3	38.33	0.95
K1*	55.83	54.31	66.74		
K2	69.31	61.94	59.79		
K3	51.32	60.21	49.93		
R**	17.99	7.64	16.81		
***F*-value**	24.24	4.44	19.74		
p*-value**	< 0.05	< 0.05	< 0.05		

* The average detection rate for each level (Ki), used to select the best level for each factor.

** The range of detection rates, used to rank the factors by their impact on the detection rate. The higher this value, the greater the impact of the given parameter on the response.

*** One-way ANOVA test

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Table S6. Validation results for 850 contaminants across 24 samples spiked at 0.001, 0.01 and 0.1 mg.kg^{-1} with corresponding screening detection limit (SDL) and limit of identification (LOI).

Compounds	No. of detections			SDL (mg.kg^{-1})	No. of identifications			LOI (mg.kg^{-1})
	0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}		0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}	
1-(3,4-Dichlorophenyl)-3-methylurea	24	24	24	0.001	24	24	24	0.001
1-(4-Nitrophenyl)-3-propylure	24	24	24	0.001	24	24	24	0.001
1,2-Benzisothiazol-3(*2H*)-one	24	24	24	0.001	22	24	24	0.01
1,3-Diphenylurea	24	24	24	0.001	24	24	24	0.001
2,3,5-Trimethacarb	24	24	24	0.001	24	24	24	0.001
2,4-Dimethylaniline	24	24	24	0.001	24	24	24	0.001
2,6-Dichlorobenzamide	24	24	24	0.001	13	22	24	0.1
2,6-Diethylaniline	24	24	24	0.001	22	24	24	0.01
2-Ethylhexyl diphenyl phosphate	24	24	24	0.001	24	23	24	0.001
2-N-Octyl-4-isothiazolin-3-one	3	24	24	0.01	0	23	24	0.01
3,4-Dichloroaniline	24	24	24	0.001	23	24	24	0.001
3,4,5-Trimethacarb	24	24	24	0.001	24	24	24	0.001
3-Hydroxycarbofuran	24	24	24	0.001	24	24	24	0.001
3-Ketocarbofuran	24	24	24	0.001	8	20	24	0.1
4-Acethylaminoantipyrine	24	24	24	0.001	24	24	24	0.001
4-Aminoantipyrine	20	22	24	0.1	10	22	24	0.1
4-Bromo-3,5-dimethylphenyl-N-methylcarbamate	24	24	24	0.001	19	24	23	0.01
4-Dimethylaminoantipyrine	17	24	24	0.01	12	24	24	0.01
4-Formylaminoantipyrine	23	24	24	0.001	16	24	24	0.01
4-Methylaminoantipyrine	10	24	24	0.01	10	24	24	0.01
5-Hydroxy-flunixin	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
8-Hydroxy-mutilin	23	24	24	0.001	0	0	13	> 0.1
Abamectin	22	23	24	0.01	0	0	0	> 0.1
Abamectin B1a	22	22	23	0.1	18	22	23	0.1
Abamectin B1b	17	21	24	0.1	9	16	24	0.1
Abate® (temephos)	24	24	24	0.001	24	24	24	0.001
Acephate	24	24	24	0.001	2	3	21	> 0.1
Acetamiprid	24	24	24	0.001	24	24	24	0.001
Acibenzolar-*S*-methyl	24	24	24	0.001	24	24	24	0.001
Aclonifen	24	24	24	0.001	0	0	0	> 0.1
Aconitine	24	24	24	0.001	24	24	24	0.001
Akton	21	24	24	0.01	3	16	22	> 0.1
Alachlor	24	24	24	0.001	0	0	0	> 0.1
Albendazole	24	24	24	0.001	24	24	24	0.001
Albendazole amino sulfone	24	24	24	0.001	24	24	24	0.001
Albendazole sulfone	24	24	24	0.001	24	24	24	0.001
Albendazole sulfoxide	24	24	24	0.001	24	24	24	0.001
Aldicarb	24	24	24	0.001	11	22	24	0.1
Aldicarb sulfone	24	24	24	0.001	24	24	24	0.001
Aldicarb sulfoxide	5	2	4	> 0.1	1	0	0	> 0.1
Allethrin	24	24	24	0.001	4	21	22	> 0.1
Allidochlor	24	24	24	0.001	0	12	24	0.1
Alloxydim sodium	22	23	24	0.01	3	21	24	0.1
Alpha-cypermethrin	0	0	1	> 0.1	0	0	0	> 0.1
Ametoctradin	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Ametryne	24	24	24	0.001	24	24	24	0.001
Amicarbazone	24	24	24	0.001	22	24	23	0.01
Amidosulfuron	24	24	24	0.001	24	24	24	0.001
Amino flubendazole	24	24	24	0.001	24	24	24	0.001
Amino mebendazole	22	24	24	0.01	22	23	24	0.01
Aminocarb	22	22	24	0.1	22	22	24	0.1
Amitraze	2	24	24	0.01	2	24	24	0.01
Amoxicillin	20	24	24	0.01	0	4	20	> 0.1
Ampicillin +4	24	23	24	0.001	19	21	23	0.1
Ancymidol	24	24	24	0.001	2	11	24	0.1
Anilazine	24	24	24	0.001	7	14	13	> 0.1
Anilofos	24	24	24	0.001	24	24	24	0.001
Antipyrine phenazone	24	24	24	0.001	24	24	24	0.001
Aspon ™	24	24	24	0.001	24	24	24	0.001
Asulam	24	24	24	0.001	24	24	24	0.001
Atraton	24	24	24	0.001	24	24	24	0.001
Atrazine	21	22	24	0.1	20	21	23	0.1
Atrazine desisopropyl	24	24	24	0.001	13	22	24	0.1
Azaconazole	24	24	24	0.001	24	24	24	0.001
Azadirachtin (technical)	17	20	18	> 0.1	0	0	0	> 0.1
Azamethiphos	24	24	24	0.001	24	24	24	0.001
Azimsulfuron	24	24	24	0.001	24	24	24	0.001
Aziprotryne	24	24	24	0.001	24	23	23	0.001
Azoxystrobin	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Barban	0	3	5	> 0.1	0	0	0	> 0.1
Beflubutamid	24	24	24	0.001	24	24	24	0.001
Benalaxyl	24	24	24	0.001	24	24	24	0.001
Benazolin	24	24	24	0.001	0	0	0	> 0.1
Benfluralin (benefin)	2	0	0	> 0.1	0	0	0	> 0.1
Benfuresate	12	16	18	> 0.1	0	1	0	> 0.1
Benodanil	24	24	24	0.001	24	24	24	0.001
Benomyl	11	13	19	> 0.1	3	6	5	> 0.1
Benoxacor	24	24	24	0.001	1	12	10	> 0.1
Bensulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Bensulide	24	24	24	0.001	22	24	24	0.01
Bentazon	24	24	24	0.001	24	24	24	0.001
Bentazon-methyl	1	0	0	> 0.1	1	0	0	> 0.1
Benthiavalicarb-isopropyl	24	24	24	0.001	24	24	24	0.001
Benzoximate	24	24	24	0.001	24	24	24	0.001
Benzoylprop ethyl	24	24	24	0.001	23	24	24	0.001
Benzthiazuron	24	24	24	0.001	24	24	24	0.001
Bioresmethrin	24	24	24	0.001	22	24	24	0.01
Bitertanole (mixture of isomers)	24	24	24	0.001	15	24	24	0.01
Bixafen	24	24	24	0.001	23	24	24	0.001
Bladex	24	24	24	0.001	24	24	24	0.001
Boscalid	24	24	24	0.001	24	24	24	0.001
Bromacil	24	24	24	0.001	24	24	24	0.001
Bromofenvinphos-ethyl	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL (mg.kg^{-1})	No. of identifications			LOI (mg.kg^{-1})
	0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}		0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}	
Bromophos-methyl	2	18	19	> 0.1	0	0	0	> 0.1
Bromuconazole (mixture of isomers)	24	24	24	0.001	24	24	24	0.001
Bupirimate	24	24	24	0.001	24	24	24	0.001
Buprofezin	24	24	24	0.001	24	24	24	0.001
Butachlor	24	24	24	0.001	20	23	24	0.01
Butafenacil	24	24	24	0.001	24	24	24	0.001
Butocarboxim	0	1	0	> 0.1	0	0	0	> 0.1
Butocarboxim sulfoxide	2	3	2	> 0.1	1	0	0	> 0.1
Butoxycarboxim	24	24	24	0.001	24	24	24	0.001
Butroxydim	24	24	24	0.001	23	24	24	0.001
Buturon	24	24	24	0.001	24	24	24	0.001
Butylate	24	24	24	0.001	18	24	24	0.01
Cadusafos	24	24	24	0.001	24	24	24	0.001
Cafenstrole	23	24	24	0.001	16	21	21	> 0.1
Carbaryl	24	24	24	0.001	21	24	24	0.01
Carbendazim	24	24	24	0.001	24	24	24	0.001
Carbetamide	24	24	24	0.001	24	24	24	0.001
Carbofuran	24	24	24	0.001	24	24	24	0.001
Carbophenothion	2	24	24	0.01	0	22	23	0.1
Carboxine	24	24	24	0.001	24	24	23	0.001
Carfentrazone-ethyl	24	24	24	0.001	24	24	24	0.001
Carprofen	24	24	24	0.001	24	24	24	0.001
Carpropamid	24	24	24	0.001	24	24	24	0.001
Cefalexine	24	24	24	0.001	9	24	24	0.01

Compounds	No. of detections			SDL (mg.kg^{-1})	No. of identifications			LOI (mg.kg^{-1})
	0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}		0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}	
Cefapirine	1	1	23	0.1	0	0	22	> 0.1
Cefazolin	24	24	24	0.001	2	4	17	> 0.1
Cefoperazone	24	24	24	0.001	24	24	24	0.001
Ceftiofur +4	24	24	24	0.001	24	24	24	0.001
Cefuroxim	24	24	24	0.001	17	11	18	> 0.1
Chinomethionate	24	24	24	0.001	23	24	24	0.001
Chlorantraniliprole	24	24	24	0.001	24	24	24	0.001
Chlorbromuron	24	24	24	0.001	17	24	24	0.01
Chlordimeform	24	24	24	0.001	23	24	24	0.001
Chlorfenapyr	7	19	20	> 0.1	0	1	14	> 0.1
Chlorfenvinphos (mixture of Z and E)	24	24	24	0.001	24	24	24	0.001
Chlorfluazuron	24	24	24	0.001	24	24	24	0.001
Chloridazon	24	24	24	0.001	24	24	24	0.001
Chlorimuron-ethyl	24	24	24	0.001	24	24	24	0.001
Chlorobenzuron	24	24	24	0.001	23	24	24	0.001
Chlorosulfuron	24	24	24	0.001	24	24	24	0.001
Chlorotoluron	24	24	24	0.001	24	24	24	0.001
Chloroxuron	24	24	24	0.001	24	24	24	0.001
Chlorpyrifos	23	24	24	0.001	19	24	24	0.01
Chlorpyrifos-methyl	22	24	24	0.01	1	13	20	> 0.1
Chlorpyrifos-oxon	24	24	24	0.001	24	24	24	0.001
Chlorthiamid	0	0	1	> 0.1	0	0	0	> 0.1
Chlorthiophos	20	24	24	0.01	0	0	0	> 0.1
Chromafenozide	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Cinidon-ethyl	23	24	24	0.001	11	18	3	> 0.1
Cinmethylin	24	23	24	0.001	20	21	24	0.1
Cinosulfuron	24	24	24	0.001	24	24	24	0.001
Cinoxacin	24	24	24	0.001	19	23	24	0.01
Ciprofloxacin	24	24	24	0.001	21	24	24	0.01
Clarithromycin	24	24	24	0.001	24	24	23	0.001
Clethodim	24	24	24	0.001	21	24	23	0.01
Climbazol	24	24	24	0.001	20	24	24	0.01
Clindamycin	24	24	24	0.001	24	24	24	0.001
Clodinafop (acid-free)	24	24	24	0.001	19	24	24	0.01
Clodinafop-propargyl	24	24	24	0.001	24	24	24	0.001
Clofentezine	24	24	24	0.001	24	24	24	0.001
Clomeprop	24	24	24	0.001	24	24	24	0.001
Cloquintocet-mexyl	24	24	24	0.001	24	24	24	0.001
Cloransulam-methyl	24	24	24	0.001	24	24	24	0.001
Clorsulon	24	24	24	0.001	24	24	24	0.001
Closantel	24	24	24	0.001	24	24	24	0.001
Clothianidin	24	24	24	0.001	24	24	24	0.001
Cloxacillin	24	24	24	0.001	19	23	24	0.01
Command (clomazone)	24	24	24	0.001	24	24	24	0.001
Coumaphos	24	24	24	0.001	23	24	24	0.001
Coumaphos-oxon	24	24	24	0.001	24	24	24	0.001
Crimidine	24	24	24	0.001	24	24	24	0.001
Crotoxyphos	24	24	24	0.001	5	10	3	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Cumyluron	24	24	24	0.001	24	22	24	0.001
Cyanofenphos	0	6	13	> 0.1	0	2	2	> 0.1
Cyanophos	24	24	24	0.001	0	0	0	> 0.1
Cyantraniliprole	24	24	24	0.001	24	24	24	0.001
Cyazofamid	24	24	24	0.001	24	23	24	0.001
Cyclanilide	24	24	24	0.001	24	24	24	0.001
Cycloate	24	24	24	0.001	8	24	24	0.01
Cyclohexamide	24	24	24	0.001	1	4	23	0.1
Cycloprothrin	0	3	8	> 0.1	0	0	0	> 0.1
Cyclosulfamuron	24	24	24	0.001	24	24	24	0.001
Cycloxidim	24	24	24	0.001	19	24	24	0.01
Cycluron	24	24	24	0.001	24	23	24	0.001
Cyflufenamid	24	24	23	0.001	23	24	23	0.001
Cyhalofop-butyl	9	14	23	0.1	3	5	11	> 0.1
Cymiazole	24	24	24	0.001	24	24	24	0.001
Cymoxanil	24	24	24	0.001	1	12	24	0.1
Cypermethrin (mixture of isomers)	0	2	5	> 0.1	0	0	0	> 0.1
Cyphenothrin	12	22	23	0.1	0	6	15	> 0.1
Cyprazine	23	24	24	> 0.1	18	20	22	> 0.1
Cyproconazole (mixture of isomers)	24	24	24	0.001	24	23	24	0.001
Cyprodinil	24	24	24	0.001	24	24	24	0.001
Cyprofuram	24	24	24	0.001	24	24	24	0.001
Cyprosulfamide	24	24	24	0.001	24	24	24	0.001
Cyromazine	22	23	24	0.01	5	15	24	0.1

Compounds	No. of detections			SDL (mg.kg^{-1})	No. of identifications			LOI (mg.kg^{-1})
	0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}		0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}	
Cythioate	24	24	24	0.001	0	2	2	> 0.1
Daimuron	24	24	24	0.001	22	24	24	0.01
Daminozide	19	24	24	0.01	0	1	7	> 0.1
Danitol	21	23	24	0.01	14	17	22	> 0.1
Danofloxacin	24	24	24	0.001	23	24	24	0.001
Dapsone	24	24	24	0.001	23	24	24	0.001
Dazomet	5	21	21	> 0.1	0	0	7	> 0.1
Dementon-*S*-methyl sulfone	24	24	24	0.001	24	24	24	0.001
Demeton S	23	24	24	0.001	18	20	19	> 0.1
Demeton-*S*-methyl	13	16	20	> 0.1	0	0	0	> 0.1
Deoxynivalenol	4	4	0	> 0.1	0	0	0	> 0.1
Desethyl atrazine	24	24	24	0.001	22	24	24	0.01
Desfuroylceftiofur cysteine disulfide (DCCD)	22	24	24	0.01	5	12	16	> 0.1
Desmedipham	24	24	24	0.001	24	24	24	0.001
Desmethyl norflurazon	24	24	24	0.001	24	24	24	0.001
Desmethyl-formamido-pirimicarb	24	24	24	0.001	24	24	24	0.001
Desmetryn	9	24	24	0.01	9	24	24	0.01
Diafenthiuron	0	0	1	> 0.1	0	0	0	> 0.1
Dialifos	24	24	24	0.001	21	22	24	0.1
Diazinon	24	24	24	0.001	24	24	24	0.001
Diazinon-O-analog	24	24	24	0.001	24	24	24	0.001
Dibrom	17	24	23	0.01	0	0	0	> 0.1
Dichlofenthion	18	24	24	0.01	1	8	19	> 0.1
Dichlormid	24	24	24	0.001	10	15	23	0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Dichlorvos	24	24	24	0.001	2	14	24	0.1
Diclazuril	23	24	24	0.001	23	24	24	0.001
Diclobutrazol (mixture of stereo isomers)	24	24	24	0.001	24	23	24	0.001
Diclocymet	24	24	24	0.001	24	24	24	0.001
Diclofenac	24	24	24	0.001	24	24	24	0.001
Diclosulam	24	24	24	0.001	24	24	24	0.001
Dicrotophos	24	24	24	0.001	24	24	24	0.001
Diethatyl-ethyl	24	24	24	0.001	24	24	24	0.001
Diethofencarb	24	24	24	0.001	24	24	24	0.001
Difenoconazole (mixture of isomers)	24	24	24	0.001	24	24	24	0.001
Difenoxurone	24	24	24	0.001	24	24	24	0.001
Difloxacin	24	24	24	0.001	24	24	24	0.001
Diflubenzuron	24	24	24	0.001	24	24	24	0.001
Diflufenicen	24	24	24	0.001	24	24	24	0.001
Dimefox	24	24	24	0.001	11	11	19	> 0.1
Dimefuron	24	24	24	0.001	24	24	24	0.001
Dimepiperate	24	24	24	0.001	24	24	23	0.001
Dimethachlor	24	24	24	0.001	24	24	24	0.001
Dimethametryn	24	24	24	0.001	24	24	24	0.001
Dimethenamid	24	24	24	0.001	24	24	24	0.001
Dimethirimol	24	24	24	0.001	24	24	24	0.001
Dimethoate	24	24	24	0.001	24	24	24	0.001
Dimethomorph	24	24	24	0.001	24	24	24	0.001
Dimethylvinphos	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Dimetilan	24	24	24	0.001	24	24	24	0.001
Dimetridazole	24	24	24	0.001	24	24	24	0.001
Dimoxystrobin	24	24	24	0.001	24	24	24	0.001
Diniconazole (E isomer)	24	24	24	0.001	24	24	24	0.001
Diniconazole (Z isomer)	24	24	24	0.001	24	24	24	0.001
Dinitramine	24	24	24	0.001	24	24	24	0.001
Dinotefuran	24	24	24	0.001	24	24	24	0.001
Dioxacarb	24	24	24	0.001	24	24	24	0.001
Dioxathion (mixture of isomers)	0	1	0	> 0.1	0	0	0	> 0.1
Diphenamid	24	24	24	0.001	24	24	24	0.001
Diphenyl phosphate	1	0	2	> 0.1	0	0	0	> 0.1
Diphenylamine	24	24	24	0.001	24	24	24	0.001
Dipropetryn	24	24	24	0.001	24	24	24	0.001
Disulfoton sulfone	24	24	24	0.001	13	22	23	0.1
Disulfoton sulfoxide	24	24	24	0.001	24	24	24	0.001
Ditalimfos	24	24	24	0.001	23	24	24	0.001
Dithianon	0	11	18	> 0.1	0	0	3	> 0.1
Dithiopyr	24	24	24	0.001	24	24	24	0.001
Diuron	24	24	24	0.001	24	24	24	0.001
DMA	24	24	24	0.001	24	24	24	0.001
DMF	24	24	24	0.001	22	24	24	0.01
DMPF	24	24	24	0.001	24	24	24	0.001
Dodemorph	24	24	24	0.001	24	24	24	0.001
Doramectin	24	24	24	0.001	23	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Dyfonate™	24	24	24	0.001	17	24	23	0.01
Edifenphos	24	24	24	0.001	24	24	24	0.001
Emamectin	7	24	24	0.01	0	24	24	0.01
Emamectin B1a	24	24	24	0.001	24	24	24	0.001
Empenthrin	9	24	24	0.01	0	3	9	> 0.1
Enrofloxacin	24	24	24	0.001	24	24	24	0.001
Epn	24	24	24	0.001	2	11	21	> 0.1
Epoxiconazole (iso)	24	24	24	0.001	24	24	24	0.001
Eprinomectin	23	24	24	0.001	21	24	24	0.01
Eprinomectin B1a	23	24	24	0.001	21	24	24	0.01
EPTC (S-ethyl dipropylthiocarbamate)	24	24	24	0.001	1	2	5	> 0.1
Erythromycin	24	24	24	0.001	24	24	24	0.001
Erythromycin	24	24	24	0.001	24	24	24	0.001
Esbiol	24	24	24	0.001	4	21	22	> 0.1
Esprocarb	24	24	24	0.001	24	24	24	0.001
Etaconazole	24	24	24	0.001	24	24	24	0.001
Ethaboxam	24	24	24	0.001	24	24	24	0.001
Ethametsulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Ethidimuron	24	24	24	0.001	23	24	24	0.001
Ethiofencarb	24	24	24	0.001	24	24	24	0.001
Ethiofencarb sulfone	24	24	24	0.001	24	24	23	0.001
Ethiofencarb sulfoxide	24	24	24	0.001	24	24	24	0.001
Ethion	24	24	24	0.001	23	23	23	0.001
Ethiozin	17	22	22	> 0.1	14	20	20	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Ethiprole	24	24	24	0.001	24	24	24	0.001
Ethirimol	24	24	24	0.001	24	24	24	0.001
Ethofumesate	24	24	24	0.001	0	0	0	> 0.1
Ethoprophos (prophos)	24	24	24	0.001	24	24	24	0.001
Ethoxyquin	6	19	24	0.1	3	15	22	> 0.1
Ethoxysulfuron	24	24	24	0.001	21	21	24	0.1
Ethyclozate	24	24	24	0.001	24	24	24	0.001
Etobenzanid	24	24	24	0.001	22	24	24	0.01
Etoxazole	24	24	24	0.001	24	24	24	0.001
Etrimfos	24	24	24	0.001	24	24	24	0.001
Famoxadone	5	0	2	> 0.1	2	0	0	> 0.1
Famphur	24	24	24	0.001	23	24	24	0.001
Fenamidone	24	24	24	0.001	24	24	24	0.001
Fenamiphos	24	24	24	0.001	24	24	24	0.001
Fenamiphos sulfone	24	24	24	0.001	24	24	24	0.001
Fenamiphos sulfoxide	24	24	24	0.001	15	8	1	> 0.1
Fenarimol	24	24	24	0.001	24	24	24	0.001
Fenazaquin	24	24	24	0.001	24	24	24	0.001
Fenazox	24	24	24	0.001	8	20	22	> 0.1
Fenbendazole	24	24	24	0.001	24	24	24	0.001
Fenbuconazole	24	24	24	0.001	24	24	24	0.001
Fenchlorazol-ethyl	24	24	24	0.001	23	24	24	0.001
Fenchlorphos-oxon	24	24	24	0.001	22	24	24	0.01
Fenclorim	3	1	5	> 0.1	0	0	0	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Fenfuram	24	24	24	0.001	24	24	24	0.001
Fenhexamid	24	24	24	0.001	24	24	24	0.001
Fenitrothion	20	23	24	0.01	7	22	24	0.1
Fenobucarb	23	24	24	0.001	23	23	24	0.001
Fenothiocarb	24	24	24	0.001	24	24	24	0.001
Fenoxanil	24	24	24	0.001	24	24	24	0.001
Fenoxaprop	24	24	24	0.001	24	24	24	0.001
Fenoxaprop-P-ethyl	24	24	24	0.001	24	24	24	0.001
Fenoxycarb	24	24	24	0.001	24	24	24	0.001
Fenpiclonil	24	24	24	0.001	24	24	24	0.001
Fenpropathrin	21	23	24	0.01	14	17	23	0.1
Fenpropidin	24	24	24	0.001	24	24	24	0.001
Fenpropimorph	24	24	24	0.001	24	24	24	0.001
Fenpyroximate	24	24	24	0.001	24	24	24	0.001
Fensulfothion	24	24	24	0.001	24	24	24	0.001
Fensulfothion-oxon	24	24	24	0.001	24	24	24	0.001
Fensulfothion-oxon sulfone	24	24	24	0.001	24	24	24	0.001
Fensulfothion sulfone	24	24	24	0.001	7	20	24	0.1
Fenthion	24	24	24	0.001	1	19	24	0.1
Fenthion-oxon	24	24	24	0.001	24	24	24	0.001
Fenthion-oxon sulfoxide	24	24	24	0.001	24	24	23	0.001
Fenthion sulfoxide	24	24	24	0.001	24	24	24	0.001
Fenthion-ethyl	24	24	24	0.001	3	24	24	0.01
Fenthion sulfone	24	24	24	0.001	1	6	17	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Fenthoxon sulfone	24	24	24	0.001	24	24	24	0.001
Fenuron	24	24	24	0.001	24	24	24	0.001
Ferimzone	10	24	24	0.01	6	23	23	0.01
Fipronil	24	24	24	0.001	22	18	24	0.1
Fipronil sulfide	23	24	24	0.001	22	24	24	0.01
Fipronil-desulfinyl	24	24	24	0.001	22	24	24	0.01
Flamprop-isopropyl	24	24	24	0.001	24	24	24	0.001
Flamprop-methyl (Metaven)	24	24	24	0.001	9	17	20	> 0.1
Flamprop-M-isopropyl	24	24	24	0.001	24	24	24	0.001
Flazasulfuron	24	24	24	0.001	3	6	4	> 0.1
Fleroxacin	24	24	24	0.001	24	24	24	0.001
Flonicamid	24	24	24	0.001	24	24	24	0.001
Florasulam	24	24	24	0.001	24	24	24	0.001
Florfénicol	24	24	24	0.001	24	24	24	0.001
Fluacrypyrim	24	24	24	0.001	23	24	24	0.001
Fluazifop	24	24	24	0.001	24	24	24	0.001
Fluazifop-butyl	24	24	24	0.001	24	24	24	0.001
Fluazifop-P-butyl	24	24	24	0.001	24	24	24	0.001
Fluazinam	24	24	24	0.001	24	24	24	0.001
Fluazuron	24	24	24	0.001	24	24	23	0.001
Flubendazole	24	24	24	0.001	24	24	24	0.001
Flubendiamide	24	24	24	0.001	24	24	24	0.001
Flucarbazone sodium	22	24	24	0.01	10	20	23	0.1
Fluchloralin	1	17	24	0.1	0	1	0	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Flucycloxuron	24	24	24	0.001	24	24	24	0.001
Fludioxonil	10	10	20	> 0.1	0	0	0	> 0.1
Flufenacet	24	24	24	0.001	23	24	24	0.001
Flufenoxuron	24	24	24	0.001	24	24	24	0.001
Flumequine	23	23	23	0.001	23	23	23	0.001
Flumestulam	24	24	24	0.001	24	24	24	0.001
Flumetralin	2	20	22	> 0.1	0	0	0	> 0.1
Flumiclorac-pentyl	24	24	24	0.001	24	24	24	0.001
Flumioxazin	24	24	24	0.001	22	24	24	0.01
Flumorph	24	24	24	0.001	24	24	24	0.001
Flunixin	24	24	24	0.001	24	24	24	0.001
Fluoglycofene-ethyl	22	24	23	0.01	14	15	16	> 0.1
Fluometuron	24	24	24	0.001	24	24	24	0.001
Fluopicolide	24	24	24	0.001	24	24	24	0.001
Fluopyram	24	24	24	0.001	24	24	24	0.001
Fluorodifen	1	1	0	> 0.1	1	1	0	> 0.1
Fluoxastrobin	24	24	24	0.001	24	24	24	0.001
Flupyradifurone	24	24	24	0.001	23	24	24	0.001
Flupyrsulfuron-methyl sodium	20	24	24	0.01	0	0	0	> 0.1
Fluquinconazole	24	24	24	0.001	24	24	24	0.001
Fluralaner	23	24	24	0.001	23	24	24	0.001
Fluridone	24	24	24	0.001	24	24	24	0.001
Flurilazole	22	18	23	0.1	0	2	19	> 0.1
Flurochloridon (iso)	24	24	24	0.001	17	24	24	0.01

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Fluroxypyr	24	24	24	0.001	24	24	24	0.001
Fluroxypyr-meptyl	24	24	24	0.001	18	24	24	0.01
Flurprimidol	24	24	24	0.001	24	24	24	0.001
Flurtamone	24	24	24	0.001	24	24	24	0.001
Flusilazole	24	24	24	0.001	24	24	24	0.001
Fluthiacet-methyl	24	24	24	0.001	24	24	24	0.001
Flutolanil	24	24	24	0.001	24	24	24	0.001
Flutriafol	24	24	24	0.001	24	24	24	0.001
Fomesafen	23	24	24	0.001	22	20	24	0.1
Foramsulfuron	24	24	24	0.001	24	24	24	0.001
Forchlorfenuron	24	24	24	0.001	24	24	24	0.001
Formetanate HCl	6	0	24	0.1	0	0	24	0.1
Fosthiazate	24	24	24	0.001	24	24	24	0.001
Fuberidazole	24	24	24	0.001	24	24	24	0.001
Furalaxyl	24	24	24	0.001	24	24	24	0.001
Furathiocarb	24	24	24	0.001	24	24	24	0.001
Furmecyclox	24	24	24	0.001	24	24	24	0.001
Fusidic acid	23	24	24	0.001	23	24	23	0.001
Gamithromycin	24	24	24	0.001	23	24	24	0.001
Guthion-ethyl	21	17	24	0.1	1	5	8	> 0.1
Guthion®	2	0	11	> 0.1	0	0	5	> 0.1
Halofenozide	24	24	24	0.001	24	24	24	0.001
Halofuginone	24	24	24	0.001	24	24	24	0.001
Halosulfuron-methyl	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Haloxyfop	9	18	3	> 0.1	0	6	0	> 0.1
Haloxyfop-2-ethoxyethyl	24	24	24	0.001	24	24	24	0.001
Haloxyfop-methyl	24	24	24	0.001	24	24	24	0.001
Haloxyfop-P-methyl	24	24	24	0.001	24	24	24	0.001
Heptenophos	24	24	24	0.001	22	24	24	0.01
Hexaconazole	24	24	24	0.001	24	24	24	0.001
Hexaflumuron	24	24	24	0.001	23	24	24	0.001
Hexazinon	24	24	24	0.001	24	24	24	0.001
Hexythiazox	24	24	24	0.001	24	24	24	0.001
HMMNI	23	24	24	0.001	20	23	24	0.01
Hydroxy-flubendazole	24	24	24	0.001	24	24	24	0.001
Hydroxy-mebendazole	24	24	24	0.001	24	24	24	0.001
Hydroxy-thiabendazole	24	24	24	0.001	24	24	24	0.001
Hymexazole	19	22	24	0.1	0	0	0	> 0.1
Imazalil	24	24	24	0.001	24	24	24	0.001
Imazamethabenz-methyl	24	24	24	0.001	24	24	24	0.001
Imazamox	24	24	24	0.001	24	24	24	0.001
Imazapic	24	24	24	0.001	24	24	24	0.001
Imazaquin	24	24	24	0.001	24	24	24	0.001
Imazethapyr	24	24	24	0.001	24	24	24	0.001
Imazosulfuron	24	24	24	0.001	24	24	24	0.001
Imibenconazole	24	24	24	0.001	24	24	24	0.001
Imidacloprid	24	24	24	0.001	24	24	24	0.001
Imidacloprid-olefin	24	24	24	0.001	22	24	24	0.01

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Inabenfide	24	24	24	0.001	24	24	24	0.001
Indaziflam	24	24	24	0.001	24	24	24	0.001
Indoxacarb	24	24	24	0.001	24	24	24	0.001
Iodofenphos	5	18	19	> 0.1	0	2	9	> 0.1
Iodosulfuron-methyl sodium	18	24	23	0.01	1	16	19	> 0.1
Ipconazole	24	24	24	0.001	24	24	24	0.001
Iprobenfos	24	24	24	0.001	24	24	24	0.001
Iprodione	20	24	24	0.01	1	6	10	> 0.1
Ipronidazole	24	24	24	0.001	24	24	24	0.001
Ipronidazole OH	24	24	24	0.001	18	24	24	0.01
Iprovalicarb	24	24	24	0.001	24	24	24	0.001
Irgarol (cybutryne)	24	24	24	0.001	24	24	24	0.001
Isazophos	24	24	24	0.001	24	24	24	0.001
Isocarbamide	24	24	24	0.001	14	21	24	0.1
Isofenphos	24	24	24	0.001	24	24	24	0.001
Isofenphos-methyl	22	23	24	0.01	19	19	24	0.1
Isofenphos-oxon	24	24	24	0.001	24	24	24	0.001
Isomethiozin	24	24	24	0.001	24	24	24	0.001
Isonoruron	24	24	24	0.001	24	24	24	0.001
Isoprocarb	24	24	24	0.001	24	24	24	0.001
Isopropalin	24	24	24	0.001	8	22	23	0.1
Isoprothiolane	24	24	24	0.001	24	24	24	0.001
Isoproturon	24	24	24	0.001	24	24	24	0.001
Isouron	24	24	24	0.001	23	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Isoxaben	24	24	24	0.001	24	24	24	0.001
Isoxadifen-ethyl	24	24	24	0.001	23	24	24	0.001
Isoxaflutole	24	24	24	0.001	20	23	23	0.01
Isoxathion	24	24	24	0.001	23	24	24	0.001
Ivermectin	24	24	24	0.001	0	0	0	> 0.1
Ivermectin B1a	24	24	24	0.001	0	16	21	> 0.1
Josamycin	24	24	23	0.001	24	24	23	0.001
Karbutilate	24	24	24	0.001	22	24	24	0.01
Ketoprofen	24	24	24	0.001	24	24	24	0.001
Ketotriclabendazole	24	24	24	0.001	24	24	24	0.001
Kresoxim Methyl	18	24	24	0.01	18	23	24	0.01
Lactofen	22	24	24	0.01	15	22	23	0.1
Lasalocid A	24	24	24	0.001	24	24	24	0.001
Lenacil	24	24	24	0.001	23	24	24	0.001
Leptophos	7	21	22	> 0.1	1	11	20	> 0.1
Levamisole	22	24	24	0.01	22	24	24	0.01
Levofloxacin	24	24	24	0.001	23	24	23	0.001
Lincomycin	24	24	24	0.001	24	24	24	0.001
Linuron	24	24	24	0.001	24	24	24	0.001
Lomefloxacin	24	24	24	0.001	24	24	24	0.001
Lufenuron	24	24	24	0.001	23	24	24	0.001
Maduramicin	19	22	23	0.1	19	22	23	0.1
Malaoxon	24	24	24	0.001	23	23	24	0.001
Malathion	24	24	24	0.001	20	22	24	0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Mandipropamid	24	24	24	0.001	24	24	24	0.001
Marbofloxacin	24	24	24	0.001	21	24	24	0.01
Mebendazole	24	24	24	0.001	24	24	24	0.001
Mefenacet	24	24	24	0.001	24	24	24	0.001
Mefenamic acid	24	24	24	0.001	24	24	24	0.001
Mefenpyr-diethyl	24	24	24	0.001	24	24	24	0.001
Mefluidide	24	24	24	0.001	24	24	24	0.001
Meloxicam	24	24	24	0.001	24	24	24	0.001
Mepanipyrim	24	24	24	0.001	24	24	24	0.001
Mephosfolan	24	24	24	0.001	24	24	24	0.001
Mepronil	24	24	24	0.001	24	24	23	0.001
Mesosulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Mesotrione	24	24	24	0.001	23	23	24	0.001
Metaflumizone	24	24	24	0.001	24	24	24	0.001
Metalaxyl	24	24	24	0.001	24	24	24	0.001
Metalaxyl-m	24	24	24	0.001	24	24	24	0.001
Metamitron	24	24	24	0.001	18	24	24	0.01
Metazachlor	24	24	24	0.001	24	24	24	0.001
Metconazole	24	24	24	0.001	24	24	24	0.001
Methabenzthiazuron	24	24	24	0.001	24	24	24	0.001
Methacrifos	8	20	21	> 0.1	0	0	0	> 0.1
Methfuroxam	24	24	24	0.001	24	24	24	0.001
Methidathion	24	24	24	0.001	4	17	23	0.1
Methiocarb	24	24	24	0.001	18	19	24	0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Methiocarb sulfone	24	24	24	0.001	19	21	24	0.1
Methiocarb sulfoxide	24	24	24	0.001	24	24	24	0.001
Methoprotryne	24	24	24	0.001	24	24	24	0.001
Methoxyfenozide	24	24	24	0.001	24	24	24	0.001
Methyl paraoxon	24	24	24	0.001	16	24	24	0.01
Methyl parathion	23	24	24	0.001	0	0	0	> 0.1
Metobromuron	24	24	24	0.001	24	24	24	0.001
Metolachlor	24	24	24	0.001	24	24	24	0.001
Metolcarb	22	24	24	0.01	17	23	24	0.01
(E)-Metominostrobin	24	24	24	0.001	24	24	24	0.001
(Z)-Metominostrobin	24	24	24	0.001	24	24	24	0.001
Metosulam	24	24	24	0.001	24	24	24	0.001
Metoxuron	24	24	24	0.001	24	24	23	0.001
Metrafenone	24	24	24	0.001	24	24	24	0.001
Metribuzin	24	24	24	0.001	24	24	24	0.001
Metronidazole	24	24	24	0.001	20	24	23	0.01
Metsulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Mevinphos	24	24	24	0.001	24	24	24	0.001
Mexacarbate	24	24	24	0.001	24	24	24	0.001
MGK-264 (mixture of isomers)	24	24	24	0.001	15	24	24	0.01
Molinate	24	24	24	0.001	9	21	24	0.1
Monensin	24	24	24	0.001	24	24	24	0.001
Monepantel	24	24	24	0.001	23	24	24	0.001
Monepantel sulfone	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Monocrotophos	24	24	24	0.001	23	24	24	0.001
Monolinuron	24	24	24	0.001	24	24	24	0.001
Monuron	24	24	24	0.001	24	24	24	0.001
Morantel	24	24	24	0.001	24	24	24	0.001
Moxidectin	24	24	24	0.001	15	24	24	0.01
N,N-Diethyl-*m*-toluamide (DEET)	24	24	24	0.001	24	24	24	0.001
N,N'-Ethylenethiourea	0	0	3	> 0.1	0	0	0	> 0.1
Nafcillin	24	24	24	0.001	22	23	24	0.01
Naphthalophos (naftalofos)	24	24	24	0.001	24	24	24	0.001
Napropamide	24	24	24	0.001	24	24	24	0.001
Naproxen	23	24	24	0.001	20	24	23	0.01
Naptalam	24	24	24	0.001	23	24	24	0.001
Narasin	24	24	24	0.001	24	24	24	0.001
Neburon	24	24	24	0.001	24	24	24	0.001
Nicosulfuron	24	24	24	0.001	23	24	24	0.001
Nigericin	24	24	24	0.001	24	24	24	0.001
Nitenpyram (ISO)	24	24	24	0.001	21	24	24	0.01
Nitralin	23	23	24	0.001	0	0	0	> 0.1
Nitroguanidine	12	20	24	0.1	0	0	0	> 0.1
Nitroxinil	24	24	24	0.001	24	24	24	0.001
Norfloxacin	24	24	24	0.001	24	24	23	0.001
Norflurazon	24	24	24	0.001	24	24	24	0.001
Noruron	24	24	24	0.001	24	24	24	0.001
Novaluron	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Novobiocin	24	24	24	0.001	23	24	24	0.001
Nuarimol	24	24	24	0.001	24	24	24	0.001
O-Acetyltylosin	24	24	24	0.001	24	24	24	0.001
Ofloxacin	24	24	24	0.001	23	24	23	0.001
Ofurace	24	24	24	0.001	24	24	24	0.001
Oleandomycin	24	24	24	0.001	22	24	24	0.01
Omethoate	1	1	0	> 0.1	0	0	0	> 0.1
Orbencarb	24	24	24	0.001	24	24	24	0.001
Orbifloxacin	24	24	24	0.001	24	24	24	0.001
Ormetoprime	24	24	24	0.001	24	24	24	0.001
Orysastrobin	24	24	24	0.001	24	24	24	0.001
Oryzalin	24	24	24	0.001	24	24	24	0.001
Oxacillin	24	24	24	0.001	24	24	24	0.001
Oxadiargyl	24	24	24	0.001	0	12	16	> 0.1
Oxadiazon	22	23	24	0.01	13	22	23	0.1
Oxadixyl	24	24	24	0.001	24	24	24	0.001
Oxasulfuron	24	24	24	0.001	24	24	24	0.001
Oxaziclomefone	24	24	24	0.001	24	24	24	0.001
Oxfendazole (fenbendazole sulfoxide)	24	24	24	0.001	24	24	24	0.001
Oxfendazole sulfone (fenbendazole sulfone)	24	24	24	0.001	24	24	24	0.001
Oxibendazole	24	24	24	0.001	24	24	24	0.001
Oxolinic acid	24	24	24	0.001	23	23	24	0.001
Oxycarboxin	24	24	24	0.001	24	24	24	0.001
Oxyclozanide	24	24	24	0.001	23	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Oxyfluorfen	15	22	24	0.1	1	8	21	> 0.1
Oxyphenbutazone	24	24	24	0.001	24	24	24	0.001
Paclobutrazol (mixture of stereo isomers)	24	24	24	0.001	24	24	24	0.001
Paraoxon-ethyl	24	24	24	0.001	23	24	24	0.001
Parathion	24	24	24	0.001	1	6	17	> 0.1
Pebulate	24	24	24	0.001	0	12	24	0.1
Penconazol	24	24	24	0.001	24	24	24	0.001
Pencycuron	24	24	24	0.001	24	24	24	0.001
Pendimethalin	24	24	24	0.001	9	20	23	0.1
Penfluron	23	24	24	0.001	23	24	24	0.001
Pénicillin-G	24	24	24	0.001	21	24	24	0.01
Penicilllin-V^{+4}	24	24	24	0.001	24	24	24	0.001
Penoxsulam	24	24	24	0.001	24	24	24	0.001
Pentanochlor	24	24	24	0.001	24	24	24	0.001
Penthiopyrad	24	24	24	0.001	24	24	24	0.001
Pethoxamid	24	24	24	0.001	24	24	24	0.001
Phenmedipham	24	24	24	0.001	24	24	24	0.001
Phenothrin	1	24	24	0.01	0	18	23	0.1
Phenthoate	24	24	24	0.001	6	20	21	> 0.1
Phenylbutazone	24	24	24	0.001	21	24	24	0.01
Phenylurea	23	24	24	0.001	23	24	24	0.001
Phorate-oxon sulfoxide	24	24	24	0.001	4	15	15	> 0.1
Phorate sulfoxide	24	24	24	0.001	24	24	24	0.001
Phorate-oxon sulfone	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Phorat sulfone	24	24	24	0.001	6	19	23	0.1
Phosalone	24	24	24	0.001	19	22	22	> 0.1
Phosfolan	24	24	24	0.001	24	24	24	0.001
Phosmet	24	24	24	0.001	23	24	24	0.001
Phosmet-oxon	24	24	24	0.001	24	24	24	0.001
Phosphamidon	24	24	24	0.001	24	24	24	0.001
Phospholan-methyl	24	24	24	0.001	23	24	24	0.001
Phoxim	24	24	24	0.001	24	24	24	0.001
Phthalylsulfathiazole (CAS)	24	24	24	0.001	24	24	24	0.001
Picolinafen	24	24	24	0.001	7	9	9	> 0.1
Picoxystrobin	24	24	24	0.001	24	24	24	0.001
Piperalin	24	24	24	0.001	24	24	24	0.001
Piperonyl butoxide	24	24	24	0.001	24	24	24	0.001
Piperophos	24	24	24	0.001	24	24	24	0.001
Pirimicarb	24	24	24	0.001	24	24	24	0.001
Pirimicarb-desmethyl	24	24	24	0.001	24	24	24	0.001
Pirimiphos-methyl	24	24	24	0.001	24	24	24	0.001
Pirimiphos-ethyl	24	24	24	0.001	24	24	24	0.001
Pirimiphos-methyl-N-desethyl	24	24	24	0.001	24	24	24	0.001
Pirlymycin	24	24	24	0.001	24	24	24	0.001
Prallethrin	24	24	24	0.001	2	15	24	0.1
Pretilachlor	24	24	24	0.001	24	24	24	0.001
Primisulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Probenazole	24	24	24	0.001	6	16	22	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Prochloraz	24	24	24	0.001	24	24	24	0.001
Procyazine	24	24	24	0.001	24	24	24	0.001
Procymidone	20	24	24	0.01	18	23	23	0.01
Profenofos	24	24	24	0.001	21	20	23	0.1
Profoxydim lithium	24	24	24	0.001	21	24	24	0.01
Prohydrojasmon	7	24	24	0.01	0	5	19	> 0.1
Promecarb	23	24	24	0.001	23	23	24	0.001
Prometon	24	24	24	0.001	24	24	24	0.001
Prometryn	24	24	24	0.001	24	24	24	0.001
Propachlor	24	24	24	0.001	24	24	24	0.001
Propanil	24	24	24	0.001	24	24	24	0.001
Propaphos	24	24	24	0.001	24	24	24	0.001
Propaquizafop	24	24	24	0.001	24	24	24	0.001
Propargite	24	24	24	0.001	23	24	24	0.001
Propazine	24	24	24	0.001	24	24	24	0.001
Propazine-2-hydroxy	24	24	24	0.001	24	24	24	0.001
Propetamphos	14	21	23	0.1	0	0	0	> 0.1
Propham	24	24	24	0.001	23	24	24	0.001
Propiconazol (mixture of isomers)	24	24	24	0.001	24	24	24	0.001
Propisochlor	24	24	24	0.001	24	24	24	0.001
Propoxur	24	24	24	0.001	23	24	24	0.001
Propyzamide (pronamide)	24	24	24	0.001	24	24	24	0.001
Proquinazid	24	24	24	0.001	24	24	24	0.001
Prosulfocarb	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL (mg.kg^{-1})	No. of identifications			LOI (mg.kg^{-1})
	0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}		0.001 mg.kg^{-1}	0.01 mg.kg^{-1}	0.1 mg.kg^{-1}	
Prosulfuron	24	24	24	0.001	24	24	24	0.001
Prothioconazole-desthio	24	24	24	0.001	24	24	24	0.001
Pymetrozine	22	24	24	0.01	22	24	24	0.01
Pyracarbolid	24	24	24	0.001	24	24	24	0.001
Pyraclofos	24	24	24	0.001	23	24	24	0.001
Pyraclostrobin	24	24	24	0.001	24	24	24	0.001
Pyraflufen-ethyl	24	24	24	0.001	24	24	24	0.001
Pyrantel	24	24	24	0.001	24	24	24	0.001
Pyrazolynate	24	24	24	0.001	24	24	24	0.001
Pyrazophos	24	24	24	0.001	24	24	24	0.001
Pyrazosulfuron-ethyl	24	24	24	0.001	24	24	24	0.001
Pyrazoxyfen	24	24	24	0.001	24	24	24	0.001
Pyrethrin (mixture of isomers)	2	4	0	> 0.1	0	0	0	> 0.1
Pyributicarb	24	24	24	0.001	24	24	24	0.001
Pyridaben	24	24	24	0.001	24	24	24	0.001
Pyridafol	24	24	24	0.001	24	24	24	0.001
Pyridalyl	24	24	24	0.001	24	24	24	0.001
Pyridaphenthion	24	24	24	0.001	24	24	24	0.001
Pyridate	24	24	24	0.001	24	24	24	0.001
Pyrifenox (mixture of isomers))	24	24	24	0.001	24	24	24	0.001
Pyrimethanil	24	24	24	0.001	24	24	24	0.001
Pyriproxyfen	24	24	24	0.001	24	24	24	0.001
Pyroquilon	24	24	24	0.001	24	24	24	0.001
Pyroxsulam	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Quinalphos	24	24	24	0.001	24	24	24	0.001
Quinclorac	24	24	24	0.001	23	24	24	0.001
Quinmerac	16	24	24	0.01	16	24	24	0.01
Quinoclamine	24	24	24	0.001	22	24	24	0.01
Quinoline	24	24	24	0.001	24	24	24	0.001
Quinoxyfen	24	24	24	0.001	24	24	24	0.001
Quizalofop	24	24	24	0.001	23	24	24	0.001
Quizalofop-ethyl	24	24	24	0.001	24	24	24	0.001
Quizalofop-P-ethyl	24	24	24	0.001	24	24	24	0.001
Rafoxanide	23	24	24	0.001	22	24	24	0.01
Reserpine	24	24	24	0.001	23	24	23	0.001
Resmethrin	24	24	24	0.001	22	24	24	0.01
Rifampicin	5	16	20	> 0.1	2	14	17	> 0.1
Rifaximine	20	22	24	0.1	18	22	24	0.1
Rimsulfuron	24	24	24	0.001	20	24	23	0.01
Robenidine	24	24	24	0.001	24	24	24	0.001
Rotenone	24	24	23	0.001	24	24	23	0.001
Roxithromycin	24	24	23	0.001	24	24	23	0.001
Saflufenacil	24	24	24	0.001	21	24	24	0.01
Salinomycin	24	24	24	0.001	24	24	24	0.001
Sarafloxacin	24	24	24	0.001	24	24	24	0.001
Schradan (DMPA)	24	24	24	0.001	24	24	24	0.001
Sebuthylazin	22	24	23	0.01	22	24	24	0.01
Sebuthylazin-desethyl	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Secbumeton	1	24	24	0.01	1	24	24	0.01
Selamectin impurity B	24	24	24	0.001	24	24	24	0.001
Sethoxydim	24	24	24	0.001	18	23	24	0.01
Siduron	24	24	24	0.001	24	24	24	0.001
Simazine	24	24	24	0.001	24	24	24	0.001
Simeconazole	24	24	24	0.001	23	24	24	0.001
Simetone	24	24	24	0.001	24	24	24	0.001
Simetryn	9	24	24	0.01	9	24	24	0.01
S-Metolachlor	24	24	24	0.001	24	24	24	0.001
Spinetoram (mixture of isomers)	1	24	24	0.01	0	24	24	0.01
Spinosad (mixure Of spinosyn A and B)	2	24	24	0.01	0	24	24	0.01
Spiramycin	24	24	24	0.001	22	24	24	0.01
Spirodiclofen	24	24	23	0.001	24	24	23	0.001
Spiromesifen	24	24	24	0.001	24	24	24	0.001
Spirotetramat	24	24	24	0.001	24	24	24	0.001
Spirotetramat-enol	24	24	24	0.001	24	24	24	0.001
Spirotetramat-enol-glucoside	24	24	24	0.001	24	23	24	0.001
Spirotetramat-mono-hydroxy	24	24	24	0.001	24	24	24	0.001
Spiroxamine (mixture of isomers)	24	24	24	0.001	24	24	24	0.001
Sulcotrione	24	24	24	0.001	7	8	7	> 0.1
Sulfacetamide	24	24	24	0.001	24	24	24	0.001
Sulfachloropyridazine	24	24	24	0.001	24	24	24	0.001
Sulfaclozine	24	24	24	0.001	24	24	24	0.001
Sulfadiazine	24	24	24	0.001	22	24	24	0.01

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Sulfadimerazine	24	24	24	0.001	24	24	24	0.001
Sulfadimethoxine	24	24	24	0.001	24	24	24	0.001
Sulfadoxine	24	24	24	0.001	24	24	24	0.001
Sulfaguanidine	21	23	24	0.01	2	4	24	0.1
Sulfallate	22	24	24	0.01	8	9	18	> 0.1
Sulfamerazine	24	24	24	0.001	24	24	24	0.001
Sulfamethizole	24	24	24	0.001	24	24	24	0.001
Sulfamethoxazole	24	24	24	0.001	24	24	24	0.001
Sulfamethoxypyridazine	24	24	24	0.001	24	24	24	0.001
Sulfamonomethoxine	24	24	24	0.001	24	24	24	0.001
Sulfamonomethoxine	24	24	24	0.001	24	24	24	0.001
Sulfanilamide	24	24	24	0.001	1	13	16	> 0.1
Sulfaphenazole	24	24	24	0.001	24	24	24	0.001
Sulfaquinoxaline	24	24	24	0.001	24	24	24	0.001
Sulfathiazole	24	24	24	0.001	24	24	24	0.001
Sulfentrazone	24	24	24	0.001	24	24	24	0.001
Sulfisoxazole	24	24	24	0.001	24	24	24	0.001
Sulfometuron-methyl	24	24	24	0.001	24	24	24	0.001
Sulfosulfuron	24	24	24	0.001	24	24	24	0.001
Sulfoxaflor	24	24	24	0.001	24	24	24	0.001
Sulfuramid	19	18	24	0.1	19	18	24	0.1
Sulprofos sulfoxide	24	24	24	0.001	24	24	24	0.001
Systhane™	24	24	24	0.001	24	24	24	0.001
Tau-fluvalinate	20	22	22	> 0.1	15	19	21	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
TDCPP	23	24	24	0.001	11	5	12	> 0.1
Tebuconazol (Folicur®)	24	24	24	0.001	24	24	24	0.001
Tebufenozide	24	24	24	0.001	24	24	24	0.001
Tebufenpyrad	24	24	24	0.001	24	24	24	0.001
Tebupirimfos	24	24	24	0.001	24	24	24	0.001
Tebutam	24	24	24	0.001	24	24	24	0.001
Tebuthiuron	24	24	24	0.001	24	24	24	0.001
Teflubenzuron	24	24	24	0.001	21	24	24	0.01
Telithromycin	24	24	24	0.001	24	24	24	0.001
Tembotrione	24	24	24	0.001	19	22	22	> 0.1
Tepraloxydim	24	24	24	0.001	23	23	24	0.001
Terbufos	1	7	6	> 0.1	0	0	0	> 0.1
Terbufos sulfone	24	24	24	0.001	24	24	24	0.001
Terbufos sulfoxide	24	24	24	0.001	24	24	24	0.001
Terbumeton	24	24	24	0.001	24	24	24	0.001
Terbumeton-desethyl	24	24	24	0.001	24	24	24	0.001
Terbuthylazine	22	24	23	0.01	22	24	24	0.01
Terbuthylazine-desethyl	24	24	24	0.001	24	24	24	0.001
Terbutol (terbucarb)	24	24	24	0.001	24	24	24	0.001
Terbutryne	24	24	24	0.001	24	24	24	0.001
Terbutylazine-2-hydroxy	24	24	24	0.001	24	24	24	0.001
Tetrachlorvinphos (ISO)	24	24	24	0.001	0	0	0	> 0.1
Tetraconazole	24	24	24	0.001	24	24	24	0.001
Tetraethyl dithiopyrophosphate	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Tetraethyl pyrophosphate	24	24	24	0.001	24	24	24	0.001
Tetramethrin	24	24	23	0.001	24	24	23	0.001
Thenylchlor	24	24	24	0.001	11	13	24	0.1
Thiabendazole	24	24	24	0.001	24	24	24	0.001
Thiacloprid	24	24	24	0.001	24	24	24	0.001
Thiamethoxam	24	24	24	0.001	24	24	24	0.001
Thiamphenicol	24	24	24	0.001	24	23	24	0.001
Thiazafluron	24	24	24	0.001	24	24	24	0.001
Thiazopyr	24	24	24	0.001	24	24	24	0.001
Thidiazuron	24	24	24	0.001	24	24	24	0.001
Thiencarbazone-methyl	24	24	24	0.001	24	24	24	0.001
Thifensulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Thifluzamide	24	24	24	0.001	0	0	0	> 0.1
Thiobencarb	24	24	24	0.001	24	24	24	0.001
Thiocarbazyl	24	24	24	0.001	24	24	24	0.001
Thiodicarb	24	24	24	0.001	24	24	24	0.001
Thiofanox	24	24	24	0.001	4	11	23	0.1
Thiofanox-sulfone	24	24	24	0.001	13	18	24	0.1
Thiofanox-sulfoxide	24	24	24	0.001	0	1	6	> 0.1
Thionazin (Zinophos™)	24	24	24	0.001	22	24	24	0.01
Thiophanate-methyl	24	24	24	0.001	20	24	24	0.01
Thiophanate-ethyl	24	24	24	0.001	13	16	18	> 0.1
Tiadinil	24	24	24	0.001	24	24	24	0.001
Tiamulin	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Tokuthion®	19	23	24	0.01	0	1	5	> 0.1
Tolclofos-methyl	21	23	24	0.01	1	18	23	0.1
Tolfenamic acid	24	24	24	0.001	24	24	24	0.001
Tolfenpyrade	24	24	24	0.001	23	24	24	0.001
Toltrazuril	24	24	24	0.001	5	6	18	> 0.1
Toltrazuril sulfone	23	24	24	0.001	22	23	24	0.01
Tolylfluanid	1	1	1	> 0.1	0	1	0	> 0.1
Topramezone	0	4	1	> 0.1	0	0	0	> 0.1
Tralkoxydim	24	24	24	0.001	24	24	24	0.001
Triadimefon	24	24	24	0.001	24	24	24	0.001
Triadimenol (Baytan®)	15	21	24	0.1	15	21	24	0.1
Triallate	24	24	24	0.001	8	22	24	0.1
Triasulfuron	24	24	24	0.001	24	24	24	0.001
Triazamate	24	24	24	0.001	24	24	24	0.001
Triaziflam	24	24	24	0.001	24	24	24	0.001
Triazophos	23	24	24	0.001	21	22	23	0.1
Triazoxid	24	24	24	0.001	24	24	24	0.001
Tribenuron-methyl	24	24	24	0.001	0	0	0	> 0.1
Tribufos (defoliant)	24	24	24	0.001	24	24	24	0.001
Trichlorfon	24	24	24	0.001	10	19	22	> 0.1
Triclabendazole	24	24	24	0.001	24	24	24	0.001
Triclabendazole sulfone	24	24	24	0.001	24	24	24	0.001
Triclabendazole sulfoxide	24	24	24	0.001	24	24	24	0.001
Tricyclazole	24	24	24	0.001	24	24	24	0.001

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$		0.001 $mg.kg^{-1}$	0.01 $mg.kg^{-1}$	0.1 $mg.kg^{-1}$	
Tridemorph (mixture of isomers)	0	24	0	0.01	0	21	0	> 0.1
Tridiphane	0	1	0	> 0.1	0	0	0	> 0.1
Trietazine	24	24	24	0.001	24	24	24	0.001
Trifloxystrobin	24	24	24	0.001	24	24	24	0.001
Trifloxystrobin metabolite	24	24	24	0.001	24	24	24	0.001
Trifloxysulfuron sodium	23	24	23	0.001	0	0	0	> 0.1
Triflumizole	24	24	24	0.001	24	24	24	0.001
Triflumuron	24	24	24	0.001	24	24	24	0.001
Trifluralin	2	0	1	> 0.1	0	0	0	> 0.1
Triflusulfuron-methyl	24	24	24	0.001	24	24	24	0.001
Triforine	23	24	24	0.001	16	24	24	0.01
Trimethoprim	24	24	24	0.001	24	24	24	0.001
Trinexapac-ethyl	24	24	24	0.001	2	18	20	> 0.1
Triphenyl phosphorothionate	24	24	24	0.001	9	20	24	0.1
Tris(2-chloroethyl) phosphate (TRCP)	24	24	24	0.001	5	15	23	0.1
Tri-*o*-cresyl phosphate (TCP)	24	24	24	0.001	24	24	24	0.001
Triticonazole	24	24	24	0.001	24	24	24	0.001
Tritosulfuron	24	24	24	0.001	22	24	24	0.01
Trovafloxacin	24	24	24	0.001	23	24	24	0.001
Tylosin	24	24	23	0.001	24	24	23	0.001
Uniconazole	24	24	24	0.001	24	23	24	0.001
Valnemulin	24	24	24	0.001	24	24	24	0.001
Vamidothion	24	24	24	0.001	24	24	24	0.001
Vamidothion sulfoxide	1	3	2	> 0.1	0	0	0	> 0.1

Compounds	No. of detections			SDL ($mg.kg^{-1}$)	No. of identifications			LOI ($mg.kg^{-1}$)
	0.001 $mg.kg^{-1}$	**0.01 $mg.kg^{-1}$**	**0.1 $mg.kg^{-1}$**		**0.001 $mg.kg^{-1}$**	**0.01 $mg.kg^{-1}$**	**0.1 $mg.kg^{-1}$**	
Vedaprofen	23	24	24	0.01	17	21	24	0.1
Vernolate	24	24	24	0.001	0	12	24	0.1
Virginiamycin M1	24	24	24	0.001	22	24	24	0.01
XMC (3,5-xylyl methylcarbamate)	21	24	24	0.01	1	11	23	0.1
Z-mevinphos	24	24	24	0.001	24	24	24	0.001
Zoxamide	24	24	24	0.001	24	24	24	0.001

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900 **Table S7.** Comparison of the results of the present study with those in the literature for the analysis of organic contaminants in seafood
901 matrices. SDL, screening detection limit; LOI, limit of identification; LOQ, limit of quantification

Contaminants (number)	**Method**	**% of contaminants SDL < 0.01 mg·kg^{-1}**	**% of contaminants LOI < 0.01 mg·kg^{-1}**	**% of contaminants LOQ < 0.01 mg·kg^{-1}**	**Reference**
Pesticides, metabolites, veterinary drugs and industrial chemicals (**850**)	QuEChUP/LC-QToF-MS	92	78	-	Preset study
Pesticides, veterinary drugs, persistent organic pollutants (POPs) and marine toxins (**756**)	QuEChERS/LC-QtoF-MS	93	-	90	(Bai et al., 2022)
Pesticides (**204**)	QuEChUP/LC-QtoF-MS	66	37	-	(Diallo et al., 2022)
Pesticides, veterinary drugs and personal care products (**182**)	QuEChUP/LC-QtoF-MS	63	54	62	(Munaretto et al., 2016)
Pesticides (**109**)	ASE[b]/GC-MS/MS	-	-	88	(Wu et al., 2011)
Pesticides and veterinary drugs (**106**)	QuEChERS/LC-MS/MS	-	-	100	(Castilla-Fernández et al., 2021)
Veterinary drugs (**96**)	QuEChERS/LC-MS/MS	-	-	96	(Park et al., 2022)
Herbicides and veterinary drugs (**84**)	QuEChERS/LC and GC-MS/MS	-	-	89	(Chang et al., 2016)

Veterinary drugs (**80**)	QuEChERS/LC-MS/MS	-	-	99	(Zhao et al., 2017)
Pesticides (**52**)	QuEChERS/LC-MS/MS	-	-	85	(Barbieri et al., 2019)
Pesticides (**50**)	GLME-MA-dSPE[c]/GC-MS/MS	-	-	76	(Kaw et al., 2021)

a '-' indicates 'not provided'
b ASE = Accelerated solvent extraction
c GLME-MA-dSPE = gas-liquid microextraction and magnetic-assisted dispersive solid phase extraction

Table S8. Target analysis results, summarising the estimated mean concentration of each identified contaminant and the concentration range for each species and for all the tested samples, expressed in $mg.kg^{-1}$ wet weight (w.w.), along with the frequency of appearance (%FoA) of each identified contaminants through target analysis in the 24 real seafood samples. SDL; screening detection limit

Compound	**LogP**	**SDL ($mg.kg^{-1}$)**	**Positif sample**	**Estimated mean concentration (*range*) ($mg.kg^{-1}$ w.w.)**						**%FoA in all samples**
				Calibration strategy A		**Calibration strategy B**		**Calibration strategy C**		
Pesticides and their TPs										
1-(3,4-Dichlorophenyl)-3-methyl urea	2.9	0.001	Oysters (n=6)	**0.043**	*(0.031-0.063)*	**0.039**	*(0.027-0.056)*	**0.038**	*(0.027-0.056)*	63
			Mussels (n=6)	**0.048**	*(0.025-0.065)*	**0.043**	*(0.023-0.058)*	**0.045**	*(0.023-0.058)*	
			Spiny lobster (n=3)	**0.009**	*(0.003-0.012)*	**0.009**	*(0.002-0.014)*	**0.008**	*(0.001-0.013)*	
Azimsulfuron	0.7	0.001	Crayfish (n=3)	**0.007**	*(0.004-0.007)*	**0.008**	*(0.005-0.010)*	**0.009**	*(0.006-0.012)*	13
Bupirimate	2.7	0.001	Spiny lobster (n=3)	**0.001**	*(0.001-0.002)*	**<SDL**	*(<SDL-0.002)*	**<SDL**	*(<SDL-0.001)*	13
Butroxydim	1.9	0.001	Oysters (n=6)	**0.014**	*(0.012-0.019)*	**0.007**	*(0.005-0.011)*	**0.008**	*(0.006-0.011)*	50
			Mussels (n=6)	**0.016**	*(0.011-0.019)*	**0.008**	*(0.004-0.012)*	**0.007**	*(0.003-0.011)*	
Cyprazine	3.1	0.001	Mussels (n=6)	**0.009**	*(0.001-0.018)*	**0.011**	*(0.002-0.021)*	**0.009**	*(0.001-0.018)*	25
DEET	2.0	0.001	Oysters (n=6)	**0.008**	*(0.006-0.011)*	**0.008**	*(0.006-0.011)*	**0.008**	*(0.006-0.011)*	100
			Mussels (n=6)	**0.008**	*(0.007-0.010)*	**0.008**	*(0.007-0.009)*	**0.007**	*(0.006-0.009)*	
			Sole (n=3)	**0.008**	*(0.004-0.011)*	**0.006**	*(0.001-0.011)*	**0.006**	*(0.001-0.011)*	
			Horse mackerel (n=3)	**0.006**	*(0.003-0.011)*	**0.003**	*(<SDL-0.011)*	**0.003**	*(<SDL-0.011)*	
			Spiny lobster (n=3)	**0.021**	*(0.016-0.026)*	**0.026**	*(0.019-0.032)*	**0.025**	*(0.018-0.030)*	
			Crayfish (n=3)	**0.036**	*(0.031-0.047)*	**0.046**	*(0.039-0.060)*	**0.047**	*(0.039-0.062)*	
Diazinon	3.8	0.001	Oysters (n=6)	**<SDL**	*(<SDL-0.004)*	**0.001**	*(<SDL-0.004)*	**0.004**	*(0.003-0.006)*	50
			Mussels (n=6)	**<SDL**	*(<SDL-0.002)*	**<SDL**	*(<SDL-0.002)*	**<SDL**	*(<SDL-0.001)*	
Diflufenicen	4.6	0.001	Oysters (n=6)	**<SDL**	*(<SDL-0.003)*	**0.001**	*(<SDL-0.004)*	**0.003**	*(0.002-0.006)*	50
			Mussels (n=6)	**0.011**	*(0.008-0.011)*	**0.011**	*(0.008-0.013)*	**0.009**	*(0.006-0.012)*	
Diphenylamine	3.5	0.001	Oysters (n=6)	**0.005**	*(0.004-0.006)*	**0.005**	*(0.004-0.006)*	**0.006**	*(0.006-0.007)*	100

			Mussels (n=6)	**0.006**	*(0.004-0.008)*	**0.005**	*(0.004-0.008)*	**0.005**	*(0.003-0.007)*	
			Sole (n=3)	**0.007**	*(0.005-0.009)*	**0.008**	*(0.006-0.010)*	**0.008**	*(0.006-0.010)*	
			Horse mackerel (n=3)	**0.006**	*(0.004-0.007)*	**0.006**	*(0.005-0.007)*	**0.006**	*(0.005-0.007)*	
			Spiny lobster (n=3)	**0.007**	*(0.006-0.009)*	**0.007**	*(0.006-0.009)*	**0.007**	*(0.005-0.009)*	
			Crayfish (n=3)	**0.008**	*(0.005-0.011)*	**0.008**	*(0.005-0.012)*	**0.009**	*(0.006-0.012)*	
Diuron	2.7	0.001	Oysters (n=6)	**0.055**	*(0.037-0.080)*	**0.050**	*(0.034-0.072)*	**0.050**	*(0.034-0.071)*	63
			Mussels (n=6)	**0.076**	*(0.064-0.086)*	**0.069**	*(0.059-0.078)*	**0.070**	*(0.059-0.078)*	
			Spiny lobster (n=3)	**0.008**	*(0.007-0.010)*	**0.009**	*(0.008-0.011)*	**0.008**	*(0.007-0.010)*	
Fenpropimorph	4.9	0.001	Oysters (n=6)	**0.008**	*(0.004-0.013)*	**0.008**	*(0.004-0.012)*	**0.009**	*(0.005-0.013)*	25
Prosulfocarb	3.9	0.001	Oysters (n=6)	**0.012**	*(0.005-0.015)*	**0.012**	*(0.005-0.015)*	**0.012**	*(0.005-0.015)*	50
			Mussels (n=6)	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	
Pyroxsulam	1.7	0.001	Spiny lobster (n=3)	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	13
Spiroxamine	4.2	0.001	Oysters (n=6)	**<SDL**	*(<SDL-0.004)*	**0.001**	*(<SDL-0.004)*	**0.003**	*(0.002-0.006)*	50
			Mussels (n=6)	**0.009**	*(0.006-0.014)*	**0.009**	*(0.006-0.013)*	**0.008**	*(0.006-0.013)*	
Tebuconazole	3.7	0.001	Spiny lobster (n=3)	**0.004**	*(0.002-0.005)*	**0.004**	*(0.002-0.005)*	**0.004**	*(0.001-0.005)*	13
Thiabendazole	2.5	0.001	Crayfish (n=3)	**0.002**	-	**0.002**	-	**0.002**	*(0.002-0.003)*	13
Veterinary drugs and their TPs										
4-Dimethylaminoantipyrine	1.0	0.001	Crayfish (n=3)	**0.010**	*(0.008-0.013)*	**0.012**	*(0.010-0.016)*	**0.011**	*(0.009-0.016)*	13
Amino flubendazole	1.6	0.001	Mussels (n=6)	**0.011**	*(0.006-0.016)*	**0.010**	*(0.006-0.014)*	**0.009**	*(0.005-0.013)*	25
Clarithromycin	3.2	0.001	Oysters (n=6)	**0.015**	*(0.006-0.028)*	**0.016**	*(0.007-0.027)*	**0.015**	*(0.007-0.025)*	50
			Mussels (n=6)	**0.004**	*(<SDL-0.011)*	**0.006**	*(0.002-0.012)*	**0.005**	*(0.001-0.012)*	
Dapsone	1	0.001	Oysters (n=6)	**0.012**	*(0.005-0.015)*	**0.012**	*(0.006-0.014)*	**0.012**	*(0.007-0.015)*	50
			Mussels (n=6)	**0.017**	*(0.002-0.033)*	**0.016**	*(0.003-0.030)*	**0.015**	*(0.001-0.031)*	
Diclofenac	4	0.001	Oysters (n=6)	**0.052**	*(0.038-0.068)*	**0.044**	*(0.032-0.057)*	**0.043**	*(0.032-0.054)*	50
			Mussels (n=6)	**0.068**	*(0.045-0.091)*	**0.057**	*(0.038-0.075)*	**0.060**	*(0.039-0.079)*	
Vedaprofen	5.7	0.001	Sole (n=3)	**0.029**	*(0.017-0.044)*	**0.042**	*(0.026-0.062)*	**0.042**	*(0.026-0.062)*	50

			Horse mackerel (n=3)	**0.027**	*(0.018-0.034)*	**0.040**	*(0.027-0.049)*	**0.040**	*(0.027-0.049)*	
			Spiny lobster (n=3)	**0.030**	*(0.022-0.037)*	**0.039**	*(0.030-0.049)*	**0.035**	*(0.026-0.043)*	
			Crayfish (n=3)	**0.030**	*(0.026-0.034)*	**0.040**	*(0.035-0.045)*	**0.046**	*(0.041-0.051)*	
Industrial chemicals										
2-Ethylhexyl diphenyl phosphate	6.3	0.001	Oysters (n=6)	**0.018**	*(0.014-0.028)*	**0.016**	*(0.013-0.024)*	**0.017**	*(0.014-0.025)*	63
			Mussels (n=6)	**0.017**	*(0.014-0.020)*	**0.015**	*(0.012-0.018)*	**0.014**	*(0.011-0.017)*	
			Spiny lobster (n=3)	**0.005**	*(0.004-0.006)*	**0.005**	*(0.005-0.007)*	**0.005**	*(0.005-0.006)*	
Triphenyl phosphorothionate	6.3	0.001	Oysters (n=6)	**0.004**	*(0.002-0.008)*	**0.005**	*(0.004-0.009)*	**0.003**	*(0.001-0.007)*	75
			Mussels (n=6)	**0.007**	*(0.003-0.009)*	**0.008**	*(0.004-0.010)*	**0.010**	*(0.006-0.012)*	
			Sole (n=3)	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	
			Crayfish (n=3)	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	
Tris(2-chloroethyl) phosphate (TRCP)	1.8	0.001	Oysters (n=6)	**0.010**	*(0.004-0.018)*	**0.010**	*(0.005-0.017)*	**0.010**	*(0.006-0.017)*	100
			Mussels (n=6)	**0.009**	*(0.007-0.014)*	**0.009**	*(0.007-0.013)*	**0.008**	*(0.006-0.013)*	
			Sole (n=3)	**0.002**	*(0.001-0.002)*	**0.002**	*(0.001-0.003)*	**0.002**	*(0.001-0.003)*	
			Horse mackerel (n=3)	**<SDL**	*(<SDL-0.002)*	**<SDL**	*(<SDL-0.002)*	**<SDL**	*(<SDL-0.002)*	
			Spiny lobster (n=3)	**0.001**	-	**<SDL**	*(<SDL)*	**<SDL**	*(<SDL)*	
			Crayfish (n=3)	**0.002**	*(0.001-0.002)*	**<SDL**	*(<SDL-0.001)*	**<SDL**	*(<SDL-0.001)*	
Tri-*o*-cresyl phosphate (TCP)	6.3	0.001	Oysters (n=6)	**0.004**	*(0.003-0.005)*	**0.004**	*(0.004-0.005)*	**0.005**	*(0.005-0.006)*	100
			Mussels (n=6)	**0.004**	*(0.003-0.005)*	**0.004**	*(0.004-0.006)*	**0.003**	*(0.003-0.005)*	
			Sole (n=3)	**0.006**	*(0.005-0.006)*	**0.005**	*(0.004-0.006)*	**0.005**	*(0.004-0.006)*	
			Horse mackerel (n=3)	**0.003**	*(0.003-0.004)*	**0.001**	*(0.001-0.002)*	**0.001**	*(0.001-0.002)*	
			Spiny lobster (n=3)	**0.003**	*(0.003-0.004)*	**0.003**	-	**<SDL**	*(<SDL)*	
			Crayfish (n=3)	**0.004**	*(0.003-0.004)*	**0.003**	*(0.003-0.004)*	**0.004**	-	

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911 **Table S9.** Suspect screening results and frequency of appearance (%FoA).

Compound	Class	Positive seafood species	%FoA
17alpha-Methyltestosterone	Antineoplastic agent	Mussels	25
2,6-Xylidine	Metabolite of lindocaine (anesthetic)	Sole	13
4-Hydroxybenzoic acid	Personal care product	Mussels	25
Allopurinol	Antigout agent	Crayfish	13
Benzocaine	Anesthetic	Crayfish	13
Betaine	Nutrient	Oysters, mussels, spiny lobster, crayfish, sole	88
Bisphenol S	Industrial chemical	Crayfish	13
Canrenone	Antimineralocorticoid	Oysters, mussels, spiny lobster, crayfish, horse mackerel	88
Chlordecone	Insecticide	Spiny lobster, crayfish	25
Chlordecole	Metabolite of chlordecone (insecticide)	Crayfish	13
Cordycepin	Antineoplastic	Oysters	25
Cytisin	Partial agonist	Mussels	25
delta9-Tetrahydrocannabinol	Cannabinoid	Oysters, mussels	50
Digitoxigenin	Cardionic agent	Oysters	25
Dihydromuronic acid	Personal care product	Crayfish	13
Dinoterb	Herbicide	Crayfish	13
Diosgenin	Antioxidant	Spiny lobster	13
Ethambutol	Antibiotic	Spiny lobster, crayfish	25
Etofylline	Lipid regulatror	Spiny lobster, crayfish	25
Fexofenadine	Antihistamine	Oysters	25
Flufenacet ESA	Metabolite of flufenacet (herbicide)	Mussels	25
Galaxolidone	Personal care product	Oysters, mussels, spiny lobster, crayfish, horse mackerel	88
Gemfibrozil	Fibrate	Oysters	25
Hydroquinidine	Antiarrhythmic agent	Horse mackerel	13
Ibuprofen	Non-steroidal anti-inflammatory drug	Oysters, mussels	50
Imidocarb	Antiprotozoal agent	Crayfish, sole, horse mackerel	38
Laurocapram	Personal care product	Spiny lobster, sole	25

Metamitron-desamino	Metabolite of metamitron (herbicide)	Mussels	25
Methylprednisolone	Immunosuppressive and anti-inflammatory drugs	Horse mackerel	13
N-ethylperfluorooctane sulfonamidoacetic acid (N-EtFOSAA)	PFOS precursor	Mussels	13
Norethindrone	Hormonal agents (progestins)	Oysters, mussels	50
Oxypurinol	Metabolite of allopunol (Antigout agent)	Crayfish	13
Phenylacetaldehyde	Personal care product	Horse mackerel	13
Progesterone	Hormonal agents (progestins)	Oysters, mussels	50
Propafenone	Antiarrhythmic agent	Mussels	25
Prostaglandin E1	Vasodilator	Oysters	25
Salicylic acid	Non-steroidal anti-inflammatory drug	Mussels	25
Sclareol	Anti-inflammatory, cholagogic and anti-cancer	Oysters	25
Tocainide	Antiarrhythmic agent	Spiny lobster, crayfish	25
Triethylene glycol bis (2-ethylhexanoate)	Industrial chemical	Spiny lobster, horse mackerel	25
Tri-isobutylphosphate	Industrial chemical	Sole	13
Tris(1,3-dichloro-2-propyl)phosphate	Industrial chemical	Mussels, crayfish, Sole	50
Tris(1-chloro-2-propyl)phosphate	Industrial chemical	Oysters, mussels, spiny lobster, crayfish, sole, horse mackerel	100
Velvione	Personal care product	Mussels, crayfish, horse mackerel	50

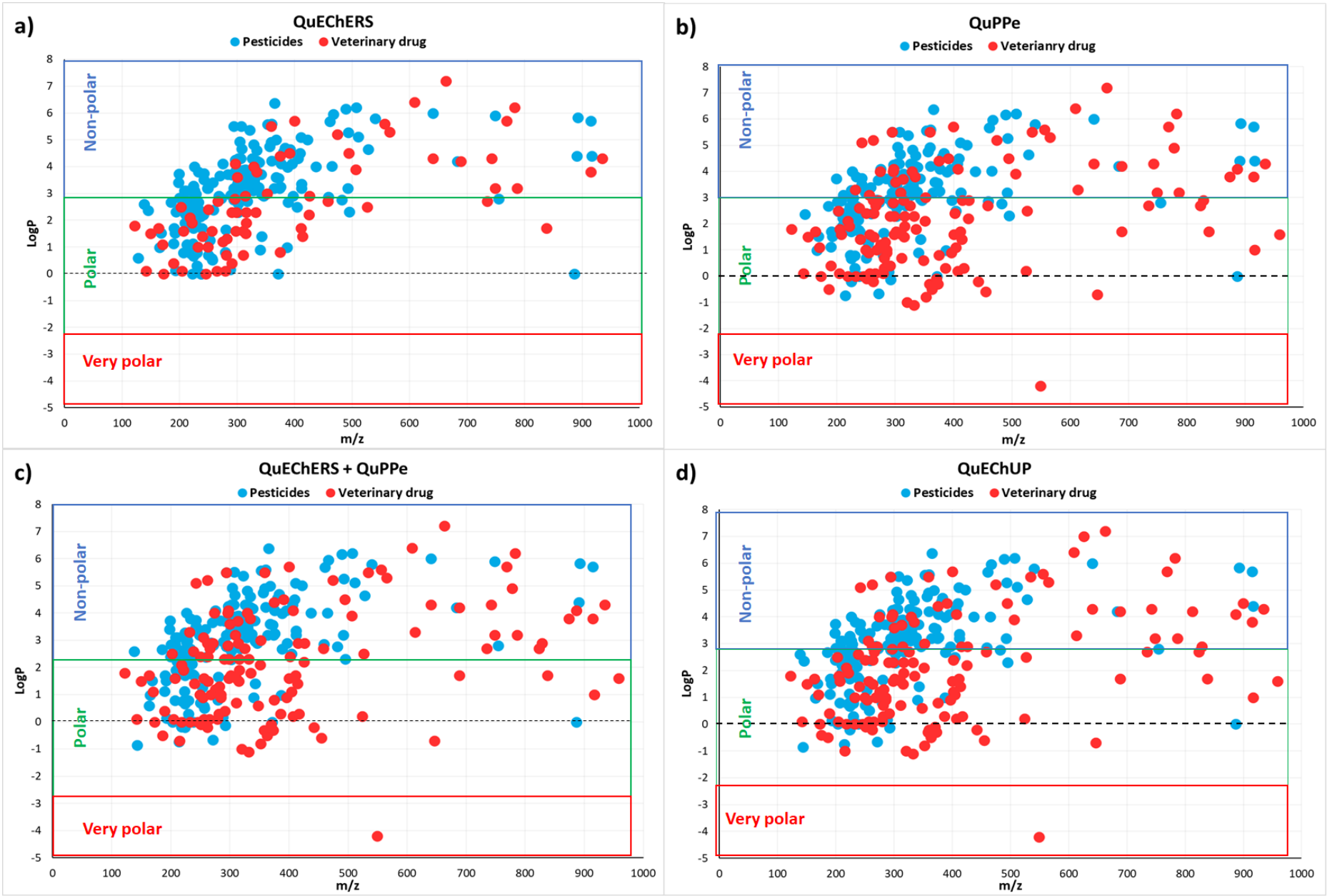
a)
QuEChERS
Pesticides
Veterinary drug
Non-polar
Polar
Very polar
LogP
m/z
b)
QuPPe
Pesticides
Veterianry drug
Non-polar
Polar
Very polar
LogP
m/z
c)
QuEChERS + QuPPe
Pesticides
Veterinary drug
Non-polar
Polar
Very polar
LogP
m/z
d)
QuEChUP
Pesticides
Veterinary drug
Non-polar
Polar
Very polar
LogP
m/z

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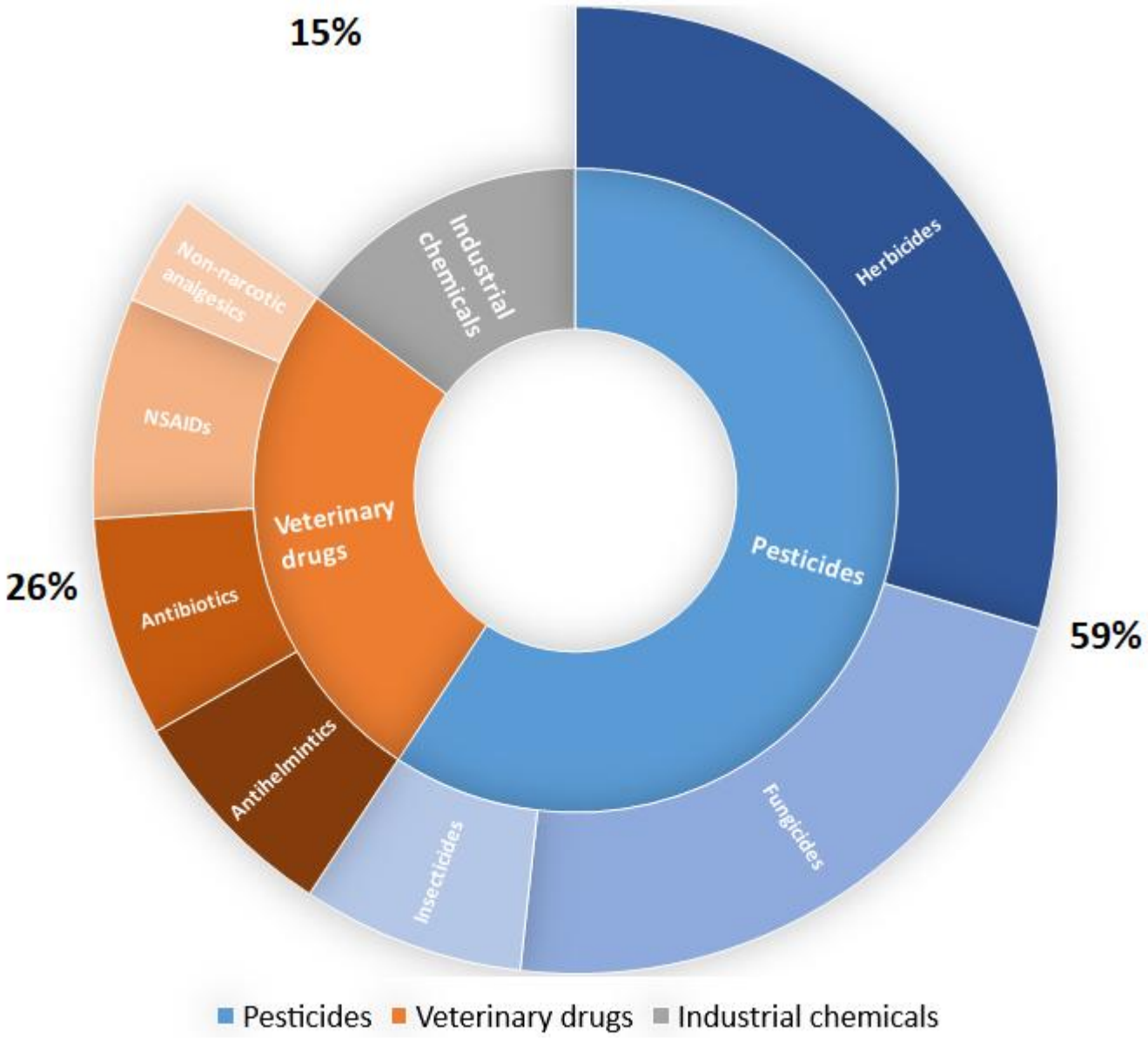
Fig. S1. Chemical coverage obtained for the QuEChERS (a), QuPPe (b), QuEChERS + QuPPe (c) and QuEChUP (d) sample preparation methods.


15%
Herbicides
Industrial chemicals
Non-narcotic analgesics
NSAIDs
Veterinary drugs
Pesticides
26%
Antibiotics
Antihelmintics
Insecticides
Fungicides
59%
Pesticides
Veterinary drugs
Industrial chemicals

916

Fig. S2. Classification of the identified compounds in seafood samples by target screening based on their main use. NSAID, non-steroidal anti-inflammatory drug

References used in SM

Bai, M., Tang, R., Li, G., She, W., Chen, G., Shen, H., Zhu, S., Zhang, H., Wu, H., 2022. High-throughput screening of 756 chemical contaminants in aquaculture products using liquid chromatography/quadrupole time-of-flight mass spectrometry. Food Chem. X 15, 100380. https://doi.org/10.1016/j.fochx.2022.100380

Barbieri, M.V., Postigo, C., Guillem-Argiles, N., Monllor-Alcaraz, L.S., Simionato, J.I., Stella, E., Barceló, D., López de Alda, M., 2019. Analysis of 52 pesticides in fresh fish muscle by QuEChERS extraction followed by LC-MS/MS determination. Sci. Total Environ. 653, 958–967. https://doi.org/10.1016/j.scitotenv.2018.10.289

Castilla-Fernández, D., Moreno-González, D., Bouza, M., Saez-Gómez, A., Ballesteros, E., García-Reyes, J.F., Molina-Díaz, A., 2021. Assessment of a specific sample cleanup for the multiresidue determination of veterinary drugs and pesticides in salmon using liquid chromatography/tandem mass spectrometry. Food Control 130, 108311. https://doi.org/10.1016/j.foodcont.2021.108311

Chang, G.-R., Chen, H.-S., Lin, F.-Y., 2016. Analysis of banned veterinary drugs and herbicide residues in shellfish by liquid chromatography-tandem mass spectrometry (LC/MS/MS) and gas chromatography-tandem mass spectrometry (GC/MS/MS). Mar. Pollut. Bull. 113, 579–584. https://doi.org/10.1016/j.marpolbul.2016.08.080

Diallo, T., Makni, Y., Lerebours, A., Thomas, H., Guérin, T., Parinet, J., 2022. Development and validation according to the SANTE guidelines of a QuEChERS-UHPLC-QTOF-MS method for the screening of 204 pesticides in bivalves. Food Chem. 386, 132871. https://doi.org/10.1016/j.foodchem.2022.132871

Kaw, H.Y., Jin, X., Liu, Y., Cai, L., Zhao, X., Wang, J., Zhou, J.L., He, M., Li, D., 2021. Gas-liquid microextraction coupled with magnetic-assisted dispersive solid-phase extraction clean-up for multi-residue pesticide analysis in fatty foods of animal origin. LWT 137, 110448. https://doi.org/10.1016/j.lwt.2020.110448

Munaretto, J.S., May, M.M., Saibt, N., Zanella, R., 2016. Liquid chromatography with high resolution mass spectrometry for identification of organic contaminants in fish fillet: screening and quantification assessment using two scan modes for data acquisition. J. Chromatogr. A 1456, 205–216. https://doi.org/10.1016/j.chroma.2016.06.018

Park, H., Choi, S.Y., Kang, H.-S., Kwon, N. ji, 2022. Multi residue determination of 96 veterinary drug residues in domestic livestock and fishery products in South Korea. Aquaculture 553, 738064. https://doi.org/10.1016/j.aquaculture.2022.738064

Wu, G., Bao, X., Zhao, S., Wu, J., Han, A., Ye, Q., 2011. Analysis of multi-pesticide residues in the foods of animal origin by GC–MS coupled with accelerated solvent extraction and gel permeation chromatography cleanup. Food Chem. 126, 646–654. https://doi.org/10.1016/j.foodchem.2010.10.105

Zhao, F., Gao, X., Tang, Z., Luo, X., Wu, M., Xu, J., Fu, X., 2017. Development of a simple multi-residue determination method of 80 veterinary drugs in Oplegnathus punctatus by liquid chromatography coupled to quadrupole Orbitrap mass spectrometry. J. Chromatogr. B 1065–1066, 20–28. https://doi.org/10.1016/j.jchromb.2017.09.013

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