



**HAL**  
open science

**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**

Thierno Diallo, Yassine Makni, Adélaïde Lerebours, Hélène Thomas, Thierry Guérin, Julien Parinet

► **To cite this version:**

Thierno Diallo, Yassine Makni, Adélaïde Lerebours, Hélène Thomas, Thierry Guérin, et al.. 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. Food Chemistry, 2023, 426, pp.136572. 10.1016/j.foodchem.2023.136572 . hal-04127649

**HAL Id: hal-04127649**

**<https://hal.science/hal-04127649v1>**

Submitted on 14 Jun 2023

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Copyright

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

5 Thierno Diallo <sup>a, b</sup>, Yassine Makni <sup>a</sup>, Adélaïde Lerebours <sup>b</sup>, Hélène Thomas <sup>b</sup>, Thierry Guérin  
6 <sup>c</sup>, Julien Parinet <sup>a, \*</sup>

7  
8  
9 <sup>a</sup> ANSES, Laboratory for Food Safety, F-94701 Maisons-Alfort, France

10 <sup>b</sup> Littoral Environnement et Sociétés (LIENSs), UMR 7266, CNRS-Université de La Rochelle, 2 rue Olympe de  
11 Gouges, F-17042 La Rochelle Cedex 01, France

12 <sup>c</sup> ANSES, Strategy and Programmes Department, F-94701 Maisons-Alfort, France

13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31 \* Corresponding Author: ANSES, Laboratory for Food Safety, F-94701 Maisons-Alfort, France

32 E-mail address: [julien.parinet@anses.fr](mailto:julien.parinet@anses.fr) (J. Parinet)

## 33 **Abstract**

34 A high-resolution mass spectrometry screening method was developed and validated based on  
35 EU SANTE/11312/2021 guidelines for the analysis of 850 multi-class contaminants in  
36 commercial seafood samples. Samples were extracted using a novel sequential QuEChUP  
37 preparation method that combines the QuEChERS and QuPPE procedures. The screening  
38 detection limits (SDLs) and limits of identification (LOIs) were equal to or lower than 0.01  
39 mg.kg<sup>-1</sup> for 92% and 78% of contaminants, respectively. This screening procedure was  
40 ultimately applied for a target screening analysis of 24 seafood samples. The concentrations  
41 of identified contaminants were assessed using semi-quantitative approach. Two identified  
42 contaminants, diuron and diclofenac, showed the highest estimated average concentrations:  
43 0.076 and 0.068 mg.kg<sup>-1</sup> respectively in mussel samples. Suspect screening was also  
44 performed. Target and suspect screening led to the identification of mixtures of contaminants  
45 (pesticides, veterinary products, industrial chemicals and personal care products) and the  
46 assessment of their frequencies of appearance (FoA).

## 47 **Keywords**

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

50

## 51 **1. Introduction**

52 Currently, there is heightened awareness of the toxicity of certain chemical compounds, such  
53 as pesticides, whose presence in the environment has been or is regulated by various  
54 legislation (Teyssere et al., 2021). Along with pesticide use, veterinary drug use has  
55 increased dramatically in recent years (Casado et al., 2019). This latter group of substances,  
56 which includes antimicrobials, hormones and non-steroidal anti-inflammatory drugs  
57 (NSAIDs), is one of the major classes of emerging contaminants (Samal et al., 2022). The  
58 main route of entry of veterinary drugs into the aquatic environment is via wastewater  
59 (including urban, industrial, agricultural and livestock wastewater), whereas pesticides enter  
60 the aquatic ecosystem via runoff, vaporisation into the atmosphere, agricultural returns,  
61 intrusion into groundwater or by adsorption or uptake by plants (Tudi et al., 2021). Once  
62 pesticides, veterinary drugs and various mixtures of contaminants enter the water, aquatic  
63 species absorb them — e.g. fish take them up through their gills — and they can accumulate  
64 and undergo metabolism in tissues (van der Oost et al., 2003). In addition, other species such  
65 as bivalves filter a large volume of water and can bioaccumulate xenobiotics in their digestive  
66 glands, making bivalves good sentinel species of environmental quality (Breitwieser et al.,  
67 2018) and therefore relevant for eco-exposome assessment. Pesticides, veterinary drugs and  
68 other contaminants that enter the food chain through aquatic ecosystems can indirectly  
69 threaten human health (Breitwieser et al., 2018; van der Oost et al., 2003). Contaminant  
70 residues in seafood are therefore a critical public health issue that needs to be addressed not  
71 only in the context of the advocated ‘One Health’ approach but also to amend the limited  
72 information available on the mixtures of contaminants to which humans are exposed.  
73 Nevertheless, few maximum residue limits (MRLs) have been set for currently employed  
74 contaminants to ensure safe seafood consumption.

75 Seafood contains a large quantity of lipids (up to 17%) and proteins (up to 27%) (ANSES,  
76 2020) that can affect the analysis of target contaminant compounds, especially because when  
77 the analytes are present at low concentrations. These usually result in signal suppression or  
78 enhancement, which affects the accuracy of the results obtained (Diallo et al., 2023).  
79 Therefore, appropriate extraction and clean-up methods must be developed to limit the  
80 presence of matrix interferents during analysis. The current popular generic solid-phase  
81 extraction method is the QuEChERS (which stands for ‘quick, easy, cheap, effective, rugged  
82 and safe’) method, owing to its rapid protocol, reliable results and affordable cost (Barbieri et  
83 al., 2019). Acetonitrile is the most widely used organic solvent for QuEChERS extraction,

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

90 Food sample preparation for the analysis of pesticides and veterinary drugs normally involves  
91 an extraction and purification step. To achieve the best extraction performance, many  
92 parameters need to be optimised, including sample amount, extraction solvent, pH, partition  
93 salt, clean-up, and concentration/dilution of the extracts, which makes optimisation complex  
94 and time consuming. The orthogonal array design, also known as the Taguchi orthogonal  
95 array (TOA) design, is a simple and effective strategy for the simultaneous optimisation of  
96 multiple experimental conditions at multiple levels (Narendran et al., 2019). It can greatly  
97 simplify the experimental optimisation without reducing the quality of the results. The TOA  
98 method has been used to optimise the QuEChERS method for wide-scope multi-residue  
99 analysis of 129 and 204 pesticides in beef (Pang et al., 2021) and bivalves (Diallo et al.,  
100 2022), respectively.

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

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

117 acquiring a MS/MS mass spectrum are data-dependent acquisition (DDA) and data-  
118 independent acquisition (DIA) (Diallo et al., 2022). The choice of acquisition mode may  
119 depend on the instrument and software available to each user, although the HRMS acquisition  
120 mode that provides the best quality and easiest-to-interpret spectra is DDA, also called  
121 information-dependent acquisition (IDA), in Sciex instruments (Diallo et al., 2022). However,  
122 only the most intense precursor ions selected by the user (TopN) are fragmented in IDA,  
123 which can lead to difficulties in complex matrices or low concentrations. The TopN must  
124 therefore be optimised to avoid or minimise the loss of pertinent MS/MS data, especially for  
125 suspect and non-targeted analyses. For targeted analyses, a precursor inclusion list (PIL) can  
126 be added. In IDA-PIL mode, the targeted precursor ions have the highest priority for  
127 fragmentation, regardless of whether these precursor ions are the most intense (Diallo et al.,  
128 2022; Makni et al., 2022).

129 The aim of this study was to develop a wide-scope screening approach for 850 multi-class  
130 chemical contaminants in 12 different commercial seafood products using a novel sample  
131 preparation method combining QuEChERS and QuPPE (called QuEChUP), followed by  
132 UHPLC-QTOF-MS analysis. The list of target contaminants included pesticides, veterinary  
133 drugs, their transformation products (TPs) and industrial chemicals from different families  
134 with very distinct physicochemical properties, used as a templates for suspect screening. To  
135 our knowledge, this study is the first to perform simultaneous analysis by HRMS for such a  
136 comprehensive list of contaminants in so many different seafood species. The TOA method  
137 was used to evaluate the optimal parameters for the sample extraction step. The developed  
138 method was validated in accordance with the criteria set by European Union  
139 SANTE/11312/2021 guidelines for qualitative multi-residue methods (European Commission,  
140 2021). For each contaminant, screening detection limits (SDLs) were established. Although  
141 not required for the validation of the qualitative screening method according to SANTE  
142 guidelines, the limits of identification (LOIs) were also established. The number of false  
143 positives was assessed using non-spiked seafood samples. To test its applicability, the  
144 screening method was applied to the analysis (target screening) of real seafood samples,  
145 including mussels, oysters, sole, horse mackerel, spiny lobster and crayfish from South-West  
146 France and the French West Indies. The concentration of the identified contaminants was  
147 estimated using different semi-quantitative strategies. To test the versatility of the method on  
148 contaminants other than those included in the validation, a suspect screening approach was

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

## 151 **2. Materials and methods**

### 152 *2.1. Chemical substances and analytical standards*

153 A kit of 745 pesticide and industrial chemical standards, divided into five mixtures (5 mg.L<sup>-1</sup>  
154 of each compound in either acetonitrile (ACN) or methanol (MeOH)), was obtained from  
155 LGC Standards (Molsheim, France). The analytical standards of 180 veterinary drugs, divided  
156 into 10 mixtures (10 mg.L<sup>-1</sup> of each compound in either ACN or MeOH), was obtained from  
157 the ANSES Fougères Laboratory (France). ACN, MeOH, purchased from Fisher Scientific  
158 (Illkirch, France), and ultrapure water (18.2 MΩ.cm), obtained by purifying distilled water  
159 with a Milli-Q system from Merck Millipore (Saint-Quentin-en-Yvelines, France), were used  
160 for the mobile phases and sample preparation. Formic acid (FA) was supplied by Fisher  
161 Scientific to prepare the LC-MS mobile phases and the extraction solvent. QuEChERS  
162 extraction pouches based on the original method (4.0 g of magnesium sulphate (MgSO<sub>4</sub>), 1.0  
163 g of sodium chloride (NaCl)) was provided by Agilent Technologies (Santa Clara, CA, USA).  
164 A dispersive solid-phase extraction (dSPE) kit containing 900 mg of MgSO<sub>4</sub>, 150 mg of  
165 primary and secondary amines (PSA) and 150 mg of octadecylsilane (C18), Enhanced Matrix  
166 Removal-lipid (EMR-lipid) dSPE, and a dispersive kit for veterinary drugs containing 900 mg  
167 Na<sub>2</sub>SO<sub>4</sub>, 50 mg PSA and 150 mg C18 end-capped (C18EC), were obtained from Agilent  
168 Technologies. Ethylenediaminetetraacetic acid disodium salt dihydrate (Na<sub>2</sub>EDTA.H<sub>2</sub>O),  
169 citric acid (≥99.5% purity) and disodium phosphate (HNa<sub>2</sub>PO<sub>4</sub>; ≥99.0% purity) were obtained  
170 from Fisher Scientific. Na<sub>2</sub>EDTA.H<sub>2</sub>O (37.18 g), citric acid (12.9 g) and HNa<sub>2</sub>PO<sub>4</sub> (10.9 g)  
171 were dissolved in 1 L of ultrapure water to prepare a 0.1 mol.L<sup>-1</sup> Na<sub>2</sub>EDTA-McIlvaine buffer  
172 solution.

### 173 *2.2. Equipment and apparatus*

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

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

### 181 2.3. *Selection and use of the contaminants*

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

### 190 2.4. *Selection and use of seafood samples*

191 Twelve of the most widely consumed seafood species in France, namely oysters, mussels,  
192 scallops (*Pecten maximus* and *Mimachlamys varia*), clams, cod, salmon, sole, anchovies and  
193 tuna, as well as spiny lobster and crayfish, used to optimise and validate the method  
194 (including to assess false positives), were purchased from local markets in March and April  
195 2022 (Maisons-Alfort, France). These 12 seafood samples were pooled and used to optimise  
196 sample preparation. To validate the method, two groups were randomly formed for each of  
197 the 12 seafood species, for a total of 24 seafood samples. To test the applicability of the  
198 screening method using target and suspect screening, two species of bivalves (mussels ( $n = 6$ )  
199 and oysters ( $n = 6$ )) and two species of fish (sole ( $n = 3$ ) and horse mackerel ( $n = 3$ )) were  
200 collected in the Pertuis-Charentais area (South-West France), and two species of crustaceans  
201 (lobster ( $n = 3$ ) and crayfish ( $n = 3$ )) were collected in Martinique (French West Indies).  
202 Before shucking (bivalves) or dissection (fish), the seafood samples were stored at 4°C  
203 overnight and then brought to room temperature. The samples were homogenised and kept at -  
204 20°C until analysis.

### 205 2.5. *Development of a homemade LC-MS/MS compound database and MS/MS* 206 *library*

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



210 the standards were performed in both ESI<sup>+</sup> and ESI<sup>-</sup> mode. The information on molecular  
211 formulae, retention time (T<sub>R</sub>), accurate m/z of the precursor ion, isotopic pattern and the  
212 MS/MS fragmentation spectrum of each of the studied contaminants were recorded and taken  
213 as reference for the automated detection and identification process in matrix samples. In total,  
214 744 and 247 spectra in ESI<sup>+</sup> and ESI<sup>-</sup>, respectively, were recorded. Data were processed and  
215 evaluated using PeakView<sup>®</sup> software version 2.2 comprising the AB Sciex MasterView<sup>™</sup>  
216 module. The MasterView<sup>™</sup> module is inter-connected to LibraryView<sup>™</sup> software and  
217 compares the experimental fragmentation spectra to those recorded in the homemade  
218 database. The term ‘detection’ was employed when a contaminant did not exceed the  
219 following thresholds: (i) T<sub>R</sub> variation ± 0.1 min and (ii) mass accuracy ± 5 ppm on the  
220 precursor ion (European Commission, 2021). The term ‘identification’ was based on the same  
221 thresholds as detection, and also satisfied an MS/MS library score of spectral similarity of  
222 >70% between the experimental and reference MS/MS fragmentation spectra using the Fit  
223 MS/MS search algorithm (Makni et al., 2022). The Fit algorithm represents the degree of  
224 similarity of the peaks and intensities of the reference spectrum with those of the experimental  
225 spectrum, ignoring the other interfering peaks in the experimental spectrum.

## 226 2.6. *Orthogonal array design for optimisation of sample preparation*

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

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

## 238 2.7. *Optimisation of sample preparation*

239 Extraction solvent, dSPE and dilution ratio were simultaneously optimised using L9 TOA. To  
240 obtain a pesticide supplementation at a concentration of 0.01 mg.kg<sup>-1</sup>, 7.5 µL of the mix  
241 containing 364 contaminants were added to 50-mL polypropylene centrifuge tubes, which

242 contained  $1.50 \pm 0.05$  g of pooled seafood sample. The tubes were stored at 4°C for 24 h to  
243 allow the contaminants to bind to the matrix. Then, 8.5 mL of the aqueous phase (Na<sub>2</sub>EDTA-  
244 McIlvaine buffer (0.1 mol.L<sup>-1</sup>)) was added to each tube, and the sample was then ground  
245 using an IKA Ultra-Turrax mixer for 3 min at 5000 rpm. Then, 10 mL of organic solvent was  
246 added to each centrifuge tube and vortexed again for 1 min. After that, a mixture of 4.0 g of  
247 MgSO<sub>4</sub> and 1.0 g of NaCl were added to the fortified samples, and the resulting mixture was  
248 centrifuged for 5 min at 4000 rpm.

249 For the purification step, there were two cases. When EMR-lipid was used as the dSPE  
250 reagent, the sorbent was activated by adding 5 mL of water to a 15 mL centrifuge tube  
251 containing the EMR-lipid and vortexed for 3 s. Then, 5 mL of the extract supernatant (50 mL  
252 polypropylene centrifuge tube) was transferred to the activated 15 mL centrifuge tube. The  
253 mixture was immediately vortexed for 1 min. The tube was centrifuged at 4000 rpm for 5  
254 min, and 5 mL of the supernatant was transferred to the polishing tube containing 0.5 g NaCl  
255 and 1.5 g MgSO<sub>4</sub> to remove excess water. When using the other dSPE reagents, 6 mL of the  
256 supernatant was transferred to a 15-mL centrifuge tube containing the dSPE reagent. The tube  
257 was vortexed for 1 min, and then centrifuged for 5 min at 4000 rpm. The supernatant was then  
258 combined with ACN according to the dilution ratio. The mixture was then vortexed, filtered  
259 and deposited into a 2-mL autosampler vial for injection in the UHPLC-QTOF system.

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

## 262 2.8. UHPLC-Q-TOF-MS conditions

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

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

## 280 2.9. Method validation

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

## 294 2.10. Data processing for real sample analysis

### 295 2.10.1. Target screening

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

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

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

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

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

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

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

### 327 *2.10.2. Suspect screening*

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

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

### 341 **3. Results and discussion**

#### 342 *3.1. Optimisation of the sample extraction and purification steps*

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

350 The values of the mean detection rates for all contaminants ranged from 49% to 83% ([Tables](#)  
351 [S4, S5](#)) for all experiments. Overall, the best performances were found with Experiment 1 and  
352 6 for pesticides and veterinary drugs, respectively. According to the R values, the factor with  
353 the greatest impact on pesticide detection was dilution (R = 23), followed by extraction  
354 solvent (R = 14) and finally the dSPE (R = 3). For veterinary drug detection, the most  
355 influential factor was solvent extraction (R = 18), then dilution (R = 17), and finally dSPE (R  
356 = 8). The effects of the three studied factors on the pesticide and veterinary drug detection  
357 rates are also shown in [Fig. 1](#). The detection rates are represented in bar charts; therefore, the  
358 greater the difference between the best and worst performing levels, the more significant the  
359 factor is. All factors were significant ( $p < 0.05$ ) for the veterinary drug detection rates, and  
360 solvent extraction and dilution were significant for the pesticide detection rates ([Tables S4,](#)  
361 [S5](#)).

##### 362 *3.1.1. Extraction solvent*

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

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

### 377 3.1.3. dSPE

378 As illustrated in Fig. 1, the best pesticide detection rates were obtained with a mixture of  
379 MgSO<sub>4</sub>/PSA/C18 as dSPE reagent, closely followed by EMR-lipid. MgSO<sub>4</sub> is commonly  
380 used as a drying salt for ACN extraction because it effectively removes residual water. PSA  
381 has been shown to remove many polar organic acids from the extract, as well as polar  
382 pigments, sugars and fatty acids, whereas C18 can retain fats, vitamins and minerals (Kim et  
383 al., 2019). For veterinary drugs, the best detection rates were obtained with EMR-lipid,  
384 followed by a mixture of PSA/Na<sub>2</sub>SO<sub>4</sub>/C18EC. EMR-lipid, whose structure is a proprietary  
385 secret, removes lipids from sample matrices (Pang et al., 2021). This sorbent allows a highly  
386 selective and efficient interaction with lipids, providing excellent extraction efficiency,  
387 precision and matrix effect (Castilla-Fernández et al., 2021). Na<sub>2</sub>SO<sub>4</sub> is also a drying agent,  
388 similar to MgSO<sub>4</sub>. This salt performed better for veterinary drugs than MgSO<sub>4</sub>, because the  
389 Mg<sup>2+</sup> ions can also form complexes with some veterinary drugs, which reduces detection rates  
390 (Gros et al., 2019). Another difference is that Na<sub>2</sub>SO<sub>4</sub> is a weak drying agent compared with  
391 MgSO<sub>4</sub>, and when added to the organic extraction solvent, the amount of water is higher than  
392 when MgSO<sub>4</sub> is used, favouring the extraction of polar compounds, such as veterinary drugs  
393 (Munaretto et al., 2016). The C18EC products are based on reversed phase, bonded and end-  
394 capped octadecylsilane silica gel particles. The non-polar sorbent is end-capped (EC), which  
395 reduces polar secondary interactions associated with surface silanol groups (Sobczak et al.,  
396 2021).

#### 397 3.1.4. Dilution

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

407 The conclusion based on the R values associated with the K1, K2, and K3 values and the main  
408 effects plot for detection is that the optimal extraction conditions for pesticides were obtained  
409 with pure ACN, MgSO<sub>4</sub>/PSA/C18 for dSPE, and the non-dilution of extracts, which  
410 corresponds to a classical QuEChERS method, and consistent with previous results (Diallo et  
411 al., 2022). For the detection of veterinary drugs, the optimal extraction conditions were  
412 obtained with ACN/MeOH, EMR-lipid as the dSPE sorbent and the non-dilution of extracts,  
413 which corresponds to a modified QuPPe method.

#### 414 3.2. Comparison of optimal conditions for the detection of pesticides and veterinary 415 drugs

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

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



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

### 439 3.3. Validation of the screening method

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

#### 445 3.3.1. Selectivity of the screening method

446 In SANTE guidelines, no criteria have been set with respect to the occurrence of false  
447 positives. However, the selectivity of the method must reduce the false positive rate to a  
448 sufficiently low level to avoid manual verification or confirmatory analysis that may reduce  
449 the effectiveness of the screening method. The number of false positives was checked by  
450 analysing 24 non-spiked seafood samples. According to the results, a total of  $42 \pm 7$  (standard  
451 deviation, SD) false positives (5% of the 850 target contaminants) were obtained across all  
452 non-spiked samples, applying the detection criteria, i.e. tolerances of  $\pm 5$  ppm and  $\pm 0.1$  min for  
453 mass accuracy and  $T_R$ , respectively. To reduce this false positive rate and to obtain a more  
454 reliable detection of contaminants, an additional criterion on the signal-to-noise (SN) ratio  
455 was added for detection. When the S/N threshold was set to  $S/N > 10$  instead of  $S/N > 3$  (as was  
456 originally the case), the number of false positives dropped drastically to  $17 \pm 4$  contaminants,  
457 representing only 2% of the 850 targeted contaminants. The addition of this extra criterion  
458 had no impact on the detection rates of contaminants, which remained unchanged. Finally,  
459 when the identification criterion was considered by adding the MS/MS library score (Fit >  
460 70%), the number of false positives dropped to  $2 \pm 1$  contaminants (0.24% of the 850 targeted



461 contaminants). These false positives were due to misattributions during automatic MS/MS  
462 matching. False positive contaminants for 1,2-benzisothiazol-3(2H)-one (C<sub>7</sub>H<sub>5</sub>NOS) and  
463 piperonyl butoxide (C<sub>19</sub>H<sub>30</sub>O<sub>5</sub>) were each detected in five non-spiked seafood samples,  
464 whereas false positives for (E)-metominostrobin (C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>) were observed in nine  
465 samples. The other false positives were only detected once each in the different samples.  
466 These results demonstrated the good selectivity of the method both in terms of detection (with  
467 S/N > 10) and identification.

### 468 3.3.2. Determination of SDL and LOI

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

484 The LOI was determined to be equal to or less than 0.001, 0.01 and 0.1 mg.kg<sup>-1</sup> for 67, 78 and  
485 85% of pesticides, respectively (Fig. 4c). Thus, 16% of the contaminants could not be  
486 validated for identification because the criteria of LOI were not met. For 82 contaminants  
487 (representing 10% of the selected contaminants), it was possible to establish the SDL at least  
488 at one of the three concentration levels, but not the LOI. For these compounds, validation was  
489 limited to detection (only the SDL could be set). Overall, the reliable identification was likely  
490 for 89% of contaminants at 0.1 mg.kg<sup>-1</sup> (Fig. 4d). This value decreased to 87% and 80% at  
491 0.01 and 0.001 mg.kg<sup>-1</sup>, respectively.

492 To check the applicability of the screening method, the resulting SDLs must be compared  
493 with the MRLs in food, established by the European Commission to ensure consumer safety.  
494 The MRL is the highest level of a contaminant or residue that is legally tolerated in food and  
495 can therefore be used. To date, no MRLs have been established for the targeted residues in  
496 seafood matrices. A general default MRL of 0.01 mg.kg<sup>-1</sup> applies where a contaminant is not  
497 specifically mentioned. Thus, the SDL and LOI obtained, in most cases less than or equal to  
498 0.01 mg.kg<sup>-1</sup>, can be considered satisfactory and the proposed methodology adequately  
499 sensitive for suspect and non-targeted screening purposes.

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

### 515 3.4. *Target screening in real seafood samples*

516 Contaminants were identified using the criteria applied in this study (see sections [2.5](#) and  
517 [2.10.1](#)). [Fig. 5](#) showed an unequivocal identification of diuron and diclofenac in a mussel  
518 sample.

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

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

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

#### 541 3.4.1. Pesticides and their transformation products (TPs)

542 For all the seafood samples, the most identified pesticides were herbicides and fungicides,  
543 most of them in the bivalve samples. The pesticides identified with 100% FoA in all seafood  
544 samples were *N,N*-diethyl-*m*-toluamide (DEET) and diphenylamine, with an estimated  
545 average concentration of 0.016 and 0.007 mg.kg<sup>-1</sup>, respectively. Diuron and its TP 1-(3,4-  
546 dichlorophenyl)-3-methyl urea) were identified with a 63% FoA, with an estimated maximum  
547 concentration of 0.078 to 0.086 mg.kg<sup>-1</sup> for diuron in mussels. Butroxydim, diazinon,  
548 diflufenicen, prosulfocarb and spiroxamine were identified in oysters and mussels (50% FoA),  
549 with an estimated average concentration ranging from below the SDL for diazinon to 0.016  
550 mg.kg<sup>-1</sup> for butroxidim. The pesticides with the lowest FoA (13%) were azimsulfuron,  
551 bupirimate, pyroxsulam, tebuconazole and thiabendiazole, which were only identified in  
552 crustacean samples (spiny lobsters or crayfish) with an estimated maximum concentration of  
553 0.009 mg.kg<sup>-1</sup> for azimsulfuron in crayfish. These pesticides found in this study have also  
554 been identified in previous reports in seafood samples (Diallo et al., 2022; Slaby et al., 2022).  
555 The extraction procedure used in these previous works was QuEChERS, followed by LC-

556 HRMS and LC-MS/MS analysis in the case of [Diallo et al. \(2022\)](#) and [Slaby et al. \(2022\)](#),  
557 respectively.

#### 558 3.4.2. *Veterinary drugs*

559 Generally, the categories of the seven identified veterinary drugs were antibiotics, NSAIDs  
560 and antihistamines. Of these, none had a FoA of 100%. Clarithromycin, dapsone and  
561 diclofenac were identified in oysters and mussels (50% FoA), with an estimated maximum  
562 concentration of 0.057 to 0.068 mg.kg<sup>-1</sup> for diclofenac in mussels. Vedaprofen was identified  
563 in crustacean and fish samples (50% FoA), with an estimated average concentration between  
564 0.027 and 0.046 mg.kg<sup>-1</sup> in these samples. The veterinary drug with the lowest FoA (13%)  
565 was 4-dimethylaminoantipyrine, which was only identified in spiny lobster. Only diclofenac  
566 was previously detected in the bivalve using a QuEChERS-LC-HRMS method ([Daniele et al.,](#)  
567 [2016](#)), the other veterinary drugs were detected in environmental samples such as surface  
568 water using solid phase extraction (SPE), following by LC-MS/MS analysis ([Ramírez-](#)  
569 [Morales et al., 2021](#)).

#### 570 3.4.3. *Industrial chemicals*

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

#### 577 3.5. *Suspect screening analysis in real seafood samples*

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

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

587 (25% FoA), fexofenadine (25% FoA) and methylprednisolone (13% FoA) (Dodder et al.,  
588 2014; Omar et al., 2019; Ramírez-Morales et al., 2021).

589 Tetrahydrocannabinol (THC), an illicit drug, was also identified in oyster and mussel samples  
590 (50% FoA). It has previously been found in fish from Argentina by suspect screening using  
591 four extraction methods (two involving SPE and two based on QuEChERS), follow by LC-  
592 HRMS analysis (Carrizo et al., 2022).

593 Two pesticide TPs (flufenacet-ethane sulfonic acid (ESA) and met amitron-desamino) were  
594 identified only in mussel samples (25% FoA). Flufenacet ESA has been reported in fish  
595 collected from north-eastern France (Slaby et al., 2022). Met amitron-desamino has been  
596 identified in environmental samples in Greece using SPE-LC-HRMS method (Nika et al.,  
597 2020).

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

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

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

## 615 **4. Conclusion**

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

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

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

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

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

## 653 **Acknowledgements**

654 This work was funded by the French National Research Agency (ANR) AlimOmic project,  
655 ANR-19-CE21-0002. Authors are very grateful to the AQUAECOS project (Amélioration de  
656 la QUALité Environnementale en zones CONchylicoles des Pertuis Charentais), funded by the  
657 Nouvelle Aquitaine Regional Council, the regional shellfish growers association (Comité  
658 Régional de la Conchyliculture de la Charente-Maritime (CRC17)), the Charente-Maritime  
659 Departmental Council (CD17) and the French Office for Biodiversity (OFB). The authors  
660 would also like to thank the Pesticides and Marine Biotoxins Unit (UPBM) of the ANSES  
661 Food Safety Laboratory (LSAL) for its technical support.

## 662 **Declaration of competing interest**

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

## 665 **5. References**

- 666 Anastassiades, M., Kolberg, D.I., Eichhorn, E., Benkenstein, A., Lukačević, S., Mack, D.,  
667 Wildgrube, C., Sigalov, I., Dörk, D., Barth, A., 2015. Quick Method for the Analysis  
668 of numerous Highly Polar Pesticides in Foods of Plant Origin via LC-MS/MS  
669 involving Simultaneous Extraction with Methanol (QuPPE-Method).
- 670 Anses, 2020. Table de composition nutritionnelle Ciqua pour le calcul des apports  
671 nutritionnels CALNUT. Consulté le 02/11/2022. <https://ciqua.anses.fr/>.
- 672 Arroyo-Manzanares, N., Campillo, N., López-García, I., Hernández-Córdoba, M., Viñas, P.,  
673 2021. High-resolution mass spectrometry for the determination of mycotoxins in  
674 biological samples. A review. *Microchem. J.* 166, 106197.  
675 <https://doi.org/10.1016/j.microc.2021.106197>
- 676 Bai, M., Tang, R., Li, G., She, W., Chen, G., Shen, H., Zhu, S., Zhang, H., Wu, H., 2022.  
677 High-throughput screening of 756 chemical contaminants in aquaculture products  
678 using liquid chromatography/quadrupole time-of-flight mass spectrometry. *Food*  
679 *Chem. X* 15, 100380. <https://doi.org/10.1016/j.fochx.2022.100380>
- 680 Barbieri, M.V., Postigo, C., Guillem-Argiles, N., Monllor-Alcaraz, L.S., Simionato, J.I.,  
681 Stella, E., Barceló, D., López de Alda, M., 2019. Analysis of 52 pesticides in fresh fish  
682 muscle by QuEChERS extraction followed by LC-MS/MS determination. *Sci. Total*  
683 *Environ.* 653, 958–967. <https://doi.org/10.1016/j.scitotenv.2018.10.289>
- 684 Breitwieser, M., Vigneau, E., Viricel, A., Becquet, V., Lacroix, C., Erb, M., Huet, V.,  
685 Churlaud, C., Le Floch, S., Guillot, B., Graber, M., Thomas, H., 2018. What is the  
686 relationship between the bioaccumulation of chemical contaminants in the variegated  
687 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



737 Catalonia). *Sci. Total Environ.* 654, 1337–1349.  
738 <https://doi.org/10.1016/j.scitotenv.2018.11.061>

739 Guo, J., Tong, M., Tang, J., Bian, H., Wan, X., He, L., Hou, R., 2019. Analysis of multiple  
740 pesticide residues in polyphenol-rich agricultural products by UPLC-MS/MS using a  
741 modified QuEChERS extraction and dilution method. *Food Chem.* 274, 452–459.  
742 <https://doi.org/10.1016/j.foodchem.2018.08.134>

743 Jansons, M., Pugajeva, I., Bartkevics, V., Karkee, H.B., 2021. LC-MS/MS characterisation  
744 and determination of dansyl chloride derivatised glyphosate, aminomethylphosphonic  
745 acid (AMPA), and glufosinate in foods of plant and animal origin. *J. Chromatogr. B*  
746 1177, 122779. <https://doi.org/10.1016/j.jchromb.2021.122779>

747 Kim, H.-Y., Lee, I.-S., Oh, J.-E., 2017. Human and veterinary pharmaceuticals in the marine  
748 environment including fish farms in Korea. *Sci. Total Environ.* 579, 940–949.  
749 <https://doi.org/10.1016/j.scitotenv.2016.10.039>

750 Kim, L., Lee, D., Cho, H.-K., Choi, S.-D., 2019. Review of the QuEChERS method for the  
751 analysis of organic pollutants: Persistent organic pollutants, polycyclic aromatic  
752 hydrocarbons, and pharmaceuticals. *Trends Environ. Anal. Chem.* 22, e00063.  
753 <https://doi.org/10.1016/j.teac.2019.e00063>

754 Makni, Y., Diallo, T., Guérin, T., Parinet, J., 2022. Improving the monitoring of multi-class  
755 pesticides in baby foods using QuEChERS-UHPLC-Q-TOF with automated  
756 identification based on MS/MS similarity algorithms. *Food Chem.* 395, 133573.  
757 <https://doi.org/10.1016/j.foodchem.2022.133573>

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

762 Narendran, S.T., Meyyanathan, S.N., Karri, V.V.S.R., 2019. Experimental design in  
763 pesticide extraction methods: A review. *Food Chem.* 289, 384–395.  
764 <https://doi.org/10.1016/j.foodchem.2019.03.045>

765 Nika, M.C., Ntaiou, K., Elytis, K., Thomaidi, V.S., Gatidou, G., Kalantzi, O.I., Thomaidis,  
766 N.S., Stasinakis, A.S., 2020. Wide-scope target analysis of emerging contaminants in  
767 landfill leachates and risk assessment using Risk Quotient methodology. *J. Hazard.*  
768 *Mater.* 394, 122493. <https://doi.org/10.1016/j.jhazmat.2020.122493>

769 Nikolopoulou, V., Ajibola, A.S., Aalizadeh, R., Thomaidis, N.S., 2023. Wide-scope target  
770 and suspect screening of emerging contaminants in sewage sludge from Nigerian  
771 WWTPs by UPLC-qToF-MS. *Sci. Total Environ.* 857, 159529.  
772 <https://doi.org/10.1016/j.scitotenv.2022.159529>

773 Omar, T.F.T., Aris, A.Z., Yusoff, F.M., Mustafa, S., 2019. Occurrence and level of emerging  
774 organic contaminant in fish and mollusk from Klang River estuary, Malaysia and  
775 assessment on human health risk. *Environ. Pollut.* 248, 763–773.  
776 <https://doi.org/10.1016/j.envpol.2019.02.060>

777 Pang, X., Liu, X., Peng, L., Chen, Z., Qiu, J., Su, X., Yu, C., Zhang, J., Weng, R., 2021.  
778 Wide-scope multi-residue analysis of pesticides in beef by ultra-high-performance  
779 liquid chromatography coupled with quadrupole time-of-flight mass spectrometry.  
780 *Food Chem.* 351, 129345. <https://doi.org/10.1016/j.foodchem.2021.129345>

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

784 Peng, Y., Fang, W., Krauss, M., Brack, W., Wang, Z., Li, F., Zhang, X., 2018. Screening  
785 hundreds of emerging organic pollutants (EOPs) in surface water from the Yangtze

786 River Delta (YRD): Occurrence, distribution, ecological risk. *Environ. Pollut.* 241,  
787 484–493. <https://doi.org/10.1016/j.envpol.2018.05.061>

788 Rajski, L., Petromelidou, S., Díaz-Galiano, F.J., Ferrer, C., Fernández-Alba, A.R., 2021.  
789 Improving the simultaneous target and non-target analysis LC-amenable pesticide  
790 residues using high speed Orbitrap mass spectrometry with combined multiple  
791 acquisition modes. *Talanta* 228, 122241. <https://doi.org/10.1016/j.talanta.2021.122241>

792 Ramírez-Morales, D., Masís-Mora, M., Montiel-Mora, J.R., Cambronero-Heinrichs, J.C.,  
793 Pérez-Rojas, G., Tormo-Budowski, R., Méndez-Rivera, M., Briceño-Guevara, S.,  
794 Gutiérrez-Quirós, J.A., Arias-Mora, V., Brenes-Alfaro, L., Beita-Sandí, W.,  
795 Rodríguez-Rodríguez, C.E., 2021. Multi-residue analysis of pharmaceuticals in water  
796 samples by liquid chromatography- mass spectrometry: Quality assessment and  
797 application to the risk assessment of urban-influenced surface waters in a metropolitan  
798 area of Central America. *Process Saf. Environ. Prot.* 153, 289–300.  
799 <https://doi.org/10.1016/j.psep.2021.07.025>

800 Schymanski, E.L., Jeon, J., Gulde, R., Fenner, K., Ruff, M., Singer, H.P., Hollender, J., 2014.  
801 Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating  
802 Confidence. *Environ. Sci. Technol.* 48, 2097–2098. <https://doi.org/10.1021/es5002105>

803 Slaby, S., Le Cor, F., Dufour, V., Auger, L., Pasquini, L., Cardoso, O., Curtet, L., Baudoin, J.-  
804 M., Wiest, L., Vulliet, E., Feidt, C., Dauchy, X., Banas, D., 2022. Distribution of  
805 pesticides and some of their transformation products in a small lentic waterbody: Fish,  
806 water, and sediment contamination in an agricultural watershed. *Environ. Pollut.* 292,  
807 118403. <https://doi.org/10.1016/j.envpol.2021.118403>

808 Sobczak, Ł., Kołodziej, D., Goryński, K., 2021. Benefits of Innovative and Fully Water-  
809 Compatible Stationary Phases of Thin-Film Microextraction (TFME) Blades.  
810 *Molecules* 26, 4413. <https://doi.org/10.3390/molecules26154413>

811 Teyssseire, R., Manangama, G., Baldi, I., Carles, C., Brochard, P., Bedos, C., Delva, F., 2021.  
812 Determinants of non-dietary exposure to agricultural pesticides in populations living  
813 close to fields: A systematic review. *Sci. Total Environ.* 761, 143294.  
814 <https://doi.org/10.1016/j.scitotenv.2020.143294>

815 Tudi, M., Daniel Ruan, H., Wang, L., Lyu, J., Sadler, R., Connell, D., Chu, C., Phung, D.T.,  
816 2021. Agriculture Development, Pesticide Application and Its Impact on the  
817 Environment. *Int. J. Environ. Res. Public Health* 18, 1112.  
818 <https://doi.org/10.3390/ijerph18031112>

819 van der Oost, R., Beyer, J., Vermeulen, N.P.E., 2003. Fish bioaccumulation and biomarkers in  
820 environmental risk assessment: a review. *Environ. Toxicol. Pharmacol.* 13, 57–149.  
821 [https://doi.org/10.1016/S1382-6689\(02\)00126-6](https://doi.org/10.1016/S1382-6689(02)00126-6)

822  
823  
824

## 825 **Figure captions**

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

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

833 **Fig. 3.** Comparison of the QuEChERS, QuPPE, QuEChERS + QuPPE and QuEChUP sample  
834 preparation methods for detection of pesticides and veterinary drugs. The error bars  
835 correspond to the standard deviation (SD) (Mean  $\pm$  SD, n = 3).

836 **Fig. 4.** Percentage of pesticides presenting screening detection limits (SDLs) (a) and limits of  
837 identification (LOIs) (b) at 0.001, 0.01, 0.1 and  $> 0.1$  mg.kg<sup>-1</sup> under optimised conditions.  
838 Detection (c) and identification rates (d) across different seafood samples spiked at 0.001,  
839 0.01 and 0.1 mg.kg<sup>-1</sup>.

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

843

844

845

846

847 **Fig. 1.**

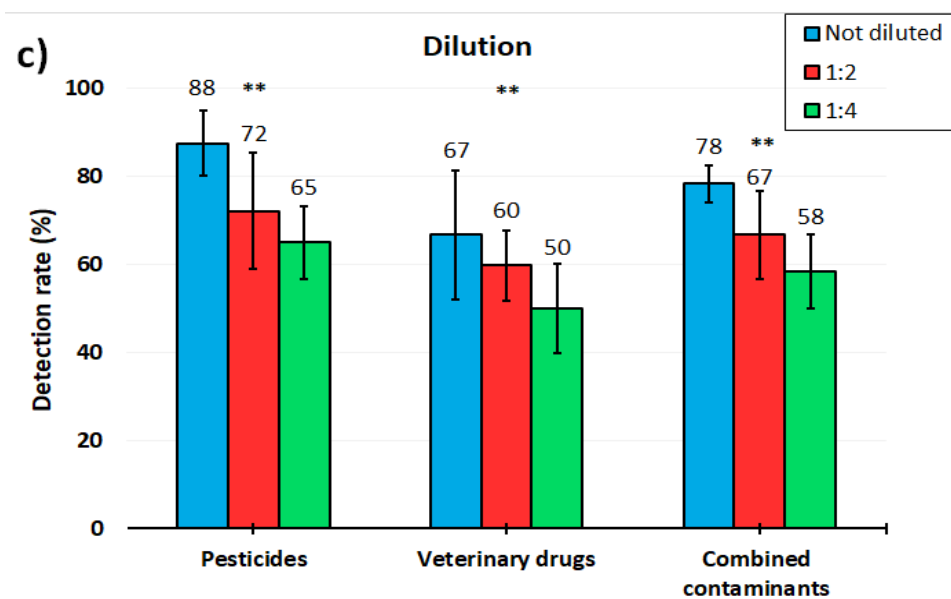
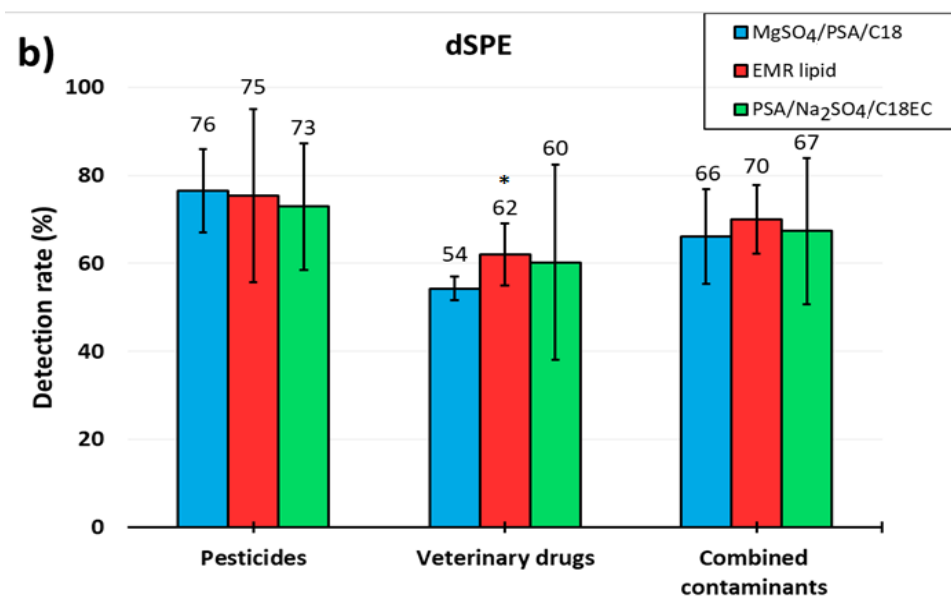
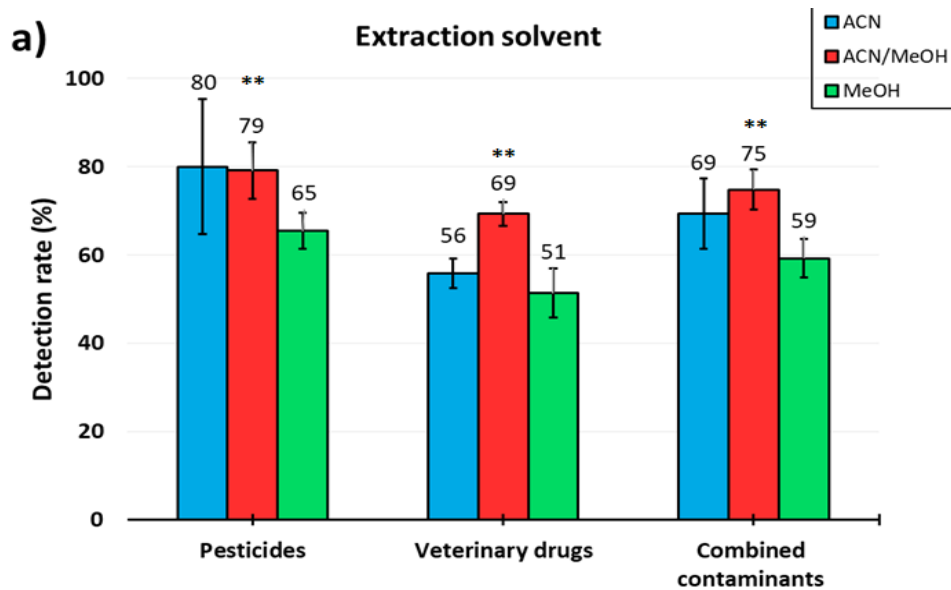


Fig. 2.

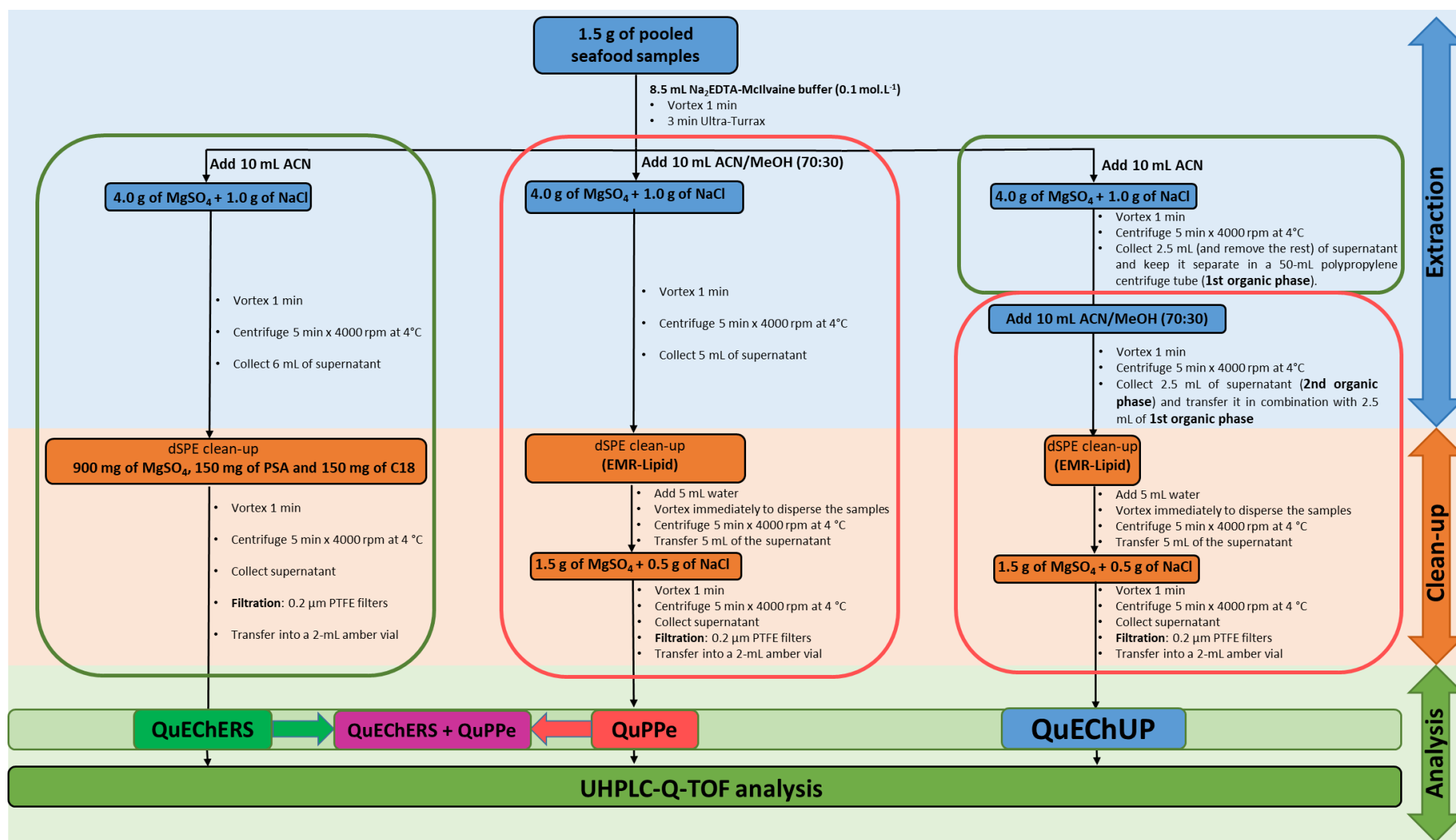
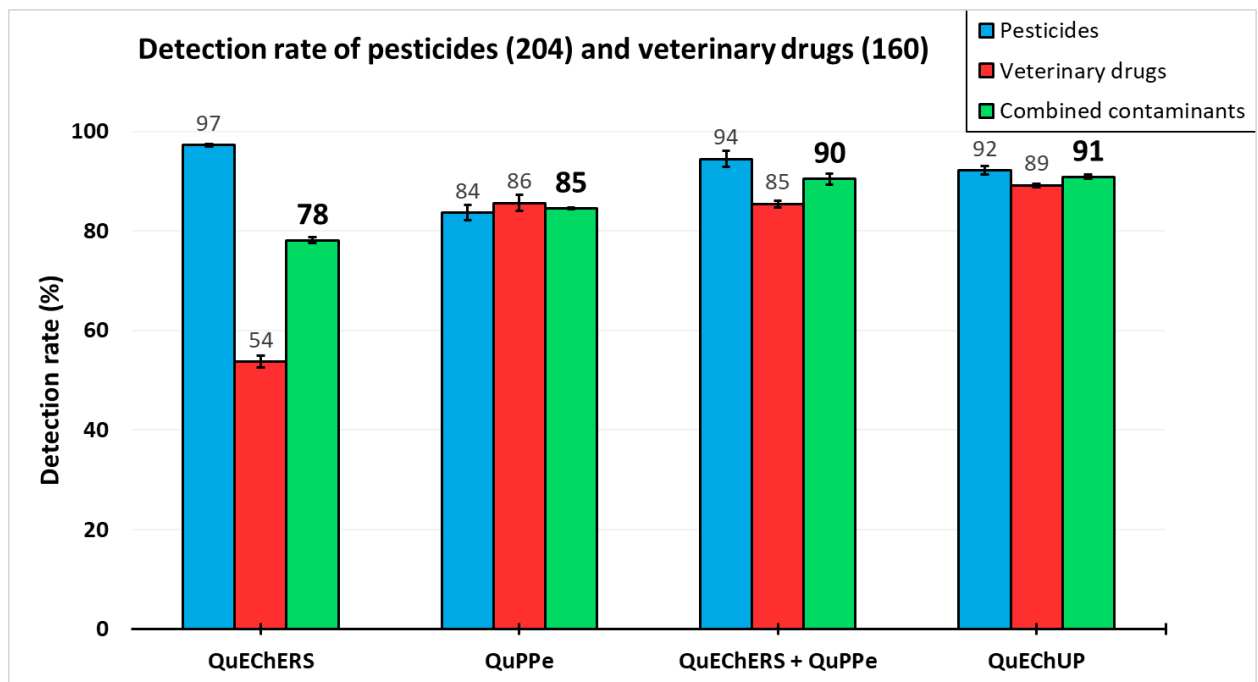




Fig. 3.

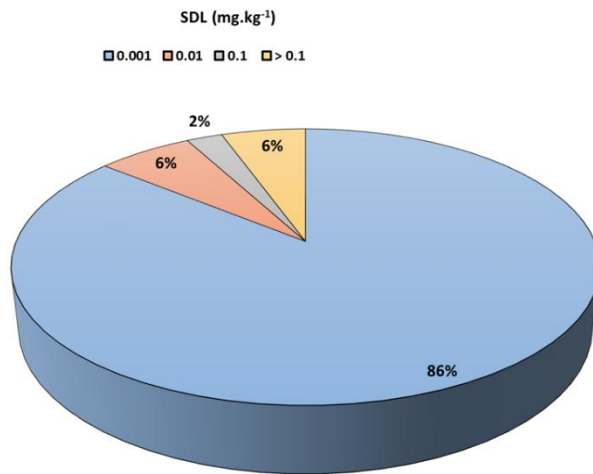


854

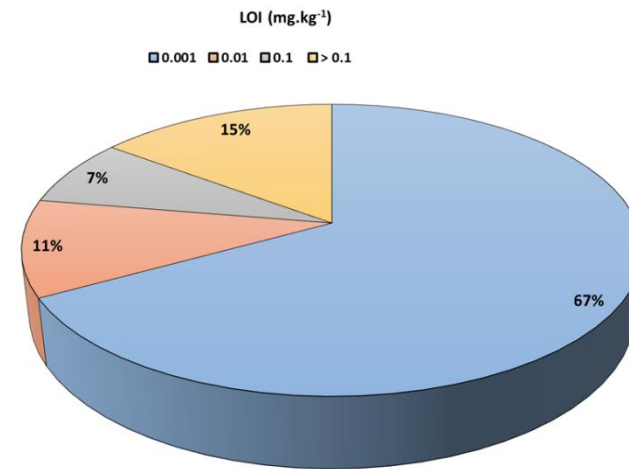
855

Fig. 4.

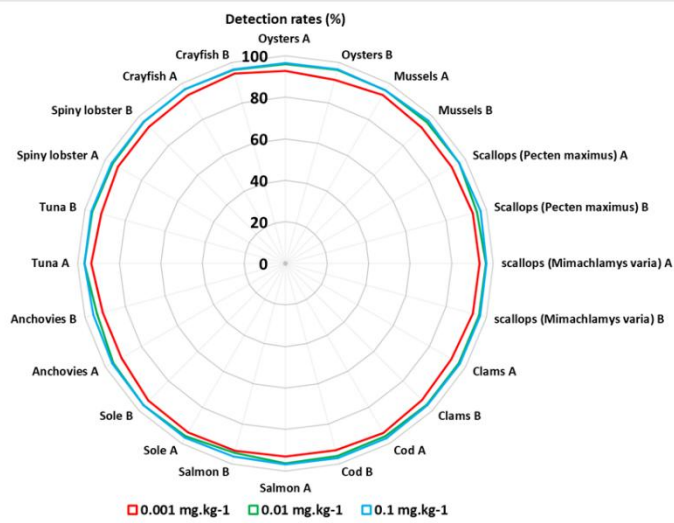
a)



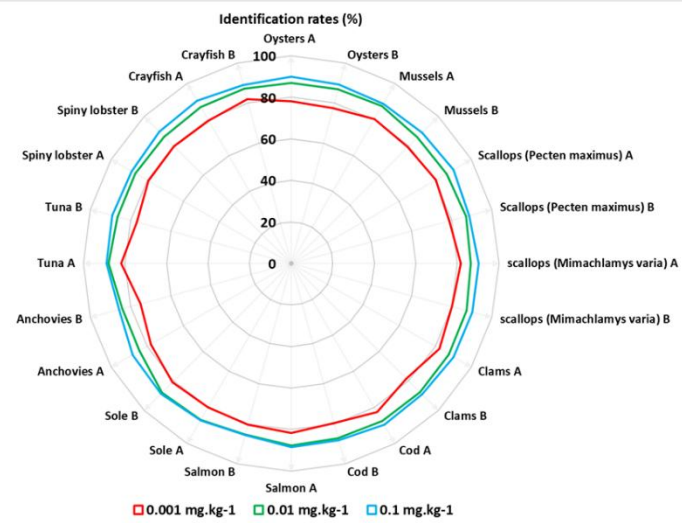
b)



c)



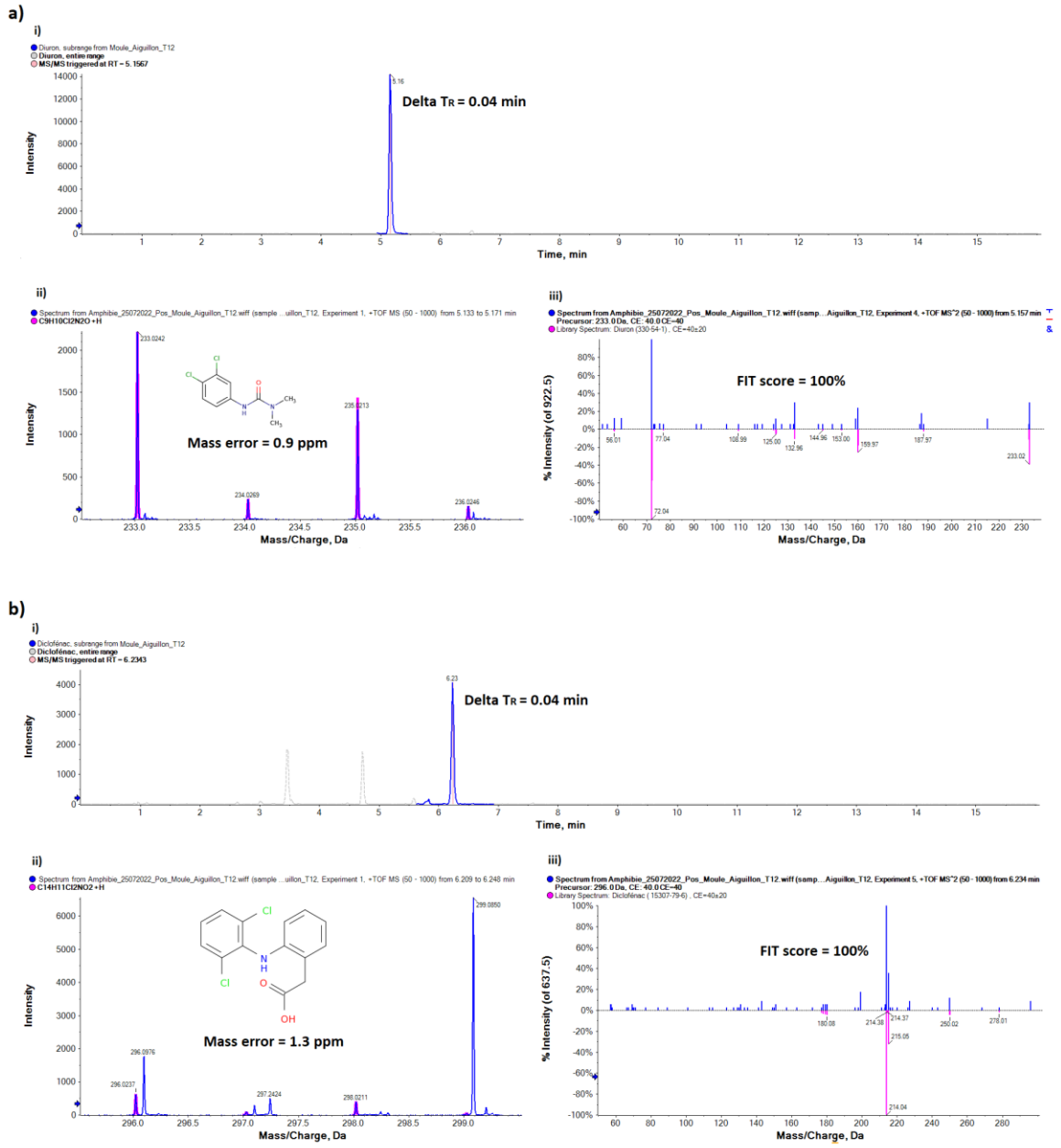
d)



856



Fig. 5.



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

Level	Factor		
	Extraction solvent	dSPE sorbent	Dilution
1	ACN	MgSO <sub>4</sub> /PSA/C18	Not diluted
2	MeOH/ACN (7:3)	EMR-lipid	1:2
3	MeOH (1% FA)	PSA/Na <sub>2</sub> SO <sub>4</sub> /C18EC	1:4

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

863

## Supplementary Materials

864

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

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
1-(3,4-Dichlorophenyl)-3-methylurea	0.01	C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M-H] <sup>-</sup>	219.00864	4.78	2.94
1-(4-Nitrophenyl)-3-propylurea	0.01	C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>	[M-H] <sup>-</sup>	224.10297	4.69	2.4**
1,2-Benzisothiazol-3(2H)-one	0.01	C <sub>7</sub> H <sub>5</sub> NOS	[M+H] <sup>+</sup>	152.01646	2.78	1.95
1,3-Diphenylurea	0.01	C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	213.10224	5.19	3
2,3,5-Trimethacarb	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	194.11756	5.35	2.5
2,4-Dimethylaniline	0.01	C <sub>8</sub> H <sub>11</sub> N	[M+H] <sup>+</sup>	122.09643	2.47	1.68
2,6-Dichlorobenzamide	0.01	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NO	[M+H] <sup>+</sup>	189.9821	2.71	0.77
2,6-Diethylaniline	0.01	C <sub>10</sub> H <sub>15</sub> N	[M+H] <sup>+</sup>	150.12773	5.75	2.7
2-Ethylhexyl diphenyl phosphate	0.01	C <sub>20</sub> H <sub>27</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	363.17197	8.64	6.3
2-N-Octyl-4-isothiazolin-3-one	0.01	C <sub>11</sub> H <sub>19</sub> NOS	[M+H] <sup>+</sup>	214.12601	6.29	2.45
3,4-Dichloroaniline	0.01	C <sub>6</sub> H <sub>5</sub> Cl <sub>2</sub> N	[M+H] <sup>+</sup>	161.98718	5.32	2.7
3,4,5-Trimethacarb	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	194.11756	5.28	2.7
3-Hydroxycarbofuran	0.01	C <sub>12</sub> H <sub>15</sub> NO <sub>4</sub>	C <sub>12</sub> H <sub>14</sub> NO <sub>3</sub> <sup>+</sup>	220.09682	3.08	0.76
3-Ketocarbofuran	0.01	C <sub>12</sub> H <sub>13</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	236.09173	4.03	1.8
4-Acethylaminoantipyrine	0.01	C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>	[M+Na] <sup>+</sup>	246.12370	2.27	0
4-Aminoantipyrine	0.01	C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	204.11314	2.24	0.1
4-Bromo-3,5-dimethylphenyl-N-methylcarbamate	0.01	C <sub>10</sub> H <sub>12</sub> BrNO <sub>2</sub>	[M+H] <sup>+</sup>	258.01242	5.91	3.1
4-Dimethylaminoantipyrine	0.01	C <sub>13</sub> H <sub>17</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	232.14444	1.98	1

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
4-Formylaminoantipyrine	0.01	C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	232.10805	2.24	0
4-Methylaminoantipyrine	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	218.12879	1.86	0
5-Hydroxy-flunixin	0.01	C <sub>14</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	313.07945	5.10	3.7
8-Hydroxy-mutilin	0.01	C <sub>20</sub> H <sub>32</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	337.23734	3.61	/
Abamectin	0.01	C <sub>48</sub> H <sub>72</sub> O <sub>14</sub>	[M+Na] <sup>+</sup>	895.48143	8.78	3.8
Abamectin B1a	0.01	C <sub>48</sub> H <sub>72</sub> O <sub>14</sub>	[M+Na] <sup>+</sup>	873.49948	8.86	3.8
Abamectin B1b	0.01	C <sub>47</sub> H <sub>70</sub> O <sub>14</sub>	[M+CH <sub>3</sub> COO] <sup>-</sup>	876.51038	/	3.5
Abate® (temephos)	0.01	C <sub>16</sub> H <sub>20</sub> O <sub>6</sub> P <sub>2</sub> S <sub>3</sub>	[M+H] <sup>+</sup>	466.99701	8.03	6
Acephate	0.01	C <sub>4</sub> H <sub>10</sub> NO <sub>3</sub> PS	C <sub>2</sub> H <sub>8</sub> O <sub>3</sub> PS <sup>+</sup>	142.99263	0.96	-0.8
Acetamiprid	0.01	C <sub>10</sub> H <sub>11</sub> ClN <sub>4</sub>	[M+H] <sup>+</sup>	223.0745	3.44	0.8
Acibenzolar- <i>S</i> -methyl	0.01	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	[M+H] <sup>+</sup>	210.99943	6.07	3.1
Aclonifen	0.01	C <sub>12</sub> H <sub>9</sub> ClN <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	265.03745	6.93	4.04
Aconitine	0.01	C <sub>34</sub> H <sub>47</sub> NO <sub>11</sub>	[M+H] <sup>+</sup>	646.32219	4.71	0.3**
Akton	0.01	C <sub>12</sub> H <sub>14</sub> Cl <sub>3</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	374.95396	8.3	4.8**
Alachlor	0.01	C <sub>14</sub> H <sub>20</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	270.12553	6.68	3.5
Albendazole	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	266.09578	4.80	2.7
Albendazole amino sulfone	0.01	C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	240.08013	1.96	1.4
Albendazole sulfone	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	298.08560	3.44	1.6
Albendazole sulfoxide	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	282.09069	2.93	1.3
Aldicarb	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	[M+Na] <sup>+</sup>	213.06682	3.8	1.13
Aldicarb sulfone	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	223.07471	3.44	0.79
Aldicarb sulfoxide	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	207.07979	0.94	-0.2
Allethrin	0.01	C <sub>19</sub> H <sub>26</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	303.19547	8.08	4.78

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Allidochlor	0.01	C <sub>8</sub> H <sub>12</sub> ClNO	[M+H] <sup>+</sup>	174.06802	4.23	1.83
Alloxydim sodium	0.01	C <sub>17</sub> H <sub>24</sub> NNaO <sub>5</sub>	[M+H] <sup>+</sup>	346.16249	7.12	/
Alpha-cypermethrin	0.01	C <sub>22</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	433.10802	8.74	6.6
Ametoctradin	0.01	C <sub>15</sub> H <sub>25</sub> N <sub>5</sub>	[M+H] <sup>-</sup>	276.21827	6.57	4.6**
Ametryne	0.01	C <sub>9</sub> H <sub>17</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	228.12774	5.03	2.98
Amicarbazone	0.01	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	242.16115	4.06	1.23
Amidosulfuron	0.01	C <sub>9</sub> H <sub>15</sub> N <sub>5</sub> O <sub>7</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	370.04857	4.77	1.63
Amino flubendazole	0.01	C <sub>14</sub> H <sub>10</sub> FN <sub>3</sub> O	[M+H] <sup>+</sup>	256.08807	3.21	1.6
Amino mebendazole	0.01	C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	238.09749	3.02	2.6
Aminocarb	0.01	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	209.12845	1.71	1.9
Amitraze	0.01	C <sub>19</sub> H <sub>23</sub> N <sub>3</sub>	[M+H] <sup>+</sup>	294.19647	8.58	5.5
Amoxicillin	0.01	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	366.11182	0.92	-2
Ampicillin +4	0.01	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	350.11690	0.95	-1.1
Ancymidol	0.01	C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	257.12845	4.26	1..91
Anilazine	0.01	C <sub>9</sub> H <sub>5</sub> Cl <sub>3</sub> N <sub>4</sub>	[M+H] <sup>+</sup>	274.96526	6.26	3.88
Anilofos	0.01	C <sub>13</sub> H <sub>19</sub> ClNO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	368.03053	7.12	3.81
Antipyrine phenazone	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	189.10224	2.88	0.4
Aspon <sup>TM</sup>	0.01	C <sub>12</sub> H <sub>28</sub> O <sub>5</sub> P <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	379.09262	8.73	6
Asulam	0.01	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	231.04341	2.25	-0.27
Atraton	0.01	C <sub>9</sub> H <sub>17</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	212.15059	3.75	2.7
Atrazine	0.01	C <sub>8</sub> H <sub>14</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	216.10105	5.12	2.6
Atrazine desisopropyl	0.01	C <sub>5</sub> H <sub>8</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	174.0541	2.51	1.1**
Avilamycin	0.01	C <sub>61</sub> H <sub>88</sub> Cl <sub>2</sub> O <sub>32</sub>	[M+H] <sup>+</sup>	1403.47085	/	/

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Azaconazole	0.01	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	300.03011	5.21	2.32
Azadirachtin	0.01	C <sub>35</sub> H <sub>44</sub> O <sub>16</sub>	[M+H] <sup>+</sup>	721.27021	5.01	1.09
Azamethiphos	0.01	C <sub>9</sub> H <sub>10</sub> ClN <sub>2</sub> O <sub>5</sub> PS	[M+H] <sup>+</sup>	324.98094	4.44	1.05
Azimsulfuron	0.01	C <sub>13</sub> H <sub>16</sub> N <sub>10</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	425.10986	5.03	0.65
Aziprotryne	0.01	C <sub>7</sub> H <sub>11</sub> N <sub>7</sub> S	[M+H] <sup>+</sup>	226.08694	6.15	3
Azoxystrobin	0.01	C <sub>22</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	404.1241	6.16	2.5
Bacitracin A	0.01	C <sub>66</sub> H <sub>103</sub> N <sub>17</sub> O <sub>16</sub> S	[M+H] <sup>+</sup>	1422.75622	/	/
Baquiloprim	0.01	C <sub>17</sub> H <sub>20</sub> N <sub>6</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	326.20877	/	/
Barban	0.01	C <sub>11</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	258.00831	6.25	3.47
Beflubutamid	0.01	C <sub>18</sub> H <sub>17</sub> F <sub>4</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	356.12682	6.96	4.7
Benalaxyl	0.01	C <sub>20</sub> H <sub>23</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	326.17507	7.04	3.4
Benazolin	0.01	C <sub>9</sub> H <sub>6</sub> ClNO <sub>3</sub> S	[M+H] <sup>+</sup>	243.98297	3.88	2.5
Bendiocarb	0.01	C <sub>11</sub> H <sub>13</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	224.09173	4.7	1.7
Benfluralin (benefin)	0.01	C <sub>13</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	336.11657	8.17	5.29
Benfuresate	0.01	C <sub>12</sub> H <sub>16</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	257.08421	6	2.41
Benodanil	0.01	C <sub>13</sub> H <sub>10</sub> INO	[M+H] <sup>+</sup>	323.98799	5.67	2.85
Benomyl	0.01	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	291.14517	6.1	2.12
Benoxacor	0.01	C <sub>11</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	260.02396	6.06	2.7
Bensulfuron-methyl	0.01	C <sub>16</sub> H <sub>18</sub> N <sub>4</sub> O <sub>7</sub> S	[M+H] <sup>+</sup>	411.0969	5.44	2.18
Bensulide	0.01	C <sub>14</sub> H <sub>24</sub> NO <sub>4</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	398.06779	7.09	4.2
Bentazon	0.01	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	241.06414	4.48	2.34
Bentazon-methyl	0.01	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	255.07979	5.32	2.31
Benthiavalicarb-isopropyl	0.01	C <sub>18</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	382.15952	5.93	2.52

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Benzoximate	0.01	C <sub>18</sub> H <sub>18</sub> ClNO <sub>5</sub>	C <sub>9</sub> H <sub>8</sub> ClO <sub>3</sub> <sup>+</sup>	199.01565	7.53	3.73
Benzoylprop ethyl	0.01	C <sub>18</sub> H <sub>17</sub> Cl <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	366.06583	7.28	4.1**
Benzthiazuron	0.01	C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> OS	[M+H] <sup>-</sup>	208.05391	3.88	1.6**
Bifenthrin	0.01	C <sub>23</sub> H <sub>22</sub> ClF <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	423.13332	/	6
Bioresmethrin	0.01	C <sub>22</sub> H <sub>26</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	339.19547	8.89	4.7
Bitertanole (mixture of isomers)	0.01	C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	338.1863	6.65	4.16
Bixafen	0.01	C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>3</sub> O	[M+H] <sup>-</sup>	414.03823	6.69	4.7**
Bladex	0.01	C <sub>9</sub> H <sub>13</sub> ClN <sub>6</sub>	[M+H] <sup>+</sup>	241.0963	4.4	2.22
Boscalid	0.01	C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	343.03995	6.32	2.96
Bromacil	0.01	C <sub>9</sub> H <sub>13</sub> BrN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>-</sup>	261.02332	4.18	2.11
Bromofenvinphos-ethyl	0.01	C <sub>12</sub> H <sub>14</sub> BrCl <sub>2</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	404.92397	7.03	3.2**
Bromophos-methyl	0.01	C <sub>8</sub> H <sub>8</sub> BrCl <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	366.85409	8.06	5.21
Bromuconazole (mixture of isomers)	0.01	C <sub>13</sub> H <sub>12</sub> BrCl <sub>2</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	377.95902	6.12	3.24
Bufen carb	0.01	C <sub>26</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	443.29043	/	/
Bupirimate	0.01	C <sub>13</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	317.16419	6.49	2.7
Buprofezin	0.01	C <sub>16</sub> H <sub>23</sub> N <sub>3</sub> OS	[M+H] <sup>+</sup>	306.16346	7.96	4.3
Butachlor	0.01	C <sub>17</sub> H <sub>26</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	312.17248	8.11	4.5
Butafenacil	0.01	C <sub>20</sub> H <sub>18</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>6</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	492.11437	6.72	3.2
Butocarboxim	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	191.08488	4	1.1
Butocarboxim sulfoxide	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	[M+Na] <sup>+</sup>	229.06174	0.96	-1.02
Butoxycarboxim	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	223.07471	3.44	-0.1
Butoxydim	0.01	C <sub>24</sub> H <sub>33</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	400.24824	8.14	1.9
Buturon	0.01	C <sub>12</sub> H <sub>13</sub> ClN <sub>2</sub> O	[M+H] <sup>+</sup>	237.07892	5.57	3**

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Butylate	0.01	C <sub>11</sub> H <sub>23</sub> NOS	[M+H] <sup>+</sup>	218.15731	7.97	4.15
Cadusafos	0.01	C <sub>10</sub> H <sub>23</sub> O <sub>2</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	271.09499	7.33	3.9
Cafenstrole	0.01	C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	351.14854	6.62	3.21
Carbaryl	0.01	C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub>	C <sub>10</sub> H <sub>9</sub> O <sup>+</sup>	145.06479	4.89	2.36
Carbendazim	0.01	C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	192.07675	2.19	1.52
Carbetamide	0.01	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	237.12337	4.04	1,75
Carbofuran	0.01	C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	222.11247	4.75	2.32
Carbophenothion	0.01	C <sub>11</sub> H <sub>16</sub> ClO <sub>2</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	342.98114	8.39	5.33
Carboxine	0.01	C <sub>12</sub> H <sub>13</sub> NO <sub>2</sub> S	[M+H] <sup>+</sup>	236.07398	5.07	2.14
Carfentrazone-ethyl	0.01	C <sub>15</sub> H <sub>14</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	412.04371	6.93	3.36
Carprofen	0.01	C <sub>15</sub> H <sub>12</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	274.06293	6.01	4
Carpropamid	0.01	C <sub>15</sub> H <sub>18</sub> Cl <sub>3</sub> NO	[M+H] <sup>+</sup>	334.05267	7.1	4.23
Cefacetriple	0.01	C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	357.08633	/	/
Cefalexine	0.01	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	348.10125	0.95	0.6
Cefapirine	0.01	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> S <sub>2</sub>	[M-H] <sup>+</sup>	424.06316	0.95	-1.1
Cefazolin	0.01	C <sub>14</sub> H <sub>14</sub> N <sub>8</sub> O <sub>4</sub> S <sub>3</sub>	[M+H] <sup>+</sup>	455.03729	2.41	-0.6
Cefoperazone	0.01	C <sub>25</sub> H <sub>27</sub> N <sub>9</sub> O <sub>8</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	646.14968	2.90	-0.7
Ceftiofur +4	0.01	C <sub>19</sub> H <sub>17</sub> N <sub>5</sub> O <sub>7</sub> S <sub>3</sub>	[M+H] <sup>+</sup>	524.03629	3.58	0.2
Ceftriaxone (CAS)	0.01	C <sub>18</sub> H <sub>18</sub> N <sub>8</sub> O <sub>7</sub> S <sub>3</sub>	[M+H] <sup>+</sup>	555.05334	/	/
Cefuroxim	0.01	C <sub>16</sub> H <sub>16</sub> N <sub>4</sub> O <sub>8</sub> S	[M-H] <sup>-</sup>	442.10271	2.58	-0.2
Cephradine	0.01	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	350.11690	0.95	/
Chinomethionate	0.01	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> OS <sub>2</sub>	[M+H] <sup>+</sup>	234.99943	7.38	3.78
Chlorantraniliprole	0.01	C <sub>18</sub> H <sub>14</sub> BrCl <sub>2</sub> N <sub>5</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	483.97579	5.68	2.76



<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Chlorbromuron	0.01	C <sub>9</sub> H <sub>10</sub> BrClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	294.96648	6.1	3.09
Chlorbufam	0.01	C <sub>11</sub> H <sub>10</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	224.04728	4.95	3.59
Chlordimeform	0.01	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub>	[M+H] <sup>+</sup>	197.084	2.64	2.89
Chlorfenapyr	0.01	C <sub>15</sub> H <sub>11</sub> BrClF <sub>3</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	408.97465	7.93	4.83
Chlorfenvinphos (mixture of Z and E)	0.01	C <sub>12</sub> H <sub>14</sub> Cl <sub>3</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	358.97681	6.93	3.81
Chlorfluazuron	0.01	C <sub>20</sub> H <sub>9</sub> Cl <sub>3</sub> F <sub>5</sub> N <sub>3</sub> O <sub>3</sub>	[M-H] <sup>-</sup>	539.97024	8.3	5.8
Chloridazon	0.01	C <sub>10</sub> H <sub>8</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	222.04287	3.19	1.14
Chlorimuron-ethyl	0.01	C <sub>15</sub> H <sub>15</sub> ClN <sub>4</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	415.04736	6.06	2.5
Chlormephos	0.01	C <sub>5</sub> H <sub>12</sub> ClO <sub>2</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	234.97777	/	3
Chlormequat chloride	0.01	C <sub>5</sub> H <sub>13</sub> Cl <sub>2</sub> N	[M+H] <sup>+</sup>	158.04978	/	/
Chlorobenzuron	0.01	C <sub>14</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	309.01921	6.64	5**
Chlorosulfuron	0.01	C <sub>12</sub> H <sub>12</sub> ClN <sub>5</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	358.03713	4.8	/
Chlorotoluron	0.01	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O	[M+H] <sup>+</sup>	213.07892	4.93	2.41
Chloroxuron	0.01	C <sub>15</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	291.08948	6.07	3.7
Chlorpyrifos	0.01	C <sub>9</sub> H <sub>11</sub> Cl <sub>3</sub> NO <sub>3</sub> PS	[M+H] <sup>+</sup>	349.93356	8.21	4.96
Chlorpyrifos-methyl	0.01	C <sub>7</sub> H <sub>7</sub> Cl <sub>3</sub> NO <sub>3</sub> PS	[M+H] <sup>+</sup>	321.90226	7.49	4.31
Chlorpyrifos-oxon	0.01	C <sub>9</sub> H <sub>11</sub> Cl <sub>3</sub> NO <sub>4</sub> P	[M+H] <sup>+</sup>	333.95641	6.48	3.5**
Chlortetracycline	0.01	C <sub>22</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>8</sub>	[M+H] <sup>+</sup>	479.12157	/	/
Chlorthiamid	0.01	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> NS	[M+H] <sup>+</sup>	205.95925	4.16	1.4**
Chlorthiophos	0.01	C <sub>11</sub> H <sub>15</sub> Cl <sub>2</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	360.96501	8.36	6**
Chromafenozide	0.01	C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>	[M-H] <sup>-</sup>	395.23292	6.65	5**
Cinidon-ethyl	0.01	C <sub>19</sub> H <sub>17</sub> Cl <sub>2</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	394.06074	7.85	4.51
Cinmethylin	0.01	C <sub>18</sub> H <sub>26</sub> O <sub>2</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	292.22711	8.08	4.62

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Cinosulfuron	0.01	C <sub>15</sub> H <sub>19</sub> N <sub>5</sub> O <sub>7</sub> S	[M+H] <sup>+</sup>	414.1078	4.57	2.04
Cinoxacin	0.01	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	263.06625	3.58	1.5
Ciprofloxacin	0.01	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	332.14050	2.46	-1.1
Clarithromycin	0.01	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>	[M+H] <sup>+</sup>	748.48417	4.89	3.16
Clarithromycin	0.01	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>	[M+H] <sup>+</sup>	748.48417	5.17	3.2
Clethodim	0.01	C <sub>17</sub> H <sub>26</sub> ClNO <sub>3</sub> S	[M+H] <sup>+</sup>	360.13947	7.86	4.21
Climbazol	0.01	C <sub>15</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	293.10513	5.02	3.76
Clindamycin	0.01	C <sub>18</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	425.18715	3.30	2.2
Clodinafop (acid-free)	0.01	C <sub>14</sub> H <sub>11</sub> ClFNO <sub>4</sub>	[M+H] <sup>+</sup>	312.04334	5.76	3.4**
Clodinafop-propargyl	0.01	C <sub>17</sub> H <sub>13</sub> ClFNO <sub>4</sub>	[M+H] <sup>+</sup>	350.05899	7.11	3.9
Clofentezine	0.01	C <sub>14</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>4</sub>	[M+H] <sup>+</sup>	303.01988	7.39	3.1
Clomeprop	0.01	C <sub>16</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M-H] <sup>-</sup>	324.05526	7.76	4.8
Cloquintocet-mexyl	0.01	C <sub>18</sub> H <sub>22</sub> ClNO <sub>3</sub>	[M+H] <sup>+</sup>	336.1361	7.9	5.03
Cloransulam-methyl	0.01	C <sub>15</sub> H <sub>13</sub> ClFN <sub>5</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	430.03827	5.41	-0.365
Clorsulon	0.01	C <sub>8</sub> H <sub>8</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>	[M-H] <sup>-</sup>	401.89140	/	1.2
Closantel	0.01	C <sub>22</sub> H <sub>14</sub> Cl <sub>2</sub> I <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	662.85946	9.00	7.2
Clothianidin	0.01	C <sub>6</sub> H <sub>8</sub> ClN <sub>5</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	250.016	3.03	0.7
Cloxacillin	0.01	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	263.06625	3.58	2.4
Command (clomazone)	0.01	C <sub>12</sub> H <sub>14</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	240.07858	5.69	2.5
Coumaphos	0.01	C <sub>14</sub> H <sub>16</sub> ClO <sub>5</sub> PS	[M+H] <sup>+</sup>	363.02174	7.33	4.13
Coumaphos-oxon	0.01	C <sub>14</sub> H <sub>16</sub> ClO <sub>6</sub> P	[M+H] <sup>+</sup>	347.04458	5.69	2.78
Crimidine	0.01	C <sub>7</sub> H <sub>10</sub> ClN <sub>3</sub>	[M+H] <sup>+</sup>	172.0636	3.73	1.31
Crotoxyphos	0.01	C <sub>14</sub> H <sub>19</sub> O <sub>6</sub> P	[M+NH <sub>4</sub> ] <sup>+</sup>	332.12575	5.89	3.3

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Crufomate	0.01	C <sub>12</sub> H <sub>19</sub> ClNO <sub>3</sub> P	[M+H] <sup>+</sup>	292.08639	6.23	3.42
Cumyluron	0.01	C <sub>17</sub> H <sub>19</sub> ClN <sub>2</sub> O	[M+H] <sup>+</sup>	303.12587	6.15	3.7
Cyanofenphos	0.01	C <sub>15</sub> H <sub>14</sub> NO <sub>2</sub> PS	[M+H] <sup>+</sup>	304.05557	7.17	4.29
Cyanophos	0.01	C <sub>9</sub> H <sub>10</sub> NO <sub>3</sub> PS	[M+H] <sup>+</sup>	244.01918	5.85	2.71
Cyantraniliprole	0.01	C <sub>19</sub> H <sub>14</sub> BrClN <sub>6</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	475.0102	5.17	3.9**
Cyazofamid	0.01	C <sub>13</sub> H <sub>13</sub> ClN <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	325.05205	6.92	3.2
Cyclanilide	0.01	C <sub>11</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	274.00323	5.71	3.25
Cycloate	0.01	C <sub>11</sub> H <sub>21</sub> NOS	[M+H] <sup>+</sup>	216.14166	7.62	3.88
Cyclohexamide	0.01	C <sub>15</sub> H <sub>23</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	282.16998	3.79	0.55
Cycloprothrin	0.01	C <sub>26</sub> H <sub>21</sub> Cl <sub>2</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	482.09204	8.52	6.2**
Cyclosulfamuron	0.01	C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	422.11288	6.36	2.05
Cycloxidim	0.01	C <sub>17</sub> H <sub>27</sub> NO <sub>3</sub> S	[M+H] <sup>+</sup>	326.17844	7.78	3.23
Cycluron	0.01	C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	199.18049	5.12	2.4**
Cyflufenamid	0.01	C <sub>20</sub> H <sub>17</sub> F <sub>5</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	413.1283	7.55	4.7
Cyhalofop-butyl	0.01	C <sub>20</sub> H <sub>20</sub> FNO <sub>4</sub>	[M+H] <sup>+</sup>	358.14491	7.75	3.31
Cymiazole	0.01	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> S	[M+H] <sup>+</sup>	219.09505	3.19	3**
Cymoxanil	0.01	C <sub>7</sub> H <sub>10</sub> N <sub>4</sub> O <sub>3</sub>	C <sub>4</sub> H <sub>6</sub> N <sub>3</sub> O <sub>2</sub> <sup>+</sup>	128.04545	3.66	0.59
Cypermethrin (mixture of isomers)	0.01	C <sub>22</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	416.08148	8.78	6.6
Cyphenothrin	0.01	C <sub>24</sub> H <sub>25</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	376.19072	8.89	6.29
Cyprazine	0.01	C <sub>9</sub> H <sub>14</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	228.10105	5.13	3.06
Cyproconazole (mixture of isomers)	0.01	C <sub>15</sub> H <sub>18</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	292.12112	6.17	2.9
Cyprodinil	0.01	C <sub>14</sub> H <sub>15</sub> N <sub>3</sub>	[M+H] <sup>+</sup>	226.13387	6.48	4
Cyprofuram	0.01	C <sub>14</sub> H <sub>14</sub> ClNO <sub>3</sub>	[M+H] <sup>+</sup>	280.0735	5.23	2.5**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Cyprosulfamide	0.01	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	375.10092	4.73	2.1**
Cyromazine	0.01	C <sub>6</sub> H <sub>10</sub> N <sub>6</sub>	[M+H] <sup>+</sup>	167.10397	0.94	-0.06
Cythioate	0.01	C <sub>8</sub> H <sub>12</sub> NO <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	297.99673	4.41	1.6**
Daimuron	0.01	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	269.16484	6.22	2.7
Daminozide	0.01	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	161.09207	0.9	-1.5
Danitol	0.01	C <sub>22</sub> H <sub>23</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	350.17507	8.59	5.7
Danofloxacin	0.01	C <sub>19</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	358.15615	2.60	-0.3
Dapsone	0.01	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	249.06923	3.02	1
Dazomet	0.01	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	163.03582	2.51	0.63
Dementon- <i>S</i> -methyl sulfone	0.01	C <sub>6</sub> H <sub>15</sub> O <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	263.01713	2.55	-0.3
Demeton O	0.01	C <sub>8</sub> H <sub>19</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	259.0586	/	3.21
Demeton S	0.01	C <sub>8</sub> H <sub>19</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	259.0586	5.51	2.09
Demeton- <i>S</i> -methyl	0.01	C <sub>6</sub> H <sub>15</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	231.0273	4.48	1.02
Deoxynivalenol	0.01	C <sub>15</sub> H <sub>20</sub> O <sub>6</sub>	[M+H] <sup>+</sup>	297.13327	0.93	-0.71
Desethyl atrazine	0.01	C <sub>6</sub> H <sub>10</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	188.06975	3.28	1.51
Desfuoylceftiofur cysteine disulfide (DCCD)	0.01	C <sub>17</sub> H <sub>20</sub> N <sub>6</sub> O <sub>7</sub> S <sub>4</sub>	[M+H] <sup>+</sup>	549.03491	/	-4.2
Desmedipham	0.01	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	301.11828	5.78	3.39
Desmethyl norflurazon	0.01	C <sub>11</sub> H <sub>7</sub> ClF <sub>3</sub> N <sub>3</sub> O	[M+H] <sup>-</sup>	290.03025	4.82	1.6**
Desmethyl-formamido-pirimicarb	0.01	C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	253.12952	4.36	0.9**
Desmetryn	0.01	C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	214.11209	4.36	2.38
Diafenthiuron	0.01	C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> OS	[M+H] <sup>+</sup>	385.23081	8.52	6
Dialifos	0.01	C <sub>14</sub> H <sub>17</sub> ClNO <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	394.00979	7.6	4.69
Diazinon	0.01	C <sub>12</sub> H <sub>21</sub> N <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	305.10833	7.39	3.81

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Diazinon-O-analog	0.01	C <sub>12</sub> H <sub>21</sub> N <sub>2</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	289.13117	5.37	2.07
Dibrom	0.01	C <sub>4</sub> H <sub>7</sub> Br <sub>2</sub> Cl <sub>2</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	380.7876	5.46	1.38
Dichlofenthion	0.01	C <sub>10</sub> H <sub>13</sub> Cl <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	314.97729	8.17	5.14
Dichlormid	0.01	C <sub>8</sub> H <sub>11</sub> Cl <sub>2</sub> NO	[M+H] <sup>+</sup>	208.02905	5.21	1.84
Dichlorvos	0.01	C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	220.95318	4.4	1.43
Diclazuril	0.01	C <sub>17</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	406.98639	6.46	4.1
Diclobutrazol	0.01	C <sub>15</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	328.09779	6.49	3.8
Diclocymet	0.01	C <sub>15</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	313.0869	6.74	4.3**
Diclofénac	0.01	C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	296.02396	6.26	4
Diclosulam	0.01	C <sub>13</sub> H <sub>10</sub> Cl <sub>2</sub> FN <sub>5</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	405.99382	5.5	0.85
Dicrotophos	0.01	C <sub>8</sub> H <sub>16</sub> NO <sub>5</sub> P	[M+H] <sup>+</sup>	238.08389	2.57	0
Diethyl-ethyl	0.01	C <sub>16</sub> H <sub>22</sub> ClNO <sub>3</sub>	[M+H] <sup>+</sup>	312.1361	6.96	3.6
Diethofencarb	0.01	C <sub>14</sub> H <sub>21</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	268.15433	6.01	2.91
Difenoconazole (mixture of isomers)	0.01	C <sub>19</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	406.07197	7.18	4.3
Difenoconazole	0.01	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	287.13902	5.28	2.54
Difloxacin	0.01	C <sub>21</sub> H <sub>19</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	400.14672	3.04	1.6
Diflubenzuron	0.01	C <sub>14</sub> H <sub>9</sub> ClF <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	311.03934	6.43	3.88
Diflufenicen	0.01	C <sub>19</sub> H <sub>11</sub> F <sub>5</sub> N <sub>2</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	395.08135	7.56	4.6**
Dimefox	0.01	C <sub>4</sub> H <sub>12</sub> FN <sub>2</sub> OP	[M+H] <sup>+</sup>	155.07441	2.66	-0.43
Dimefuron	0.01	C <sub>15</sub> H <sub>19</sub> ClN <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	339.12184	5.64	2.51
Dimepiperate	0.01	C <sub>15</sub> H <sub>21</sub> NOS	[M+H] <sup>+</sup>	264.14166	7.7	4.02
Dimethachlor	0.01	C <sub>13</sub> H <sub>18</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	256.10988	5.58	2.17
Dimethametryn	0.01	C <sub>11</sub> H <sub>21</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	256.15904	6.36	3.9

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Dimethenamid	0.01	C <sub>12</sub> H <sub>18</sub> ClNO <sub>2</sub> S	[M+H] <sup>+</sup>	276.08195	6.11	2.15
Dimethirimol	0.01	C <sub>11</sub> H <sub>19</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	210.16009	3.01	1.5**
Dimethoate	0.01	C <sub>5</sub> H <sub>12</sub> NO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	230.0069	3.33	0.78
Dimethomorph	0.01	C <sub>21</sub> H <sub>22</sub> ClNO <sub>4</sub>	[M+H] <sup>+</sup>	388.13101	5.85	2.68
Dimethylvinphos	0.01	C <sub>10</sub> H <sub>10</sub> Cl <sub>3</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	330.94551	6.19	3.13
Dimetilan	0.01	C <sub>10</sub> H <sub>16</sub> N <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	241.12952	3.41	0.27
Dimetridazole	0.01	C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	142.06110	2.36	0.1
Dimoxystrobin	0.01	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	327.17032	6.75	3.9**
Diniconazole (E isomer)	0.01	C <sub>15</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	326.08214	6.82	4.3
Diniconazole (Z isomer)	0.01	C <sub>15</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O	[M-H] <sup>+</sup>	326.08214	6.82	4.3
Dinitramine	0.01	C <sub>11</sub> H <sub>13</sub> F <sub>3</sub> N <sub>4</sub> O <sub>4</sub>	[M+H] <sup>-</sup>	323.09617	7.18	4.3
Dinotefuran	0.01	C <sub>7</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	203.11387	1.83	-0.55
Dioxacarb	0.01	C <sub>11</sub> H <sub>13</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	224.09173	3.37	0.67
Dioxathion (mixture of isomers)	0.01	C <sub>12</sub> H <sub>26</sub> O <sub>6</sub> P <sub>2</sub> S <sub>4</sub>	[M+H] <sup>+</sup>	457.01603	6.02	3
Diphenamid	0.01	C <sub>16</sub> H <sub>17</sub> NO	[M+H] <sup>+</sup>	240.13829	5.62	2.17
Diphenyl phosphate	0.01	C <sub>12</sub> H <sub>11</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	251.04677	8.52	1.4**
Diphenylamine	0.01	C <sub>12</sub> H <sub>11</sub> N	[M+H] <sup>+</sup>	170.09643	6.57	3.5
Dipropetryn	0.01	C <sub>11</sub> H <sub>21</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	256.15904	6.37	3.81
Disosultap	0.01	C <sub>5</sub> H <sub>11</sub> NNa <sub>2</sub> O <sub>6</sub> S <sub>4</sub>	[M+H] <sup>+</sup>	355.93374	/	/
Disulfoton sulfone	0.01	C <sub>8</sub> H <sub>19</sub> O <sub>4</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	307.02559	5.65	1.87
Disulfoton sulfoxide	0.01	C <sub>8</sub> H <sub>19</sub> O <sub>3</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	291.03067	5	1.73
Ditalimfos	0.01	C <sub>12</sub> H <sub>14</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	300.04539	6.63	3.48
Dithianon	0.01	C <sub>14</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	296.9787	6.45	2.84

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Dithiopyr	0.01	C <sub>15</sub> H <sub>16</sub> F <sub>5</sub> NO <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	402.06154	7.82	4.75
Diuron	0.01	C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	233.02429	5.2	2.68
DMA	0.01	C <sub>8</sub> H <sub>11</sub> N	[M+H] <sup>+</sup>	122.09643	2.55	1.8
DMF	0.01	C <sub>9</sub> H <sub>11</sub> NO	[M+H] <sup>+</sup>	150.09134	3.98	1.5
DMPF	0.01	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>	[M+H] <sup>+</sup>	163.12298	2.43	1.7
DMST	0.01	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	215.08488	4.46	1.2**
Dodemorph	0.01	C <sub>18</sub> H <sub>35</sub> NO	[M+H] <sup>+</sup>	282.27914	5.1	5.8**
Dodine	0.01	C <sub>15</sub> H <sub>33</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	288.26455	/	1.15
Doramectin	0.01	C <sub>50</sub> H <sub>74</sub> O <sub>14</sub>	[M+Na] <sup>+</sup>	921.49708	9.18	4.4
Doxycycline	0.01	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>	[M+H] <sup>+</sup>	445.16054	/	/
Dyfonate <sup>TM</sup>	0.01	C <sub>10</sub> H <sub>15</sub> OPS <sub>2</sub>	[M+H] <sup>+</sup>	247.03747	7.39	3.94
Edifenphos	0.01	C <sub>14</sub> H <sub>15</sub> O <sub>2</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	311.03239	6.91	3.48
Emamectin	0.01	C <sub>49</sub> H <sub>75</sub> NO <sub>13</sub>	[M+H] <sup>+</sup>	886.53112	6.92	5
Emamectin B1a	0.01	C <sub>49</sub> H <sub>75</sub> NO <sub>13</sub>	[M+H] <sup>+</sup>	886.53112	8.12	4.1
Empenthrin	0.01	C <sub>18</sub> H <sub>26</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	275.20056	8.82	/
Enrofloxacin	0.01	C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	360.17180	2.71	-0.2
Epi CTC	0.01	C <sub>22</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>8</sub>	[M+H] <sup>+</sup>	479.12157	/	/
Epi OTC	0.01	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub>	[M+H] <sup>+</sup>	461.15546	/	/
Epi tetra	0.01	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>	[M+H] <sup>+</sup>	445.16054	/	/
Epn	0.01	C <sub>14</sub> H <sub>14</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	324.04539	7.56	4.78
Epoxiconazole (iso)	0.01	C <sub>17</sub> H <sub>13</sub> ClFN <sub>3</sub> O	[M+H] <sup>+</sup>	330.08039	6.29	3.44
Eprinomectin	0.01	C <sub>50</sub> H <sub>75</sub> NO <sub>14</sub>	[M+H] <sup>+</sup>	914.52603	8.46	5.7
Eprinomectin B1a	0.01	C <sub>50</sub> H <sub>75</sub> NO <sub>14</sub>	[M+H] <sup>+</sup>	914.52603	8.48	3.8

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
EPTC (S-ethyl dipropylthiocarbamate)	0.01	C <sub>9</sub> H <sub>19</sub> NOS	[M+H] <sup>+</sup>	190.12601	6.91	3.21
Erythromycin	0.01	C <sub>37</sub> H <sub>67</sub> NO <sub>13</sub>	[M+H] <sup>+</sup>	734.46852	4.15	3.06
Erythromycin	0.01	C <sub>37</sub> H <sub>67</sub> NO <sub>13</sub>	[M+H] <sup>+</sup>	734.46852	4.30	2.7
Esbiol	0.01	C <sub>19</sub> H <sub>26</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	303.19547	8.07	/
Esprocarb	0.01	C <sub>15</sub> H <sub>23</sub> NOS	[M+H] <sup>+</sup>	266.15731	8.06	4.6
Etaconazole	0.01	C <sub>14</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	328.06141	6.34	3.1
Ethaboxam	0.01	C <sub>14</sub> H <sub>16</sub> N <sub>4</sub> OS <sub>2</sub>	[M+H] <sup>+</sup>	321.08383	5.1	/
Ethametsulfuron-methyl	0.01	C <sub>15</sub> H <sub>18</sub> N <sub>6</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	411.10813	4.93	1.59
Ethephone	0.01	C <sub>2</sub> H <sub>6</sub> ClO <sub>3</sub> P	[M+H] <sup>+</sup>	144.98159	/	/
Ethidimuron	0.01	C <sub>7</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	265.04236	3.07	/
Ethiofencarb	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub> S	[M+H] <sup>+</sup>	226.08963	5.05	2.04
Ethiofencarb sulfone	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>4</sub> S	[M+H] <sup>+</sup>	258.07946	3.03	/
Ethiofencarb sulfoxide	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>3</sub> S	[M+H] <sup>+</sup>	242.08454	2.95	/
Ethion	0.01	C <sub>9</sub> H <sub>22</sub> O <sub>4</sub> P <sub>2</sub> S <sub>4</sub>	[M+H] <sup>+</sup>	384.9949	8.22	5.07
Ethiozin	0.01	C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> OS	[M+H] <sup>+</sup>	229.11176	5.19	2.08
Ethiprole	0.01	C <sub>13</sub> H <sub>9</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>4</sub> OS	[M-H] <sup>-</sup>	396.9899	5.85	2.9
Ethirimol	0.01	C <sub>11</sub> H <sub>19</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	210.16009	3.07	2.22
Ethofenprox	0.01	C <sub>25</sub> H <sub>28</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	377.21112	/	7.05
Ethofumesate	0.01	C <sub>13</sub> H <sub>18</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	287.09477	6.28	2.7
Ethoprophos (prophos)	0.01	C <sub>8</sub> H <sub>19</sub> O <sub>2</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	243.06369	6.38	3.59
Ethoxyquin	0.01	C <sub>14</sub> H <sub>19</sub> NO	[M+H] <sup>+</sup>	218.15394	6.19	4.05
Ethoxysulfuron	0.01	C <sub>15</sub> H <sub>18</sub> N <sub>4</sub> O <sub>7</sub> S	[M+H] <sup>+</sup>	399.0969	6.07	/
Ethyclozate	0.01	C <sub>11</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	239.05818	5.28	/



<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Etobenzanid	0.01	C <sub>16</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	340.05018	7.25	/
Etoxazole	0.01	C <sub>21</sub> H <sub>23</sub> F <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	360.17696	8.46	5.59
Etrimfos	0.01	C <sub>10</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub> PS	[M+H] <sup>+</sup>	293.07194	7.21	/
Famoxadone	0.01	C <sub>22</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	375.13393	7.21	4.65
Famphur	0.01	C <sub>10</sub> H <sub>16</sub> NO <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	326.02803	5.8	2.2
Fenamidone	0.01	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> OS	[M+H] <sup>+</sup>	312.11651	6.19	2.8
Fenamiphos	0.01	C <sub>13</sub> H <sub>22</sub> NO <sub>3</sub> PS	[M+H] <sup>+</sup>	304.11308	6.17	3.23
Fenamiphos sulfone	0.01	C <sub>13</sub> H <sub>22</sub> NO <sub>5</sub> PS	[M+H] <sup>+</sup>	336.10291	4.58	/
Fenamiphos sulfoxide	0.01	C <sub>13</sub> H <sub>22</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	320.108	4.04	/
Fenarimol	0.01	C <sub>17</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	331.03995	6.17	3.6
Fenazaflor	0.01	C <sub>15</sub> H <sub>7</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	374.99094	/	/
Fenazaquin	0.01	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	307.18049	8.51	5.51
Fenazox	0.01	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	199.08659	7.02	#N/A
Fenbendazole	0.01	C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	300.08013	5.45	3.6
Fenbuconazole	0.01	C <sub>19</sub> H <sub>17</sub> ClN <sub>4</sub>	[M+H] <sup>+</sup>	337.12145	6.5	3.23
Fenchlorazol-ethyl	0.01	C <sub>12</sub> H <sub>8</sub> Cl <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	403.91031	7.51	/
Fenchlorphos-oxon	0.01	C <sub>8</sub> H <sub>8</sub> Cl <sub>3</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	304.92986	6.17	/
Fenclorim	0.01	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	[M+H] <sup>+</sup>	224.99808	/	4.2**
Fenfuram	0.01	C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	202.08626	5.14	2.2**
Fenhexamid	0.01	C <sub>14</sub> H <sub>17</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	302.07091	6.31	3.51
Fenitrothion	0.01	C <sub>9</sub> H <sub>12</sub> NO <sub>5</sub> PS	[M+H] <sup>+</sup>	278.02466	6.58	3.3
Fenobucarb	0.01	C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	208.13321	5.87	2.78
Fenothiocarb	0.01	C <sub>13</sub> H <sub>19</sub> NO <sub>2</sub> S	[M+H] <sup>+</sup>	254.12093	6.76	3.3

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Fenoxanil	0.01	C <sub>15</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	329.08181	6.89	4.5
Fenoxaprop	0.01	C <sub>16</sub> H <sub>12</sub> ClNO <sub>5</sub>	[M+H] <sup>+</sup>	334.04768	6.22	3.4**
Fenoxaprop-P-ethyl	0.01	C <sub>18</sub> H <sub>16</sub> ClNO <sub>5</sub>	[M+H] <sup>+</sup>	362.07898	7.7	4.1**
Fenoxycarb	0.01	C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	302.13868	5.94	4.3
Fenpiclonil	0.01	C <sub>11</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub>	[M+H] <sup>+</sup>	236.99808	5.72	4.3**
Fenpropathrin	0.01	C <sub>22</sub> H <sub>23</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	350.17507	8.6	6
Fenpropidin	0.01	C <sub>19</sub> H <sub>31</sub> N	[M+H] <sup>+</sup>	274.25293	5.25	5.5
Fenpropimorph	0.01	C <sub>20</sub> H <sub>33</sub> NO	[M+H] <sup>+</sup>	304.26349	5.34	4.93
Fenpyroximate	0.01	C <sub>24</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	422.20743	8.46	5.01
Fensulfothion	0.01	C <sub>11</sub> H <sub>17</sub> O <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	309.03787	5.37	2.23
Fensulfothion-oxon	0.01	C <sub>11</sub> H <sub>17</sub> O <sub>5</sub> PS	[M+H] <sup>+</sup>	293.06071	3.56	1.4**
Fensulfothion-oxon sulfone	0.01	C <sub>11</sub> H <sub>17</sub> O <sub>6</sub> PS	[M+H] <sup>+</sup>	309.05563	4.11	1.5**
Fensulfothion sulfone	0.01	C <sub>11</sub> H <sub>17</sub> O <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	325.03278	5.94	2.6**
Fenthion	0.01	C <sub>10</sub> H <sub>15</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	279.0273	7.14	4.1
Fenthion-oxon	0.01	C <sub>10</sub> H <sub>15</sub> O <sub>4</sub> PS	[M+H] <sup>+</sup>	263.05015	5.37	2.4**
Fenthion-oxon sulfoxide	0.01	C <sub>10</sub> H <sub>15</sub> O <sub>5</sub> PS	[M+H] <sup>+</sup>	279.04506	3.03	1**
Fenthion sulfoxide	0.01	C <sub>10</sub> H <sub>15</sub> O <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	295.02222	4.76	2.7**
Fenthion-ethyl	0.01	C <sub>12</sub> H <sub>19</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	307.0586	7.86	5**
Fenthion sulfone	0.01	C <sub>10</sub> H <sub>15</sub> O <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	311.01713	5.41	2.8**
Fenthoxon sulfone	0.01	C <sub>10</sub> H <sub>15</sub> O <sub>6</sub> PS	[M+H] <sup>+</sup>	295.03998	3.57	1.1**
Fentin acetate as Fentin	0.01	C <sub>20</sub> H <sub>18</sub> O <sub>2</sub> Sn	[M+H] <sup>+</sup>	411.04016	/	3.43
Fenuron	0.01	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	165.10224	3.19	0.98
Ferimzone	0.01	C <sub>15</sub> H <sub>18</sub> N <sub>4</sub>	[M+H] <sup>+</sup>	255.16042	4.37	3.5**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Fipronil	0.01	C <sub>12</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>4</sub> OS	[M+H] <sup>-</sup>	436.94598	6.87	4
Fipronil sulfide	0.01	C <sub>12</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>4</sub> S	[M-H] <sup>-</sup>	420.95107	7.3	5.5**
Fipronil-desulfinyl	0.01	C <sub>12</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>4</sub>	[M+H] <sup>-</sup>	388.979	7.05	4.6**
Flamprop-isopropyl	0.01	C <sub>19</sub> H <sub>19</sub> ClFNO <sub>3</sub>	[M+H] <sup>+</sup>	364.11103	7.25	4**
Flamprop-methyl (Metaven)	0.01	C <sub>17</sub> H <sub>15</sub> ClFNO <sub>3</sub>	[M+H] <sup>+</sup>	336.07973	6.47	3.2**
Flamprop-M-isopropyl	0.01	C <sub>19</sub> H <sub>19</sub> ClFNO <sub>3</sub>	[M+H] <sup>+</sup>	364.11103	7.25	4**
Flazasulfuron	0.01	C <sub>13</sub> H <sub>12</sub> F <sub>3</sub> N <sub>5</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	408.0584	5.48	1.08
Fleroxacin	0.01	C <sub>17</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	370.13730	2.43	-0.1
Flonicamid	0.01	C <sub>9</sub> H <sub>6</sub> F <sub>3</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	230.05357	2.71	0.3
Florasulam	0.01	C <sub>12</sub> H <sub>8</sub> F <sub>3</sub> N <sub>5</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	360.03727	4.63	1.22
Florfenicol	0.01	C <sub>12</sub> H <sub>14</sub> Cl <sub>2</sub> FNO <sub>4</sub> S	[M+H] <sup>+</sup>	375.03429	3.33	0.8
Florfenicol amine	0.01	C <sub>10</sub> H <sub>14</sub> FNO <sub>3</sub> S	[M+H] <sup>+</sup>	270.05706	/	/
Fluacrypyrim	0.01	C <sub>20</sub> H <sub>21</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	427.14753	7.64	4.1**
Fluazifop	0.01	C <sub>15</sub> H <sub>12</sub> F <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	328.07912	5.77	2.9**
Fluazifop-butyl	0.01	C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	384.14172	8.04	4.5
Fluazifop-P-butyl	0.01	C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	384.14172	8.03	4.5**
Fluazinam	0.01	C <sub>13</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>4</sub> O <sub>4</sub>	[M-H] <sup>-</sup>	464.95866	7.9	4.01
Fluazuron	0.01	C <sub>20</sub> H <sub>10</sub> Cl <sub>2</sub> F <sub>5</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	506.00921	7.89	6.1**
Flubendazole	0.01	C <sub>16</sub> H <sub>12</sub> FN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	314.09355	4.68	2.9
Flubendiamide	0.01	C <sub>23</sub> H <sub>22</sub> F <sub>7</sub> IN <sub>2</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	683.03061	6.88	4.2
Flucarbazone sodium	0.01	C <sub>12</sub> H <sub>10</sub> F <sub>3</sub> N <sub>4</sub> NaO <sub>6</sub> S	[M+H] <sup>+</sup>	419.02436	4.21	-1.85
Fluchloralin	0.01	C <sub>12</sub> H <sub>13</sub> ClF <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	356.06195	7.69	5.07
Flucycloxuron	0.01	C <sub>25</sub> H <sub>20</sub> ClF <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	484.1234	8.11	6.1**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Flucythrinate	0.01	C <sub>26</sub> H <sub>23</sub> F <sub>2</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	452.16679	/	6.2
Fludioxonil	0.01	C <sub>12</sub> H <sub>6</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	249.04701	8.21	4.12
Flufenacet	0.01	C <sub>14</sub> H <sub>13</sub> F <sub>4</sub> N <sub>3</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	364.07374	6.7	3.2
Flufenoxuron	0.01	C <sub>21</sub> H <sub>11</sub> ClF <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	489.04352	8.09	6.16
Flumequine	0.01	C <sub>14</sub> H <sub>12</sub> FNO <sub>3</sub>	[M+H] <sup>+</sup>	262.08740	4.73	2.9
Flumestulam	0.01	C <sub>12</sub> H <sub>9</sub> F <sub>2</sub> N <sub>5</sub> O <sub>2</sub> S	[M-H] <sup>-</sup>	326.05178	7.76	0.21
Flumetralin	0.01	C <sub>16</sub> H <sub>12</sub> ClF <sub>4</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	422.05252	8.23	5.2**
Flumiclorac-pentyl	0.01	C <sub>21</sub> H <sub>23</sub> ClFNO <sub>5</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	441.1587	7.88	4.8**
Flumioxazin	0.01	C <sub>19</sub> H <sub>15</sub> FN <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	355.10886	5.84	2.55
Flumorph	0.01	C <sub>21</sub> H <sub>22</sub> FNO <sub>4</sub>	[M+H] <sup>+</sup>	372.16056	5.3	3.4**
Flunixin	0.01	C <sub>14</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	297.08454	5.71	4.1
Fluoglycofene-ethyl	0.01	C <sub>18</sub> H <sub>13</sub> ClF <sub>3</sub> NO <sub>7</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	465.06709	7.69	3.6**
Fluometuron	0.01	C <sub>10</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O	[M-H] <sup>-</sup>	233.08962	5	2.42
Fluopicolide	0.01	C <sub>14</sub> H <sub>8</sub> Cl <sub>3</sub> F <sub>3</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	382.97271	6.41	3.26
Fluopyram	0.01	C <sub>16</sub> H <sub>11</sub> ClF <sub>6</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	397.05369	6.46	4.5**
Fluorodifen	0.01	C <sub>13</sub> H <sub>7</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	329.03798	7.01	3.7**
Fluotrimazol	0.01	C <sub>22</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub>	[M+H] <sup>+</sup>	380.13691	/	5.7**
Fluoxastrobin	0.01	C <sub>21</sub> H <sub>16</sub> ClFN <sub>4</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	459.0866	6.69	2.86
Flupyradifurone	0.01	C <sub>12</sub> H <sub>11</sub> ClF <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	289.05499	3.72	2.3**
Flupyrsulfuron-methyl sodium	0.01	C <sub>15</sub> H <sub>13</sub> F <sub>3</sub> N <sub>5</sub> NaO <sub>7</sub> S	[M+H] <sup>+</sup>	488.04583	5.79	/
Fluquinconazole	0.01	C <sub>16</sub> H <sub>8</sub> Cl <sub>2</sub> FN <sub>5</sub> O	[M+H] <sup>+</sup>	376.01627	6.34	3.24
Fluralaner	0.01	C <sub>22</sub> H <sub>17</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	556.06239	7.39	5.6
Flurenol-butyl	0.01	C <sub>18</sub> H <sub>18</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	283.13287	/	3.6**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Flurenol-methyl	0.01	C <sub>15</sub> H <sub>12</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	241.08592	4.36	2.3**
Fluridone	0.01	C <sub>19</sub> H <sub>14</sub> F <sub>3</sub> NO	[M+H] <sup>+</sup>	330.11003	5.86	1.87
Flurilazole	0.01	C <sub>11</sub> H <sub>13</sub> Cl <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	278.03453	3.66	2**
Flurochloridon (ISO)	0.01	C <sub>12</sub> H <sub>10</sub> Cl <sub>2</sub> F <sub>3</sub> NO	[M+H] <sup>+</sup>	312.01643	6.56	3.4**
Fluroxypyr	0.01	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> FN <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	254.9734	4.03	2.2
Fluroxypyr-meptyl	0.01	C <sub>15</sub> H <sub>21</sub> Cl <sub>2</sub> FN <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	367.0986	8.43	5.4**
Flurprimidol	0.01	C <sub>15</sub> H <sub>15</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	313.11584	5.92	3.3**
Flurtamone	0.01	C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> NO <sub>2</sub>	[M+H] <sup>-</sup>	334.10494	5.95	4.5**
Flusilazole	0.01	C <sub>16</sub> H <sub>15</sub> F <sub>2</sub> N <sub>3</sub> Si	[M+H] <sup>+</sup>	316.10761	6.51	3.7
Fluthiacet-methyl	0.01	C <sub>15</sub> H <sub>15</sub> ClFN <sub>3</sub> O <sub>3</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	404.03002	6.92	3.77
Flutolanil	0.01	C <sub>17</sub> H <sub>16</sub> F <sub>3</sub> NO <sub>2</sub>	[M+H] <sup>-</sup>	324.12059	6.56	3.7
Flutriafol	0.01	C <sub>16</sub> H <sub>13</sub> F <sub>2</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	302.10995	4.98	2.29
Fomesafen	0.01	C <sub>15</sub> H <sub>10</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>6</sub> S	[M-H] <sup>-</sup>	456.02385	6.13	2.4**
Foramsulfuron	0.01	C <sub>17</sub> H <sub>20</sub> N <sub>6</sub> O <sub>7</sub> S	[M+H] <sup>+</sup>	453.1187	4.2	0.17
Forchlorfenuron	0.01	C <sub>12</sub> H <sub>10</sub> ClN <sub>3</sub> O	[M-H] <sup>-</sup>	248.05852	4.95	3.2
Formetanate HCl	0.01	C <sub>11</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	222.1237	0.95	/
Fosthiazate	0.01	C <sub>9</sub> H <sub>18</sub> NO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	284.05385	5.05	1.68
Fuberidazole	0.01	C <sub>11</sub> H <sub>8</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	185.07094	2.55	2.67
Furalaxyl	0.01	C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	302.13868	5.94	2.61
Furathiocarb	0.01	C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	383.16352	7.97	4.7
Furmecyclox	0.01	C <sub>14</sub> H <sub>21</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	252.15942	6.94	3.1**
Fusidic acid	0.01	C <sub>31</sub> H <sub>48</sub> O <sub>6</sub>	[M+H] <sup>-</sup>	534.37892	7.46	5.5
Gamithromycin	0.01	C <sub>40</sub> H <sub>76</sub> N <sub>2</sub> O <sub>12</sub>	[M+H] <sup>+</sup>	777.54710	3.89	4.9

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Guthion-ethyl	0.01	C <sub>12</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	346.04435	6.67	3.4**
Guthion®	0.01	C <sub>10</sub> H <sub>12</sub> N <sub>3</sub> O <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	318.01305	5.92	2.75
Halofenozide	0.01	C <sub>18</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	331.12078	5.99	3.22
Halofuginone	0.01	C <sub>16</sub> H <sub>17</sub> BrClN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	414.02146	3.40	1.4
Halosulfuron-methyl	0.01	C <sub>13</sub> H <sub>15</sub> ClN <sub>6</sub> O <sub>7</sub> S	[M+H] <sup>+</sup>	435.04842	6.05	1.3**
Haloxyfop	0.01	C <sub>15</sub> H <sub>11</sub> ClF <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	362.04015	6.47	4.2**
Haloxyfop-2-ethoxyethyl	0.01	C <sub>19</sub> H <sub>19</sub> ClF <sub>3</sub> NO <sub>5</sub>	[M+H] <sup>+</sup>	434.09766	7.81	4.7**
Haloxyfop-methyl	0.01	C <sub>16</sub> H <sub>13</sub> ClF <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	376.0558	7.51	4.5**
Haloxyfop-P-methyl	0.01	C <sub>16</sub> H <sub>13</sub> ClF <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	376.0558	7.52	4.5**
Heptenophos	0.01	C <sub>9</sub> H <sub>12</sub> ClO <sub>4</sub> P	[M+H] <sup>+</sup>	251.02345	5.31	2.32
Hexaconazole	0.01	C <sub>14</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	314.08214	6.52	3.9
Hexaflumuron	0.01	C <sub>16</sub> H <sub>8</sub> Cl <sub>2</sub> F <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>-</sup>	460.98889	7.37	5.68
Hexazinone	0.01	C <sub>12</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	253.1659	4.13	1.85
Hexythiazox	0.01	C <sub>17</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	353.1085	8.23	5.57
HMMNI	0.01	C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	175.08257	1.81	-0.4
Hydroxy-flubendazole	0.01	C <sub>16</sub> H <sub>14</sub> FN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	316.10920	3.56	1.9
Hydroxy-mebendazole	0.01	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	298.11862	3.30	2.3
Hydroxy-thiabendazole	0.01	C <sub>10</sub> H <sub>7</sub> N <sub>3</sub> OS	[M+H] <sup>+</sup>	218.03826	1.84	2.1
Hymexazole	0.01	C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	100.0393	1.73	0.1**
Imazalil	0.01	C <sub>14</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	297.0556	4.47	3.82
Imazamethabenz-methyl	0.01	C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	289.15467	4.14	2.6**
Imazamox	0.01	C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	306.14483	3.19	0.73
Imazapic	0.01	C <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	276.13427	3.3	0.39

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Imazaquin	0.01	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	312.13427	4.45	2.5**
Imazethapyr	0.01	C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	290.14992	3.95	1
Imazosulfuron	0.01	C <sub>14</sub> H <sub>13</sub> ClN <sub>6</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	413.04294	5.53	1.49
Imibenconazole	0.01	C <sub>17</sub> H <sub>13</sub> Cl <sub>3</sub> N <sub>4</sub> S	[M+H] <sup>-</sup>	410.99993	7.69	5.8**
Imidacloprid	0.01	C <sub>9</sub> H <sub>10</sub> ClN <sub>5</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	256.05958	3.19	0.57
Imidacloprid-olefin	0.01	C <sub>9</sub> H <sub>8</sub> ClN <sub>5</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	254.04393	2.6	2**
Imidocarb dipropionate	0.01	C <sub>25</sub> H <sub>32</sub> N <sub>6</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	497.25069	/	/
Imiprothrin (mixture of isomers)	0.01	C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	319.16523	6.51	2.9
Inabenfide	0.01	C <sub>19</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	339.08948	5.55	3.7**
Indanofan	0.01	C <sub>20</sub> H <sub>17</sub> ClO <sub>3</sub>	[M+H] <sup>+</sup>	341.0939	5.47	4.1**
Indaziflam	0.01	C <sub>16</sub> H <sub>20</sub> FN <sub>5</sub>	[M+H] <sup>+</sup>	302.17755	5.78	3.2**
Indoxacarb	0.01	C <sub>22</sub> H <sub>17</sub> ClF <sub>3</sub> N <sub>3</sub> O <sub>7</sub>	[M+H] <sup>+</sup>	528.07799	7.52	4.65
Iodofenphos	0.01	C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> IO <sub>3</sub> PS	[M+H] <sup>+</sup>	412.84264	8.14	5.51
Iodosulfuron-methyl sodium	0.01	C <sub>14</sub> H <sub>13</sub> IN <sub>5</sub> NaO <sub>6</sub> S	[M+H] <sup>+</sup>	529.96018	5.57	/
Ipreconazole	0.01	C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	321.21727	6.08	4.1**
Iprobenfos	0.01	C <sub>13</sub> H <sub>21</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	289.10218	6.61	3
Iprodione	0.01	C <sub>13</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	330.04067	6.49	3.34
Ipronidazole	0.01	C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	170.09240	3.79	1.1
Ipronidazole OH	0.01	C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	186.08732	2.79	-0.5
Iprovalicarb	0.01	C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	321.21727	6.14	3.37**
Irgarol (cybutryne)	0.01	C <sub>11</sub> H <sub>19</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	254.14339	5.99	3.95
Isazophos	0.01	C <sub>9</sub> H <sub>17</sub> ClN <sub>3</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	314.04896	6.89	3.82
Isocarbamide	0.01	C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	186.1237	3.14	0.8**

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Isofenphos	0.01	C <sub>15</sub> H <sub>24</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	346.12365	7.64	4.12
Isofenphos-methyl	0.01	C <sub>14</sub> H <sub>22</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	332.108	7.27	3.8**
Isofenphos-oxon	0.01	C <sub>15</sub> H <sub>24</sub> NO <sub>5</sub> P	[M+H] <sup>+</sup>	330.14649	6.02	2.4**
Isomethiozin	0.01	C <sub>12</sub> H <sub>20</sub> N <sub>4</sub> OS	[M+H] <sup>+</sup>	269.14306	6.2	3.5**
Isonoruron	0.01	C <sub>13</sub> H <sub>22</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	223.18049	5.46	2.3**
Isoprocarb	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	194.11756	5.34	2.31
Isopropalin	0.01	C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	310.17613	8.73	5.6**
Isoprothiolane	0.01	C <sub>12</sub> H <sub>18</sub> O <sub>4</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	291.07193	6.59	2.88
Isoproturon	0.01	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	207.14919	5.19	2.87
Isouron	0.01	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	212.13935	4.34	1.6**
Isoxaben	0.01	C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	333.18088	6.4	3.94
Isoxadifen-ethyl	0.01	C <sub>18</sub> H <sub>17</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	296.12812	7.03	3.5
Isoxaflutole	0.01	C <sub>15</sub> H <sub>12</sub> F <sub>3</sub> NO <sub>4</sub> S	[M+H] <sup>+</sup>	360.05119	6	2.32
Isoxathion	0.01	C <sub>13</sub> H <sub>16</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	314.06104	7.53	3.73
Ivermectin	0.01	C <sub>48</sub> H <sub>74</sub> O <sub>14</sub>	[M+Na] <sup>+</sup>	897.49708	9.69	5.83
Ivermectin B1a	0.01	C <sub>48</sub> H <sub>74</sub> O <sub>14</sub>	[M+Na] <sup>+</sup>	875.51513	9.74	3.8
Josamycin	0.01	C <sub>42</sub> H <sub>69</sub> NO <sub>15</sub>	[M+H] <sup>+</sup>	828.47400	5.49	2.9
Karbutilate	0.01	C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	280.16557	4.62	1.7**
Ketoprofen	0.01	C <sub>16</sub> H <sub>14</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	255.10157	5.26	3.12
Ketotriclabendazole	0.01	C <sub>13</sub> H <sub>7</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	328.96459	5.90	4
Kresoxim-methyl	0.01	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	314.13868	6.86	3.4
Lactofen	0.01	C <sub>19</sub> H <sub>15</sub> ClF <sub>3</sub> NO <sub>7</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	479.08274	7.97	4.81
Lambda cyhalothrin	0.01	C <sub>23</sub> H <sub>19</sub> ClF <sub>3</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	450.10783	/	7



<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Lasalocid A	0.01	C <sub>34</sub> H <sub>54</sub> O <sub>8</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	608.41569	9.37	6.4
Lenacil	0.01	C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	235.1441	4.59	1.7**
Leptophos	0.01	C <sub>13</sub> H <sub>10</sub> BrCl <sub>2</sub> O <sub>2</sub> PS	[M+H] <sup>+</sup>	412.87485	8.86	6.3**
Levamisole	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> S	[M+H] <sup>+</sup>	205.07940	2.07	1.8
Levofloxacin	0.01	C <sub>18</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	362.15106	2.32	-0.39
Lincomycin	0.01	C <sub>18</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	407.22104	0.95	0.2
Linuron	0.01	C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	249.01921	5.96	3.2
Lomefloxacin	0.01	C <sub>17</sub> H <sub>19</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	352.14672	2.58	-0.8
Lontrel (clopyralid)	0.01	C <sub>6</sub> H <sub>3</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	191.96136	/	1.06
Lufenuron	0.01	C <sub>17</sub> H <sub>8</sub> Cl <sub>2</sub> F <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	510.9857	7.89	5.12
Maduramicin	0.01	C <sub>47</sub> H <sub>83</sub> NO <sub>17</sub>	[M+H] <sup>+</sup>	934.57338	10.58	4.3
Magnamycin A	0.01	C <sub>42</sub> H <sub>67</sub> NO <sub>16</sub>	[M+H] <sup>+</sup>	842.45326	/	/
Malaaxon	0.01	C <sub>10</sub> H <sub>19</sub> O <sub>7</sub> PS	[M+H] <sup>+</sup>	315.06619	4.68	0.6**
Malathion	0.01	C <sub>10</sub> H <sub>19</sub> O <sub>6</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	331.04335	6.53	2.36
Mandipropamid	0.01	C <sub>23</sub> H <sub>22</sub> ClNO <sub>4</sub>	[M+H] <sup>+</sup>	412.13101	6.23	3.2
Marbofloxacin	0.01	C <sub>17</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	363.14631	2.31	-0.5
Mebendazole	0.01	C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	296.10297	4.48	2.8
Mecarbam	0.01	C <sub>10</sub> H <sub>20</sub> NO <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	330.05933	6.84	2.29
Mefenacet	0.01	C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	299.08488	6.26	3.23
Mefenamic acid	0.01	C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub>	[M-H] <sup>-</sup>	242.11756	6.83	5.1
Mefenpyr-diethyl	0.01	C <sub>16</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	373.07164	7.41	3.9**
Mefluidide	0.01	C <sub>11</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	311.06718	4.61	2.02
Meloxicam	0.01	C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	352.04203	5.49	3

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Mepanipyrim	0.01	C <sub>14</sub> H <sub>13</sub> N <sub>3</sub>	[M+H] <sup>+</sup>	224.11822	6.46	3.28
Mephosfolan	0.01	C <sub>8</sub> H <sub>16</sub> NO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	270.0382	4.27	1**
Mepiquat chloride	0.01	C <sub>7</sub> H <sub>16</sub> ClN	[M+H] <sup>+</sup>	150.1044	/	-2.82
Mepronil	0.01	C <sub>17</sub> H <sub>19</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	270.14886	6.49	3.66
Mesosulfuron-methyl	0.01	C <sub>17</sub> H <sub>21</sub> N <sub>5</sub> O <sub>9</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	504.08535	4.96	-0.48
Mesotrione	0.01	C <sub>14</sub> H <sub>13</sub> NO <sub>7</sub> S	[M+H] <sup>+</sup>	340.04855	4.34	0.9
Metaflumizone	0.01	C <sub>24</sub> H <sub>16</sub> F <sub>6</sub> N <sub>4</sub> O <sub>2</sub>	[M-H] <sup>-</sup>	507.12502	7.8	6.2**
Metalaxyl	0.01	C <sub>15</sub> H <sub>21</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	280.15433	5.21	1.65
Metalaxyl-M	0.01	C <sub>15</sub> H <sub>21</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	280.15433	5.21	1.6**
Metamitron	0.01	C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O	[M+H] <sup>+</sup>	203.09274	3.03	0.83
Metazachlor	0.01	C <sub>14</sub> H <sub>16</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	278.10547	5.48	2.7**
Metconazole	0.01	C <sub>17</sub> H <sub>22</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	320.15242	6.75	3.85
Methabenzthiazuron	0.01	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> OS	[M+H] <sup>+</sup>	222.06956	4.89	2.64
Methacrifos	0.01	C <sub>7</sub> H <sub>13</sub> O <sub>5</sub> PS	[M+H] <sup>+</sup>	241.02941	5.91	1.9**
Methamidophos	0.01	C <sub>2</sub> H <sub>8</sub> NO <sub>2</sub> PS	[M+H] <sup>+</sup>	142.00862	0.92	-0.8
Methazine	0.01	C <sub>11</sub> H <sub>19</sub> N <sub>7</sub>	[M+H] <sup>+</sup>	250.17747	/	/
Methfuroxam	0.01	C <sub>14</sub> H <sub>15</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	230.11756	5.91	3**
Methidathion	0.01	C <sub>6</sub> H <sub>11</sub> N <sub>2</sub> O <sub>4</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	302.96914	5.87	2.2
Methiocarb	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub> S	C <sub>9</sub> H <sub>13</sub> OS <sup>+</sup>	169.06816	5.82	2.92
Methiocarb sulfone	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>4</sub> S	[M+H] <sup>+</sup>	258.07946	3.67	1.6**
Methiocarb sulfoxide	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>3</sub> S	[M+H] <sup>+</sup>	242.08454	2.96	1.5**
Methomyl	0.01	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	163.05358	/	0.6
Methomyl oxime	0.01	C <sub>3</sub> H <sub>7</sub> NOS	[M+H] <sup>+</sup>	106.03211	/	0.2**

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Methoprotryne	0.01	C <sub>11</sub> H <sub>21</sub> N <sub>5</sub> OS	[M+H] <sup>+</sup>	272.15396	5.09	2.82
Methoxyfenozide	0.01	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>-</sup>	313.15467	6.43	3.7
Methyl paraoxon	0.01	C <sub>8</sub> H <sub>10</sub> NO <sub>6</sub> P	[M+H] <sup>+</sup>	248.03185	4.27	1.3**
Methyl parathion	0.01	C <sub>8</sub> H <sub>10</sub> NO <sub>5</sub> PS	[M+H] <sup>+</sup>	264.00901	6.25	2.86
Metobromuron	0.01	C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	259.00767	5.34	2.38
Metolachlor	0.01	C <sub>15</sub> H <sub>22</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	284.14118	6.71	3.13
Metolcarb	0.01	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	166.08626	4.32	1.7
(E)-Metominostrobin	0.01	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	285.12337	5.52	3.2**
(Z)-Metominostrobin	0.01	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	285.12337	5.58	3.2**
Metosulam	0.01	C <sub>14</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>5</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	418.01381	5.02	3.08
Metoxuron	0.01	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	229.07383	3.99	1.6**
Metrafenone	0.01	C <sub>19</sub> H <sub>21</sub> BrO <sub>5</sub>	[M+H] <sup>+</sup>	409.06451	7.65	4.6**
Metribuzin	0.01	C <sub>8</sub> H <sub>14</sub> N <sub>4</sub> OS	[M+H] <sup>+</sup>	215.09611	4.49	1.7
Metronidazole	0.01	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	172.07167	1.86	0
Metronidazole OH	0.01	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	188.06658	0.95	/
Metsulfuron-methyl	0.01	C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	382.08158	4.55	2.2
Mevinphos	0.01	C <sub>7</sub> H <sub>13</sub> O <sub>6</sub> P	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> P <sup>+</sup>	193.02604	3.54	0.13
Mexacarbate	0.01	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	223.1441	3.48	2.56
MGK-264 (mixture of isomers)	0.01	C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	276.19581	7.42	3.7
Molinate	0.01	C <sub>9</sub> H <sub>17</sub> NOS	[M+H] <sup>+</sup>	188.11036	6.31	3.21
Monensin	0.01	C <sub>36</sub> H <sub>62</sub> O <sub>11</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	688.46304	9.94	4.2
Monepantel	0.01	C <sub>20</sub> H <sub>13</sub> F <sub>6</sub> N <sub>3</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	474.07054	7.23	5.2
Monepantel sulfone	0.01	C <sub>20</sub> H <sub>13</sub> F <sub>6</sub> N <sub>3</sub> O <sub>4</sub> S	[M-H] <sup>-</sup>	506.06037	6.85	3.9

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Monocrotophos	0.01	C <sub>7</sub> H <sub>14</sub> NO <sub>5</sub> P	[M+H] <sup>+</sup>	224.06824	2.29	-0.2
Monolinuron	0.01	C <sub>9</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	215.05818	5.14	2.3
Monuron	0.01	C <sub>9</sub> H <sub>11</sub> ClN <sub>2</sub> O	[M+H] <sup>+</sup>	199.06327	4.31	1.94
Morantel	0.01	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> S	[M+H] <sup>+</sup>	221.11070	3.07	1.9
Morpholine	0.01	C <sub>4</sub> H <sub>9</sub> NO	[M+H] <sup>+</sup>	88.07569	/	-0.86
Moxidectin	0.01	C <sub>37</sub> H <sub>53</sub> NO <sub>8</sub>	[M+H] <sup>+</sup>	640.38439	9.31	4.3
N,N-Diethyl- <i>m</i> -toluamide (DEET)	0.01	C <sub>12</sub> H <sub>17</sub> NO	[M+H] <sup>+</sup>	192.13829	5.23	2.02
N,N'-Ethylenethiourea	0.01	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S	[M+H] <sup>+</sup>	103.03245	0.9	-0.5
Nafcillin	0.01	C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S	[M-H] <sup>-</sup>	415.13222	5.22	2.9
Nalidixic acid	0.01	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	233.09207	4.68	/
Naphthalophos (naftalofos)	0.01	C <sub>16</sub> H <sub>16</sub> NO <sub>6</sub> P	[M+H] <sup>+</sup>	350.0788	5.76	2.4**
Napropamide	0.01	C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	272.16451	6.49	3.36
Naproxen	0.01	C <sub>14</sub> H <sub>14</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	231.10157	5.35	3.3
Naptalam	0.01	C <sub>18</sub> H <sub>13</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	292.09682	4.49	3.5**
Narasin	0.01	C <sub>43</sub> H <sub>72</sub> O <sub>11</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	782.54129	10.37	6.2
Neburon	0.01	C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	275.07125	6.8	4.1
Neospiramycin	0.01	C <sub>36</sub> H <sub>62</sub> N <sub>2</sub> O <sub>11</sub>	[M+H] <sup>+</sup>	716.46919	/	/
Nereistoxin oxalate	0.01	C <sub>7</sub> H <sub>13</sub> NO <sub>4</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	240.03588	/	/
Nicarbazin (DNC)	0.01	C <sub>19</sub> H <sub>18</sub> N <sub>6</sub> O <sub>6</sub>	[M+H] <sup>+</sup>	444.16261	/	/
Nicosulfuron	0.01	C <sub>15</sub> H <sub>18</sub> N <sub>6</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	411.10813	4.05	/
Nigericin	0.01	C <sub>40</sub> H <sub>68</sub> O <sub>11</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	742.50999	10.84	4.3
Nitenpyram (ISO)	0.01	C <sub>11</sub> H <sub>15</sub> ClN <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	271.09563	2.25	-0.66
Nitralin	0.01	C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	346.10673	6.84	3.7**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Nitrapyrin (2-chloro-6-(trichloromethyl)pyridine)	0.01	C <sub>6</sub> H <sub>3</sub> Cl <sub>4</sub> N	[M+H] <sup>+</sup>	231.9063	/	3.4
Nitroguanidine	0.01	CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	105.0407	/	-0.89
Nitroxinil	0.01	C <sub>7</sub> H <sub>3</sub> IN <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	290.92612	4.37	2.3
Norfloxacin	0.01	C <sub>16</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	320.14050	2.36	-1
Norflurazon	0.01	C <sub>12</sub> H <sub>9</sub> ClF <sub>3</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	304.0459	5.34	2.3
Noruron	0.01	C <sub>13</sub> H <sub>22</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	223.18049	5.52	2.3**
Novaluron	0.01	C <sub>17</sub> H <sub>9</sub> ClF <sub>8</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>-</sup>	493.01959	7.54	5.27
Novobiocin	0.01	C <sub>31</sub> H <sub>36</sub> N <sub>2</sub> O <sub>11</sub>	[M-H] <sup>-</sup>	613.23919	6.88	3.3
Nuarimol	0.01	C <sub>17</sub> H <sub>12</sub> ClFN <sub>2</sub> O	[M+H] <sup>+</sup>	315.0695	5.62	3.18
O-Acetyltylosin	0.01	C <sub>48</sub> H <sub>79</sub> NO <sub>18</sub>	[M+H] <sup>+</sup>	958.53699	4.79	1.6
Ofloxacin	0.01	C <sub>18</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	362.15106	2.43	-0.4
Ofurace	0.01	C <sub>14</sub> H <sub>16</sub> ClNO <sub>3</sub>	[M+H] <sup>+</sup>	282.08915	5.09	2.7**
Oleandomycin	0.01	C <sub>35</sub> H <sub>61</sub> NO <sub>12</sub>	[M+H] <sup>+</sup>	688.42665	4.29	1.7
Omethoate	0.01	C <sub>5</sub> H <sub>12</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	214.02974	0.92	-0.74
Orbencarb	0.01	C <sub>12</sub> H <sub>16</sub> ClNOS	[M+H] <sup>+</sup>	258.07139	7.36	3.4**
Orbifloxacin	0.01	C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	396.15295	2.74	0.9
Ormetoprim	0.01	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	275.15025	2.41	1.2
Oryastrobin	0.01	C <sub>18</sub> H <sub>25</sub> N <sub>5</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	392.19285	6.23	2.5**
Oryzalin	0.01	C <sub>12</sub> H <sub>18</sub> N <sub>4</sub> O <sub>6</sub> S	[M-H] <sup>-</sup>	347.10198	6.47	3.73
Oxacillin	0.01	C <sub>19</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S	[M-H] <sup>-</sup>	402.11182	4.72	2.4
Oxadiargyl	0.01	C <sub>15</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	341.04542	7.35	4.1**
Oxadiazon	0.01	C <sub>15</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	345.07672	8.15	4.8
Oxadixyl	0.01	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	279.13393	4.24	0.8

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Oxamyl	0.01	C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	242.05698	2.93	-0.47
Oxasulfuron	0.01	C <sub>17</sub> H <sub>18</sub> N <sub>4</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	407.10198	4.4	1.6**
Oxaziclomefone	0.01	C <sub>20</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	376.08656	7.98	5.2**
Oxfendazole (fenbendazole sulfoxide)	0.01	C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	316.07504	3.49	2.3
Oxfendazole sulfone (fenbendazole sulfone)	0.01	C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	332.06995	4.15	2.3
Oxibendazole	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	250.11862	3.79	2.4
Oximino oxamyl	0.01	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	163.05358	/	1.2**
Oxolinic acid	0.01	C <sub>13</sub> H <sub>11</sub> NO <sub>5</sub>	[M+H] <sup>+</sup>	262.07100	3.82	-0.2
Oxycarboxin	0.01	C <sub>12</sub> H <sub>13</sub> NO <sub>4</sub> S	[M+H] <sup>+</sup>	268.06381	3.84	0.77
Oxyclozanide	0.01	C <sub>13</sub> H <sub>6</sub> Cl <sub>5</sub> NO <sub>3</sub>	[M-H] <sup>-</sup>	399.88631	6.83	5.7
Oxydemeton-methyl (demeton-S-)	0.01	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	247.02222	/	-0.74
Oxyfluorfen	0.01	C <sub>15</sub> H <sub>11</sub> ClF <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	362.04015	7.98	4.73
Oxyphenbutazone	0.01	C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	[M-H] <sup>-</sup>	325.15467	5.36	2.7
Oxytetracycline	0.01	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub>	[M+H] <sup>+</sup>	461.15546	/	/
Paclobutrazol	0.01	C <sub>15</sub> H <sub>20</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	294.13677	5.83	3.2
Paraoxon-ethyl	0.01	C <sub>10</sub> H <sub>14</sub> NO <sub>6</sub> P	[M+H] <sup>+</sup>	276.06315	5.28	1.98
Parathion	0.01	C <sub>10</sub> H <sub>14</sub> NO <sub>5</sub> PS	[M+H] <sup>+</sup>	292.04031	7.1	3.83
Pebulate	0.01	C <sub>10</sub> H <sub>21</sub> NOS	[M+H] <sup>+</sup>	204.14166	7.57	3.83
Penconazol	0.01	C <sub>13</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub>	[M-H] <sup>+</sup>	284.07158	6.7	3.72
Pencycuron	0.01	C <sub>19</sub> H <sub>21</sub> ClN <sub>2</sub> O	[M+H] <sup>-</sup>	329.14152	7.42	4.8**
Pendimethalin	0.01	C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	282.14483	8.22	5.2
Penfluron	0.01	C <sub>15</sub> H <sub>9</sub> F <sub>5</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>-</sup>	345.0657	6.73	4**
Penicillin-G	0.01	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S	[M-H] <sup>-</sup>	335.10601	4.07	1.8

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Penicilllin-V <sup>4</sup>	0.01	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S	[M-H] <sup>-</sup>	351.10092	4.43	2.1
Penoxsulam	0.01	C <sub>16</sub> H <sub>14</sub> F <sub>5</sub> N <sub>5</sub> O <sub>5</sub> S	[M-H] <sup>-</sup>	484.07086	5.37	-0.354
Pentachlorocyanobenzene	0.01	C <sub>7</sub> Cl <sub>5</sub> N	[M+H] <sup>+</sup>	275.85168	/	/
Pentanochlor	0.01	C <sub>13</sub> H <sub>18</sub> ClNO	[M+H] <sup>+</sup>	240.11497	6.89	4.3**
Penthiopyrad	0.01	C <sub>16</sub> H <sub>20</sub> F <sub>3</sub> N <sub>3</sub> OS	[M-H] <sup>-</sup>	360.1352	7.03	4**
Pethoxamid	0.01	C <sub>16</sub> H <sub>22</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	296.14118	6.66	3.5**
Phenmedipham	0.01	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	301.11828	5.78	3.6**
Phenothrin	0.01	C <sub>23</sub> H <sub>26</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	351.19547	9.11	7.54
Phenthoate	0.01	C <sub>12</sub> H <sub>17</sub> O <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	321.03787	7.15	3.7**
Phénylbutazone	0.01	C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	309.15975	6.64	3.2
Phenylurea	0.01	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	137.07094	2.34	0.8**
Phorate	0.01	C <sub>7</sub> H <sub>17</sub> O <sub>2</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	261.02011	/	3.56
Phorate-oxon sulfoxide	0.01	C <sub>7</sub> H <sub>17</sub> O <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	261.03787	3.03	1.8**
Phorate sulfoxide	0.01	C <sub>7</sub> H <sub>17</sub> O <sub>3</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	277.01502	5	3.5**
Phorate-oxon	0.01	C <sub>7</sub> H <sub>17</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	213.07088	/	2.1**
Phorate-oxon sulfone	0.01	C <sub>7</sub> H <sub>17</sub> O <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	277.03278	3.66	2**
Phorat sulfone	0.01	C <sub>7</sub> H <sub>17</sub> O <sub>4</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	293.00994	5.71	3.7**
Phosalone	0.01	C <sub>12</sub> H <sub>15</sub> ClNO <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	367.99414	7.45	4.38
Phosfolan	0.01	C <sub>7</sub> H <sub>14</sub> NO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	256.02255	3.72	0.6**
Phosmet	0.01	C <sub>11</sub> H <sub>12</sub> NO <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	318.00182	6.03	2.95
Phosmet-oxon	0.01	C <sub>11</sub> H <sub>12</sub> NO <sub>5</sub> PS	[M+H] <sup>+</sup>	302.02466	4.07	1.1**
Phosphamidon	0.01	C <sub>10</sub> H <sub>19</sub> ClNO <sub>5</sub> P	[M+H] <sup>+</sup>	300.07622	4.11	0.8
Phospholan-methyl	0.01	C <sub>5</sub> H <sub>10</sub> NO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	227.99125	2.58	1.1**

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Phoxim	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	299.06138	7.04	4.4**
Phthalylsulfathiazole (CAS)	0.01	C <sub>17</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>	[M-H] <sup>-</sup>	404.03694	3.16	1.1
Picolinafen	0.01	C <sub>19</sub> H <sub>12</sub> F <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	377.09077	7.85	4.9**
Picoxystrobin	0.01	C <sub>18</sub> H <sub>16</sub> F <sub>3</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	368.11042	7.03	3.6
Piperalin	0.01	C <sub>16</sub> H <sub>21</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	330.10221	4.56	4.31
Piperonyl butoxide	0.01	C <sub>19</sub> H <sub>30</sub> O <sub>5</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	356.24315	7.92	4.75
Piperophos	0.01	C <sub>14</sub> H <sub>28</sub> NO <sub>3</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	354.1321	7.59	4.2**
Pirimicarb	0.01	C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	239.15025	3.91	1.7
Pirimicarb-desmethyl	0.01	C <sub>10</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	225.1346	2.68	1.6**
Pirimiphos-methyl	0.01	C <sub>11</sub> H <sub>20</sub> N <sub>3</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	306.10358	7.47	4.12
Pirimiphos-ethyl	0.01	C <sub>13</sub> H <sub>24</sub> N <sub>3</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	334.13488	8.17	5
Pirimiphos-methyl-N-desethyl	0.01	C <sub>9</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	278.07228	5.36	3.7**
Pirlymycin	0.01	C <sub>17</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	411.17150	3.09	1.7
Prallethrin	0.01	C <sub>19</sub> H <sub>24</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	301.17982	7.58	4.49
Pretilachlor	0.01	C <sub>17</sub> H <sub>26</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	312.17248	7.69	4.1**
Primisulfuron-methyl	0.01	C <sub>15</sub> H <sub>12</sub> F <sub>4</sub> N <sub>4</sub> O <sub>7</sub> S	[M+H] <sup>-</sup>	469.04356	6.19	/
Probenazole	0.01	C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub> S	[M+H] <sup>+</sup>	224.03759	4.96	1.4**
Prochloraz	0.01	C <sub>15</sub> H <sub>16</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	376.03809	6.62	4.1
Procyazine	0.01	C <sub>10</sub> H <sub>13</sub> ClN <sub>6</sub>	[M+H] <sup>+</sup>	253.0963	4.55	2.4**
Procymidone	0.01	C <sub>13</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	284.02396	6.64	3**
Profenofos	0.01	C <sub>11</sub> H <sub>15</sub> BrClO <sub>3</sub> PS	[M+H] <sup>+</sup>	374.94017	7.68	4.68
Profoxydim lithium	0.01	C <sub>24</sub> H <sub>32</sub> ClNO <sub>4</sub> S	[M+H] <sup>+</sup>	466.18133	8.88	/
Prohydrojasmon	0.01	C <sub>15</sub> H <sub>26</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	255.19547	7.5	3.6**



<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Promecarb	0.01	C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	208.13321	5.87	3.1
Prometon	0.01	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	226.16624	4.41	2.99
Prometryn	0.01	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	242.14339	5.88	3.51
Propachlor	0.01	C <sub>11</sub> H <sub>14</sub> ClNO	[M+H] <sup>+</sup>	212.08367	5.49	2.18
Propamocarb	0.01	C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	189.15975	0.96	1.12
Propamocarb HCl	0.01	C <sub>9</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	225.13643	2.64	/
Propanil	0.01	C <sub>9</sub> H <sub>9</sub> Cl <sub>2</sub> NO	[M+H] <sup>-</sup>	218.0134	5.69	3.07
Propaphos	0.01	C <sub>13</sub> H <sub>21</sub> O <sub>4</sub> PS	[M+H] <sup>+</sup>	305.0971	6.75	3.67
Propaquizafop	0.01	C <sub>22</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	444.13208	7.84	4.6
Propargite	0.01	C <sub>19</sub> H <sub>26</sub> O <sub>4</sub> S	[M+NH <sub>4</sub> ] <sup>+</sup>	368.18901	8.36	5
Propazine	0.01	C <sub>9</sub> H <sub>16</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	230.1167	6.53	2.93
Propazine-2-hydroxy	0.01	C <sub>9</sub> H <sub>17</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	212.15059	3.71	0.6**
Propetamphos	0.01	C <sub>10</sub> H <sub>20</sub> NO <sub>4</sub> PS	[M+H] <sup>+</sup>	282.09235	6.5	3.82
Propham	0.01	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>	C <sub>7</sub> H <sub>8</sub> NO <sub>2</sub> <sup>+</sup>	138.05496	5.41	2.6
Propiconazol (mixture of isomers)	0.01	C <sub>15</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	342.07706	6.87	3.72
Propisochlor	0.01	C <sub>15</sub> H <sub>22</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	284.14118	6.71	3.9**
Propoxur	0.01	C <sub>11</sub> H <sub>15</sub> NO <sub>3</sub>	C <sub>8</sub> H <sub>10</sub> NO <sub>3</sub> <sup>+</sup>	168.06552	4.65	1.52
Propyzamide (pronamide)	0.01	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> NO	[M+H] <sup>+</sup>	256.02905	6.31	3.43
Proquinazid	0.01	C <sub>14</sub> H <sub>17</sub> IN <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	373.04076	8.68	3.7**
Prosulfocarb	0.01	C <sub>14</sub> H <sub>21</sub> NOS	[M+H] <sup>+</sup>	252.14166	7.8	3.9**
Prosulfuron	0.01	C <sub>15</sub> H <sub>16</sub> F <sub>3</sub> N <sub>5</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	420.09479	5.87	-0.21
Prothioconazole	0.01	C <sub>14</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub> OS	[M+H] <sup>+</sup>	344.03857	6.8	3.82
Prothioconazole-desthio	0.01	C <sub>14</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	312.06649	6.24	2.7**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Pymetrozine	0.01	C <sub>10</sub> H <sub>11</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	218.10364	1.62	-0.18
Pyracarbolid	0.01	C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	218.11756	4.88	2.1**
Pyraclofos	0.01	C <sub>14</sub> H <sub>18</sub> ClN <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	361.05371	7.16	3.8**
Pyraclostrobin	0.01	C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	388.10586	7.3	3.99
Pyraflufen-ethyl	0.01	C <sub>15</sub> H <sub>13</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	413.02772	7.12	3.49
Pyrantel	0.01	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S	[M+H] <sup>+</sup>	207.09505	2.50	1.6
Pyrazolynate	0.01	C <sub>19</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	439.02806	7.48	3.8**
Pyrazophos	0.01	C <sub>14</sub> H <sub>20</sub> N <sub>3</sub> O <sub>5</sub> PS	[M+H] <sup>+</sup>	374.09341	7.27	3.1**
Pyrazosulfuron-ethyl	0.01	C <sub>14</sub> H <sub>18</sub> N <sub>6</sub> O <sub>7</sub> S	[M+H] <sup>+</sup>	415.10305	5.93	0.7**
Pyrazoxyfen	0.01	C <sub>20</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	403.06107	6.96	3.7**
Pyrethrin (mixture of isomers)	0.01	C <sub>22</sub> H <sub>28</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	373.20095	7.57	4.3
Pyributicarb	0.01	C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	331.14748	8.21	5.2**
Pyridaben	0.01	C <sub>19</sub> H <sub>25</sub> ClN <sub>2</sub> OS	[M+H] <sup>+</sup>	365.14489	8.82	6.37
Pyridafol	0.01	C <sub>10</sub> H <sub>7</sub> ClN <sub>2</sub> O	[M+H] <sup>+</sup>	207.03197	3.48	2.4**
Pyridalyl	0.01	C <sub>18</sub> H <sub>14</sub> Cl <sub>4</sub> F <sub>3</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	491.9725	9.59	7.59
Pyridaphenthion	0.01	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub> PS	[M+H] <sup>+</sup>	341.07194	6.32	3.3**
Pyridate	0.01	C <sub>19</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	379.12415	9.25	6.6**
Pyrifenox (mixture of isomers)	0.01	C <sub>14</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	295.03995	5.56	2.5**
Pyrimethanil	0.01	C <sub>12</sub> H <sub>13</sub> N <sub>3</sub>	[M+H] <sup>+</sup>	200.11822	5.49	2.84
Pyriproxyfen	0.01	C <sub>20</sub> H <sub>19</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	322.14377	8.11	5.37
Pyroquilon	0.01	C <sub>11</sub> H <sub>11</sub> NO	[M+H] <sup>+</sup>	174.09134	4.07	1.57
Pyroxulam	0.01	C <sub>14</sub> H <sub>13</sub> F <sub>3</sub> N <sub>6</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	435.0693	4.66	1.7**
Quinalphos	0.01	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	299.06138	7.04	4.4**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Quinclorac	0.01	C <sub>10</sub> H <sub>5</sub> Cl <sub>2</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	241.97701	3.81	2.97
Quinine	0.01	C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	325.19105	2.91	/
Quinine sulfate	0.01	C <sub>40</sub> H <sub>54</sub> N <sub>4</sub> O <sub>10</sub> S	[M+H] <sup>+</sup>	783.36334	/	/
Quinmerac	0.01	C <sub>11</sub> H <sub>8</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	222.03163	3.21	2.7**
Quinoclamine	0.01	C <sub>10</sub> H <sub>6</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	208.01598	4.36	2.1**
Quinoline	0.01	C <sub>9</sub> H <sub>7</sub> N	[M+H] <sup>+</sup>	130.06513	2.1	2.03
Quinoxifen	0.01	C <sub>15</sub> H <sub>8</sub> Cl <sub>2</sub> FNO	[M+H] <sup>+</sup>	308.00397	8	4.66
Quizalofop	0.01	C <sub>17</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	345.06366	6.27	3.6**
Quizalofop-ethyl	0.01	C <sub>19</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	373.09496	7.75	4.28
Quizalofop-P-ethyl	0.01	C <sub>19</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	373.09496	7.74	4.3
Rafoxanide	0.01	C <sub>19</sub> H <sub>11</sub> Cl <sub>2</sub> I <sub>2</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	625.82783	/	7
Reserpine	0.01	C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>9</sub>	[M+H] <sup>+</sup>	609.28066	4.84	3.2
Resmethrin	0.01	C <sub>22</sub> H <sub>26</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	339.19547	8.89	5.43
Rifampicin	0.01	C <sub>43</sub> H <sub>58</sub> N <sub>4</sub> O <sub>12</sub>	[M+H] <sup>+</sup>	823.41240	5.94	2.7
Rifamycin	0.01	C <sub>37</sub> H <sub>47</sub> NO <sub>12</sub>	[M+H] <sup>+</sup>	698.31710	/	/
Rifaximin	0.01	C <sub>43</sub> H <sub>51</sub> N <sub>3</sub> O <sub>11</sub>	[M+H] <sup>+</sup>	786.35964	6.24	3.2
Rimsulfuron	0.01	C <sub>14</sub> H <sub>17</sub> N <sub>5</sub> O <sub>7</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	432.06422	4.77	-1.47
Robenidine	0.01	C <sub>15</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>5</sub>	[M+H] <sup>+</sup>	334.06208	5.57	3.8
Ronidazole	0.01	C <sub>6</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	201.06183	/	/
Rotenone	0.01	C <sub>23</sub> H <sub>22</sub> O <sub>6</sub>	[M+H] <sup>+</sup>	395.14892	6.72	4.1
Roxithromycin	0.01	C <sub>41</sub> H <sub>76</sub> N <sub>2</sub> O <sub>15</sub>	[M+H] <sup>+</sup>	837.53185	4.99	1.7
Saflufenacil	0.01	C <sub>17</sub> H <sub>17</sub> ClF <sub>4</sub> N <sub>4</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	501.06171	5.99	2.1**
Salinomycin	0.01	C <sub>42</sub> H <sub>70</sub> O <sub>11</sub>	[M+NH <sub>4</sub> ] <sup>+</sup>	768.52564	9.98	5.7

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Sarafloxacin	0.01	C <sub>20</sub> H <sub>17</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	386.13107	2.98	0.3
Schradan (DMPA)	0.01	C <sub>8</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub> P <sub>2</sub>	[M+H] <sup>+</sup>	287.13964	3.05	-0.3
Sebuthylazin	0.01	C <sub>9</sub> H <sub>16</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	230.1167	5.9	3.1**
Sebuthylazin-desethyl	0.01	C <sub>7</sub> H <sub>12</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	202.0854	3.98	2.2**
Secbumeton	0.01	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	226.16624	4.45	3.2**
Selamectin impurity B	0.01	C <sub>43</sub> H <sub>63</sub> NO <sub>11</sub>	[M+H] <sup>+</sup>	770.44739	9.65	5.4**
Semduramicin	0.01	C <sub>45</sub> H <sub>76</sub> O <sub>16</sub>	[M+H] <sup>+</sup>	873.52061	7.59	/
Sethoxydim	0.01	C <sub>17</sub> H <sub>29</sub> NO <sub>3</sub> S	[M+H] <sup>+</sup>	328.19409	8.09	/
S-Hydroprene	0.01	C <sub>17</sub> H <sub>30</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	267.23186	/	6.5
Siduron	0.01	C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O	[M+H] <sup>+</sup>	233.16484	5.77	3.8
Silthiofam	0.01	C <sub>13</sub> H <sub>21</sub> NOSSi	[M+H] <sup>+</sup>	268.11859	/	/
Simazine	0.01	C <sub>7</sub> H <sub>12</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	202.0854	4.4	2.18
Simeconazole	0.01	C <sub>14</sub> H <sub>20</sub> FN <sub>3</sub> OSi	[M+H] <sup>+</sup>	294.14325	6.16	/
Simeton	0.01	C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	198.13494	3.36	1.8
Simetryn	0.01	C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	214.11209	4.41	2.8
S-Metolachlor	0.01	C <sub>15</sub> H <sub>22</sub> ClNO <sub>2</sub>	[M+H] <sup>+</sup>	284.14118	6.72	3.1
Spinetoram (mixture of isomers)	0.01	C <sub>42</sub> H <sub>69</sub> NO <sub>10</sub>	[M+H] <sup>+</sup>	748.49942	6.94	5.9**
Spinosad (mixture of spinosyn A and D)	0.01	C <sub>41</sub> H <sub>65</sub> NO <sub>10</sub>	[M+H] <sup>+</sup>	732.46812	6.34	4.9**
Spiramycin	0.01	C <sub>43</sub> H <sub>74</sub> N <sub>2</sub> O <sub>14</sub>	[M+H] <sup>+</sup>	843.52128	3.33	2.1
Spirodiclofen	0.01	C <sub>21</sub> H <sub>24</sub> Cl <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	411.11244	8.81	5.1
Spiromesifen	0.01	C <sub>23</sub> H <sub>30</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	371.22169	8.7	4.55
Spirotetramat	0.01	C <sub>21</sub> H <sub>27</sub> NO <sub>5</sub>	[M+H] <sup>+</sup>	374.1962	6.04	3.2**
Spirotetramat-enol	0.01	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	302.17507	4.45	2.4**

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Spirotetramat-enol-glucoside	0.01	C <sub>24</sub> H <sub>33</sub> NO <sub>8</sub>	[M+H] <sup>+</sup>	464.22789	2.38	0.5**
Spirotetramat-mono-hydroxy	0.01	C <sub>21</sub> H <sub>27</sub> NO <sub>5</sub>	[M+H] <sup>+</sup>	374.1962	6.04	2.1**
Spiroxamine (mixture of isomers)	0.01	C <sub>18</sub> H <sub>35</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	298.27406	5.39	4.2**
Sulbactam	0.01	C <sub>8</sub> H <sub>11</sub> NO <sub>5</sub> S	[M+NH <sub>4</sub> ] <sup>+</sup>	256.02502	/	/
Sulcotrione	0.01	C <sub>14</sub> H <sub>13</sub> ClO <sub>5</sub> S	[M+H] <sup>+</sup>	329.0245	4.61	1.5**
Sulfacetamide	0.01	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	215.04849	/	-1
Sulfachloropyridazine	0.01	C <sub>10</sub> H <sub>9</sub> ClN <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	285.02075	3.12	1
Sulfaclozine	0.01	C <sub>10</sub> H <sub>9</sub> ClN <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	285.02075	3.79	0.9
Sulfadiazine	0.01	C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	251.05972	2.07	-0.1
Sulfadimerazine	0.01	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	279.09102	2.79	0.1
Sulfadimethoxine	0.01	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	311.08085	3.86	1.6
Sulfadoxine	0.01	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	311.08085	3.35	0.7
Sulfaguanidine	0.01	C <sub>7</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	215.05972	0.95	-0.7
Sulfallate	0.01	C <sub>8</sub> H <sub>14</sub> ClNS <sub>2</sub>	[M+H] <sup>+</sup>	224.0329	7.25	3.15
Sulfamerazine	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	265.07537	2.46	0.14
Sulfamerazine	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	265.07537	2.46	0.1
Sulfamethizole	0.01	C <sub>9</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	271.03180	2.64	2.9
Sulfamethoxazole	0.01	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	254.05939	3.25	0.9
Sulfamethoxypyridazine	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	281.07029	2.98	0.3
Sulfamonomethoxine	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	281.07029	3	0.8
Sulfamonomethoxine	0.01	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	281.07029	2.72	0.7
Sulfanilamide	0.01	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	173.03793	/	-0.6
Sulfaphenazole	0.01	C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	315.09102	3.93	1.5

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Sulfaquinoxaline	0.01	C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	301.07537	3.89	1.7
Sulfathiazole	0.01	C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	256.02090	2.13	0.1
Sulfentrazone	0.01	C <sub>11</sub> H <sub>10</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	386.98915	4.91	0.99
Sulfisoxazole	0.01	C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	268.07504	3.44	1
Sulfometuron-methyl	0.01	C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	365.09142	4.73	1.2
Sulfosulfuron	0.01	C <sub>16</sub> H <sub>18</sub> N <sub>6</sub> O <sub>7</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	471.07512	5.3	-0.77
Sulfoxaflor	0.01	C <sub>10</sub> H <sub>10</sub> F <sub>3</sub> N <sub>3</sub> OS	[M+H] <sup>+</sup>	278.05695	3.91	0.8
Sulfluramid	0.01	C <sub>10</sub> H <sub>6</sub> F <sub>17</sub> NO <sub>2</sub> S	[M-H] <sup>-</sup>	527.99206	8.32	5.6**
Sulprofos sulfoxide	0.01	C <sub>12</sub> H <sub>19</sub> O <sub>3</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	339.03067	6.37	3.5**
Systhane <sup>TM</sup>	0.01	C <sub>15</sub> H <sub>17</sub> ClN <sub>4</sub>	[M+H] <sup>+</sup>	289.12145	6.16	2.94
Tau-fluvalinate	0.01	C <sub>26</sub> H <sub>22</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	503.13438	9.02	7.7**
TDCPP	0.01	C <sub>9</sub> H <sub>15</sub> Cl <sub>6</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	430.88829	6.89	3.65
Tebuconazole (Folicur®)	0.01	C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	308.15242	6.49	3.7
Tebufenozide	0.01	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>18</sub> H <sub>21</sub> N <sub>2</sub> O <sub>2</sub> <sup>+</sup>	297.15975	6.82	4.25
Tebufenpyrad	0.01	C <sub>18</sub> H <sub>24</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	334.16807	7.86	4.61
Tebupirimfos	0.01	C <sub>13</sub> H <sub>23</sub> N <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	319.12398	8.21	4.2
Tebutam	0.01	C <sub>15</sub> H <sub>23</sub> NO	[M+H] <sup>+</sup>	234.18524	6.72	3.4**
Tebuthiuron	0.01	C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> OS	[M+H] <sup>+</sup>	229.11176	4.06	1.79
Teflubenzuron	0.01	C <sub>14</sub> H <sub>6</sub> Cl <sub>2</sub> F <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	380.98152	7.46	4.56
Telithromycin	0.01	C <sub>43</sub> H <sub>65</sub> N <sub>5</sub> O <sub>10</sub>	[M+H] <sup>+</sup>	812.48042	3.89	4.2
Tembotrione	0.01	C <sub>17</sub> H <sub>16</sub> ClF <sub>3</sub> O <sub>6</sub> S	[M+NH <sub>4</sub> ] <sup>+</sup>	458.06465	5.97	-1.09
Tepraloxydim	0.01	C <sub>17</sub> H <sub>24</sub> ClNO <sub>4</sub>	[M+H] <sup>-</sup>	342.14666	6.44	2.6**
Terbufos	0.01	C <sub>9</sub> H <sub>21</sub> O <sub>2</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	289.05141	8.09	4.48

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Terbufos sulfone	0.01	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	321.04124	6.33	2.5**
Terbufos sulfoxide	0.01	C <sub>9</sub> H <sub>21</sub> O <sub>3</sub> PS <sub>3</sub>	[M+H] <sup>+</sup>	305.04633	5.74	2.2**
Terbumeton	0.01	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	226.16624	4.41	3.1**
Terbumeton-desethyl	0.01	C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	198.13494	3.27	2.1**
Terbutaline sulfate	0.01	C <sub>24</sub> H <sub>40</sub> N <sub>2</sub> O <sub>10</sub> S	[M+H] <sup>+</sup>	549.24764	/	/
Terbutylazine	0.01	C <sub>9</sub> H <sub>16</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	230.1167	5.96	3.4
Terbutylazine-desethyl	0.01	C <sub>7</sub> H <sub>12</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	202.0854	4.4	2**
Terbutol (terbucarb)	0.01	C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	278.21146	7.52	5.2**
Terbutryn	0.01	C <sub>10</sub> H <sub>19</sub> N <sub>5</sub> S	[M+H] <sup>+</sup>	242.14339	5.88	3.74
Terbutylazine-2-hydroxy	0.01	C <sub>9</sub> H <sub>17</sub> N <sub>5</sub> O	[M+H] <sup>+</sup>	212.15059	2.69	0.3**
Tetrachlorvinphos (ISO)	0.01	C <sub>10</sub> H <sub>9</sub> C <sub>14</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	366.90367	6.65	3.53
Tetraconazole	0.01	C <sub>13</sub> H <sub>11</sub> Cl <sub>2</sub> F <sub>4</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	372.02881	6.33	3.56
Tetracycline	0.01	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>	[M+H] <sup>+</sup>	445.16054	/	/
Tetraethyl dithiopyrophosphate	0.01	C <sub>8</sub> H <sub>20</sub> O <sub>5</sub> P <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	323.03002	7.36	3.99
Tetraethyl pyrophosphate	0.01	C <sub>8</sub> H <sub>20</sub> O <sub>7</sub> P <sub>2</sub>	[M+H] <sup>+</sup>	291.07571	4.04	/
Tetramethrin	0.01	C <sub>19</sub> H <sub>25</sub> NO <sub>4</sub>	[M+H] <sup>+</sup>	332.18564	7.96	4.73
Thenylchlor	0.01	C <sub>16</sub> H <sub>18</sub> ClNO <sub>2</sub> S	[M+H] <sup>+</sup>	324.08195	6.69	3.8**
Thiabendazole	0.01	C <sub>10</sub> H <sub>7</sub> N <sub>3</sub> S	[M+H] <sup>+</sup>	202.04335	2.43	2.47
Thiacloprid	0.01	C <sub>10</sub> H <sub>9</sub> ClN <sub>4</sub> S	[M+H] <sup>+</sup>	253.03092	3.9	1.26
Thiamethoxam	0.01	C <sub>8</sub> H <sub>10</sub> ClN <sub>5</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	292.02657	2.63	-0.13
Thiamphenicol	0.01	C <sub>12</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>5</sub> S	[M+H] <sup>+</sup>	373.03863	2.48	-0.3
Thiazafurion	0.01	C <sub>6</sub> H <sub>7</sub> F <sub>3</sub> N <sub>4</sub> OS	[M+H] <sup>+</sup>	241.03654	4.41	0.8**
Thiazopyr	0.01	C <sub>16</sub> H <sub>17</sub> F <sub>5</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	397.10037	7.3	3.89

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Thidiazuron	0.01	C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> OS	[M+H] <sup>-</sup>	221.04916	4.09	1.77
Thiencarbazone-methyl	0.01	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>7</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	391.03767	4.54	1.2**
Thifensulfuron-methyl	0.01	C <sub>12</sub> H <sub>13</sub> N <sub>5</sub> O <sub>6</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	388.038	4.41	/
Thifluzamide	0.01	C <sub>13</sub> H <sub>6</sub> Br <sub>2</sub> F <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	528.84733	6.91	6**
Thiobencarb	0.01	C <sub>12</sub> H <sub>16</sub> ClNOS	[M+H] <sup>+</sup>	258.07139	7.36	3.4
Thiocarbazyl	0.01	C <sub>16</sub> H <sub>25</sub> NOS	[M+H] <sup>+</sup>	280.17296	8.55	/
Thiocyclam hydrogen oxalate	0.01	C <sub>7</sub> H <sub>13</sub> NO <sub>4</sub> S <sub>3</sub>	[M+H] <sup>+</sup>	272.00795	/	/
Thiodicarb	0.01	C <sub>10</sub> H <sub>18</sub> N <sub>4</sub> O <sub>4</sub> S <sub>3</sub>	[M+H] <sup>+</sup>	355.0563	4.71	1.62
Thiofanox	0.01	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S	[M+Na] <sup>+</sup>	241.09812	5.02	2.2**
Thiofanox sulfone	0.01	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	251.10601	3.38	0.9**
Thiofanox sulfoxide	0.01	C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	235.11109	2.8	0.8**
Thionazin (Zinophos <sup>TM</sup> )	0.01	C <sub>8</sub> H <sub>13</sub> N <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	249.04573	5.66	2**
Thiophanate-methyl	0.01	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	343.05293	4.48	2.6**
Thiophanate-ethyl	0.01	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	371.08423	5.49	3.3**
Tiadinil	0.01	C <sub>11</sub> H <sub>10</sub> ClN <sub>3</sub> OS	[M+H] <sup>-</sup>	268.03059	6.13	3**
Tiamulin	0.01	C <sub>28</sub> H <sub>47</sub> NO <sub>4</sub> S	[M+H] <sup>+</sup>	494.32986	4.86	4.5
Tiamulin fumarate	0.01	C <sub>32</sub> H <sub>51</sub> NO <sub>8</sub> S	[M+H] <sup>+</sup>	610.34082	/	/
Ticarcillin	0.01	C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	385.05226	/	/
Tildipirosin	0.01	C <sub>41</sub> H <sub>71</sub> N <sub>3</sub> O <sub>8</sub>	[M+H] <sup>+</sup>	751.55794	/	/
Tilmicosin	0.01	C <sub>46</sub> H <sub>80</sub> N <sub>2</sub> O <sub>13</sub>	[M+Na] <sup>+</sup>	891.55526	9.33	/
Tokuthion®	0.01	C <sub>11</sub> H <sub>15</sub> Cl <sub>2</sub> O <sub>2</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	344.97009	8.96	4.9**
Tolclofos-methyl	0.01	C <sub>9</sub> H <sub>11</sub> Cl <sub>2</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	300.96164	7.47	4.56
Tolfenamic acid	0.01	C <sub>14</sub> H <sub>12</sub> ClNO <sub>2</sub>	[M-H] <sup>-</sup>	262.06293	7.02	5.2



<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Tolfenpyrade	0.01	C <sub>21</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	384.14733	7.84	4.7**
Toltrazuril	0.01	C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S	[M+H] <sup>+</sup>	426.07299	6.76	2.9
Toltrazuril sulfone	0.01	C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	458.06282	6.09	2.7
Tolyfluanid	0.01	C <sub>10</sub> H <sub>13</sub> Cl <sub>2</sub> FN <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	[M+H] <sup>+</sup>	346.98523	7.35	3.9
Topramezone	0.01	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	364.09617	3.57	1.44
Tralkoxydim	0.01	C <sub>20</sub> H <sub>27</sub> NO <sub>3</sub>	[M+H] <sup>+</sup>	330.20637	8.24	4.1**
Triadimefon	0.01	C <sub>14</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	294.10038	6.27	2.77
Triadimenol (Baytan®)	0.01	C <sub>14</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	296.11603	5.78	3.56
Triallate	0.01	C <sub>10</sub> H <sub>16</sub> Cl <sub>3</sub> NOS	[M+H] <sup>+</sup>	304.0091	8.5	4.6
Triasulfuron	0.01	C <sub>14</sub> H <sub>16</sub> ClN <sub>5</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	402.06334	4.75	-0.59
Triazamate	0.01	C <sub>13</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	315.14854	6.69	2.7**
Triaziflam	0.01	C <sub>17</sub> H <sub>24</sub> FN <sub>5</sub> O	[M+H] <sup>+</sup>	334.20377	6.12	3.5**
Triazophos	0.01	C <sub>12</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	314.07228	6.58	3.34
Triazoxid	0.01	C <sub>10</sub> H <sub>6</sub> ClN <sub>5</sub> O	[M+H] <sup>+</sup>	248.03336	4.56	0.9**
Tribenuron-methyl	0.01	C <sub>15</sub> H <sub>17</sub> N <sub>5</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	396.09723	5.55	0.78
Tribufos (defoliant)	0.01	C <sub>12</sub> H <sub>27</sub> OPS <sub>3</sub>	[M+H] <sup>+</sup>	315.10345	8.89	3.2**
Trichlorfon	0.01	C <sub>4</sub> H <sub>8</sub> Cl <sub>3</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	256.92986	2.9	0.51
Triclabendazole	0.01	C <sub>14</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>2</sub> OS	[M+H] <sup>+</sup>	358.95739	6.97	5.5
Triclabendazole sulfone	0.01	C <sub>14</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>3</sub> S	[M+H] <sup>+</sup>	390.94722	6.50	4.5
Triclabendazole sulfoxide	0.01	C <sub>14</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S	[M+H] <sup>+</sup>	374.95231	6.16	4.4
Tricyclazole	0.01	C <sub>9</sub> H <sub>7</sub> N <sub>3</sub> S	[M+H] <sup>+</sup>	190.04335	3.57	1.7
Tridemorph (mixture of isomers)	0.01	C <sub>19</sub> H <sub>39</sub> NO	[M+H] <sup>+</sup>	298.31044	6.43	6.9**
Tridiphane	0.01	C <sub>10</sub> H <sub>7</sub> Cl <sub>5</sub> O	[M+H] <sup>+</sup>	320.89832	/	4.7**

Compound	MRL (mg.kg <sup>-1</sup> )*	Formula [M]	Ion	Theoretical m/z	T <sub>R</sub> (min)	LogP
Trietazine	0.01	C <sub>9</sub> H <sub>16</sub> ClN <sub>5</sub>	[M+H] <sup>+</sup>	230.1167	6.58	3.34
Trifloxystrobin	0.01	C <sub>20</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	409.13697	7.64	4.5
Trifloxystrobin metabolite	0.01	C <sub>19</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	395.12132	6.71	4.3**
Trifloxysulfuron sodium	0.01	C <sub>14</sub> H <sub>13</sub> F <sub>3</sub> N <sub>5</sub> NaO <sub>6</sub> S	[M+H] <sup>+</sup>	460.05091	5.07	/
Triflumizole	0.01	C <sub>15</sub> H <sub>15</sub> ClF <sub>3</sub> N <sub>3</sub> O	[M+H] <sup>+</sup>	346.09285	7.12	2.9
Triflumuron	0.01	C <sub>15</sub> H <sub>10</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	359.04048	7	4.91
Trifluralin	0.01	C <sub>13</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	[M+H] <sup>+</sup>	336.11657	8.17	5.34
Triflusulfuron-methyl	0.01	C <sub>17</sub> H <sub>19</sub> F <sub>3</sub> N <sub>6</sub> O <sub>6</sub> S	[M+H] <sup>+</sup>	493.11117	6.22	3.1**
Triforine	0.01	C <sub>10</sub> H <sub>14</sub> Cl <sub>6</sub> N <sub>4</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	434.92917	5.3	2.2
Trimethoprim	0.01	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	291.14517	2.20	0.4
Trinexapac-ethyl	0.01	C <sub>13</sub> H <sub>16</sub> O <sub>5</sub>	[M+H] <sup>+</sup>	253.10705	5.52	0.9**
Triphenyl phosphorothionate	0.01	C <sub>18</sub> H <sub>15</sub> O <sub>3</sub> PS	[M+H] <sup>+</sup>	343.05523	8.21	6.3**
Tris(2-chloroethyl) phosphate (TRCP)	0.01	C <sub>6</sub> H <sub>12</sub> Cl <sub>3</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	284.96116	4.71	1.78
Tri- <i>o</i> -cresyl phosphate (TCP)	0.01	C <sub>21</sub> H <sub>21</sub> O <sub>4</sub> P	[M+H] <sup>+</sup>	369.12502	8.28	6.34
Triticonazole	0.01	C <sub>17</sub> H <sub>20</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	318.13677	6.03	3.29
Tritosulfuron	0.01	C <sub>13</sub> H <sub>9</sub> F <sub>6</sub> N <sub>5</sub> O <sub>4</sub> S	[M-H] <sup>-</sup>	446.03522	5.93	3.1**
Trovafloxacin	0.01	C <sub>20</sub> H <sub>15</sub> F <sub>3</sub> N <sub>4</sub> O <sub>3</sub>	[M+H] <sup>+</sup>	417.11690	3.33	0.3
Tulathromycin	0.01	C <sub>41</sub> H <sub>79</sub> N <sub>3</sub> O <sub>12</sub>	[M+H] <sup>+</sup>	806.57365	/	/
Tylosin	0.01	C <sub>46</sub> H <sub>77</sub> NO <sub>17</sub>	[M+H] <sup>+</sup>	916.52643	4.55	1
Tylvalosin	0.01	C <sub>53</sub> H <sub>87</sub> NO <sub>19</sub>	[M+H] <sup>+</sup>	1042.59451	/	/
Uniconazole	0.01	C <sub>15</sub> H <sub>18</sub> ClN <sub>3</sub> O	[M+H] <sup>+</sup>	292.12112	6.22	3.6**
Valnemulin	0.01	C <sub>31</sub> H <sub>52</sub> N <sub>2</sub> O <sub>5</sub> S	[M+H] <sup>+</sup>	565.36697	5.17	5.3
Vamidothion	0.01	C <sub>8</sub> H <sub>18</sub> NO <sub>4</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	288.04877	2.92	0.16

<b>Compound</b>	<b>MRL (mg.kg<sup>-1</sup>)*</b>	<b>Formula [M]</b>	<b>Ion</b>	<b>Theoretical m/z</b>	<b>T<sub>R</sub> (min)</b>	<b>LogP</b>
Vamidothion sulfoxide	0.01	C <sub>8</sub> H <sub>18</sub> NO <sub>5</sub> PS <sub>2</sub>	[M+H] <sup>+</sup>	304.04368	0.93	-1.1
Vedaprofen	0.01	C <sub>19</sub> H <sub>22</sub> O <sub>2</sub>	[M+H] <sup>+</sup>	300.19581	7.62	5.7
Vernolate	0.01	C <sub>10</sub> H <sub>21</sub> NOS	[M+H] <sup>+</sup>	204.14166	7.57	/
Virginiamycin M1	0.01	C <sub>28</sub> H <sub>35</sub> N <sub>3</sub> O <sub>7</sub>	[M+H] <sup>+</sup>	526.25478	5.1	2.5
XMC (3,5-xylol methylcarbamate)	0.01	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	180.10191	4.97	2.23
Z-mevinphos	0.01	C <sub>7</sub> H <sub>13</sub> O <sub>6</sub> P	[M+H] <sup>+</sup>	193.02604	3.06	1.2**
Zoxamide	0.01	C <sub>14</sub> H <sub>16</sub> Cl <sub>3</sub> NO <sub>2</sub>	[M+H] <sup>+</sup>	336.03194	7.2	3.76

867 \* General default maximum residue limit (MRL) value in seafood matrices

868 \*\* LogP predicted by XLogP3 (PubChem)

869

**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

870

871

872

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

<b>Instrument</b>	<b>Parameter</b>	<b>Condition</b>
UHPLC	Column temperature	50°C
	Injection volume	10 µL
	Flow rate	0.5 mL.min <sup>-1</sup>
	Mobile phase	A: H <sub>2</sub> O 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	

873

874

**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
<b>K1*</b>	80.01	76.42	87.53		
<b>K2</b>	79.14	75.33	72.11		
<b>K3</b>	65.47	72.88	64.98		
<b>R**</b>	14.54	3.54	22.55		
<b>F-value</b>	15.01	0.74	29.97		
<b>p-value***</b>	< 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

**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
<b>K1*</b>	55.83	54.31	66.74		
<b>K2</b>	69.31	61.94	59.79		
<b>K3</b>	51.32	60.21	49.93		
<b>R**</b>	17.99	7.64	16.81		
<b>F-value</b>	24.24	4.44	19.74		
<b>p-value***</b>	< 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

880 **Table S6.** Validation results for 850 contaminants across 24 samples spiked at 0.001, 0.01 and 0.1 mg.kg<sup>-1</sup> with corresponding screening  
 881 detection limit (SDL) and limit of identification (LOI).

Compounds	No. of detections			SDL (mg.kg <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
1-(3,4-Dichlorophenyl)-3-methylurea	24	24	24	0.001	24	24	24	0.001
1-(4-Nitrophenyl)-3-propylurea	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>®</sup> (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- <i>S</i> -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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>TM</sup>	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Diethyl-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
Difenoxyurone	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Epoiconazole (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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
Fentoxon 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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Flupyrasulfuron-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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
Haloxifop	9	18	3	> 0.1	0	6	0	> 0.1
Haloxifop-2-ethoxyethyl	24	24	24	0.001	24	24	24	0.001
Haloxifop-methyl	24	24	24	0.001	24	24	24	0.001
Haloxifop-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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Mepanipyrin	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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- <i>m</i> -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
Norfloracin	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Ormetoprim	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>+4</sup>	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Pyraclufos	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Quinoxifen	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 (mixture 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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>TM</sup>	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Terbutylazine	22	24	23	0.01	22	24	24	0.01
Terbutylazine-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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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 <sup>TM</sup> )	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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
Tolyfluanid	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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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- <i>o</i> -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 <sup>-1</sup> )	No. of identifications			LOI (mg.kg <sup>-1</sup> )
	0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>		0.001 mg.kg <sup>-1</sup>	0.01 mg.kg <sup>-1</sup>	0.1 mg.kg <sup>-1</sup>	
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

882

883

884

885

886

887

888

889

890

891

892

893

894

895

896

897

898

899

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			Reference
		SDL < 0.01 mg·kg <sup>-1</sup>	LOI < 0.01 mg·kg <sup>-1</sup>	LOQ < 0.01 mg·kg <sup>-1</sup>	
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 <sup>b</sup> /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 ( <b>80</b> )	QuEChERS/LC-MS/MS	-	-	99	(Zhao et al., 2017)
Pesticides ( <b>52</b> )	QuEChERS/LC-MS/MS	-	-	85	(Barbieri et al., 2019)
Pesticides ( <b>50</b> )	GLME-MA-dSPE <sup>c</sup> /GC-MS/MS	-	-	76	(Kaw et al., 2021)

---

902 a '-' indicates 'not provided'

903 b ASE = Accelerated solvent extraction

904 c GLME-MA-dSPE = gas-liquid microextraction and magnetic-assisted dispersive solid phase extraction

905

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

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

			Mussels (n=6)	<b>0.006</b>	(0.004-0.008)	<b>0.005</b>	(0.004-0.008)	<b>0.005</b>	(0.003-0.007)	
			Sole (n=3)	<b>0.007</b>	(0.005-0.009)	<b>0.008</b>	(0.006-0.010)	<b>0.008</b>	(0.006-0.010)	
			Horse mackerel (n=3)	<b>0.006</b>	(0.004-0.007)	<b>0.006</b>	(0.005-0.007)	<b>0.006</b>	(0.005-0.007)	
			Spiny lobster (n=3)	<b>0.007</b>	(0.006-0.009)	<b>0.007</b>	(0.006-0.009)	<b>0.007</b>	(0.005-0.009)	
			Crayfish (n=3)	<b>0.008</b>	(0.005-0.011)	<b>0.008</b>	(0.005-0.012)	<b>0.009</b>	(0.006-0.012)	
Diuron	2.7	0.001	Oysters (n=6)	<b>0.055</b>	(0.037-0.080)	<b>0.050</b>	(0.034-0.072)	<b>0.050</b>	(0.034-0.071)	63
			Mussels (n=6)	<b>0.076</b>	(0.064-0.086)	<b>0.069</b>	(0.059-0.078)	<b>0.070</b>	(0.059-0.078)	
			Spiny lobster (n=3)	<b>0.008</b>	(0.007-0.010)	<b>0.009</b>	(0.008-0.011)	<b>0.008</b>	(0.007-0.010)	
Fenpropimorph	4.9	0.001	Oysters (n=6)	<b>0.008</b>	(0.004-0.013)	<b>0.008</b>	(0.004-0.012)	<b>0.009</b>	(0.005-0.013)	25
Prosulfocarb	3.9	0.001	Oysters (n=6)	<b>0.012</b>	(0.005-0.015)	<b>0.012</b>	(0.005-0.015)	<b>0.012</b>	(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)	<b>0.001</b>	(<SDL-0.004)	<b>0.003</b>	(0.002-0.006)	50
			Mussels (n=6)	<b>0.009</b>	(0.006-0.014)	<b>0.009</b>	(0.006-0.013)	<b>0.008</b>	(0.006-0.013)	
Tebuconazole	3.7	0.001	Spiny lobster (n=3)	<b>0.004</b>	(0.002-0.005)	<b>0.004</b>	(0.002-0.005)	<b>0.004</b>	(0.001-0.005)	13
Thiabendazole	2.5	0.001	Crayfish (n=3)	<b>0.002</b>	-	<b>0.002</b>	-	<b>0.002</b>	(0.002-0.003)	13

### Veterinary drugs and their TPs

4-Dimethylaminoantipyrine	1.0	0.001	Crayfish (n=3)	<b>0.010</b>	(0.008-0.013)	<b>0.012</b>	(0.010-0.016)	<b>0.011</b>	(0.009-0.016)	13
Amino flubendazole	1.6	0.001	Mussels (n=6)	<b>0.011</b>	(0.006-0.016)	<b>0.010</b>	(0.006-0.014)	<b>0.009</b>	(0.005-0.013)	25
Clarithromycin	3.2	0.001	Oysters (n=6)	<b>0.015</b>	(0.006-0.028)	<b>0.016</b>	(0.007-0.027)	<b>0.015</b>	(0.007-0.025)	50
			Mussels (n=6)	<b>0.004</b>	(<SDL-0.011)	<b>0.006</b>	(0.002-0.012)	<b>0.005</b>	(0.001-0.012)	
Dapsone	1	0.001	Oysters (n=6)	<b>0.012</b>	(0.005-0.015)	<b>0.012</b>	(0.006-0.014)	<b>0.012</b>	(0.007-0.015)	50
			Mussels (n=6)	<b>0.017</b>	(0.002-0.033)	<b>0.016</b>	(0.003-0.030)	<b>0.015</b>	(0.001-0.031)	
Diclofenac	4	0.001	Oysters (n=6)	<b>0.052</b>	(0.038-0.068)	<b>0.044</b>	(0.032-0.057)	<b>0.043</b>	(0.032-0.054)	50
			Mussels (n=6)	<b>0.068</b>	(0.045-0.091)	<b>0.057</b>	(0.038-0.075)	<b>0.060</b>	(0.039-0.079)	
Vedaprofen	5.7	0.001	Sole (n=3)	<b>0.029</b>	(0.017-0.044)	<b>0.042</b>	(0.026-0.062)	<b>0.042</b>	(0.026-0.062)	50

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

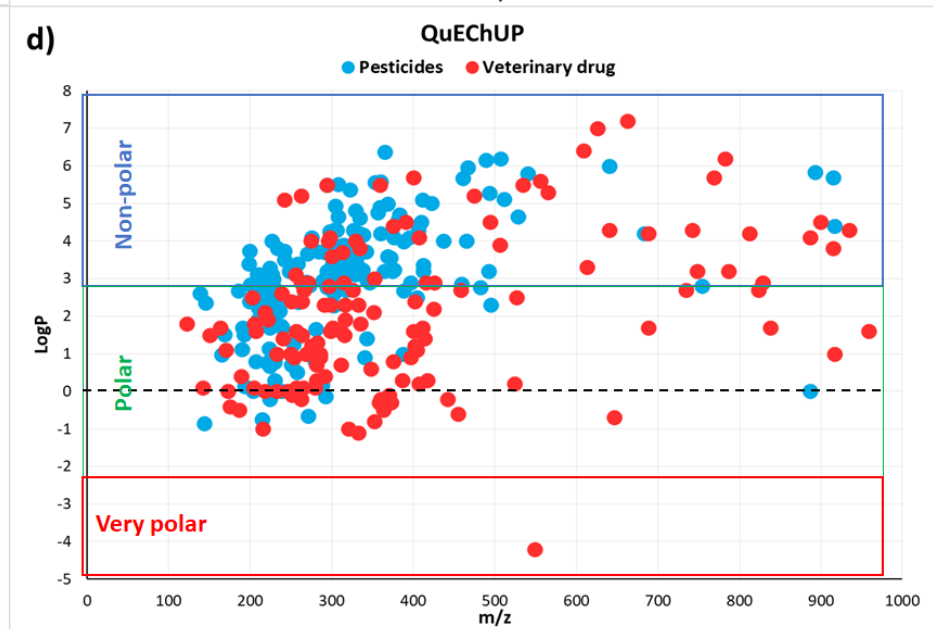
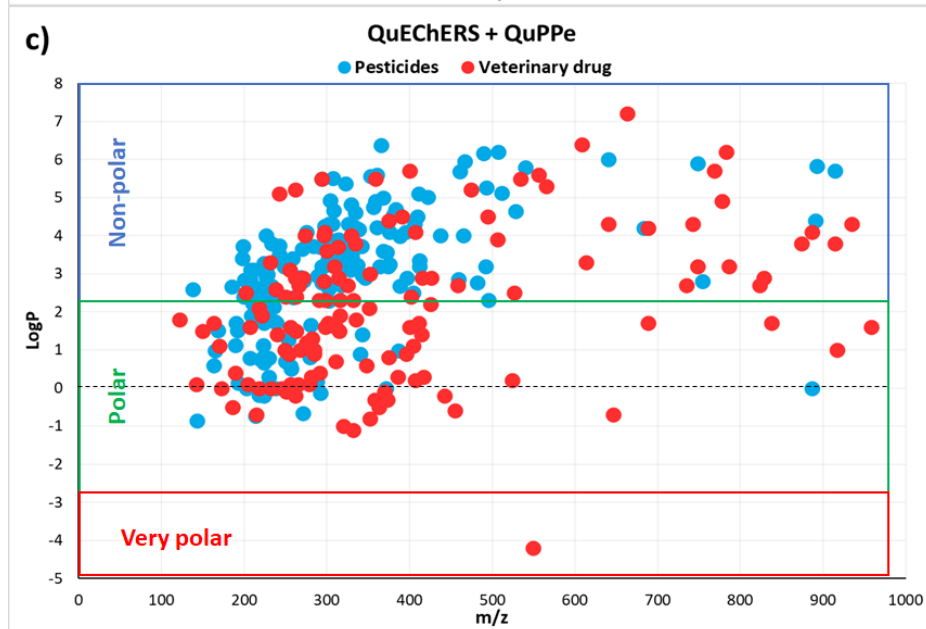
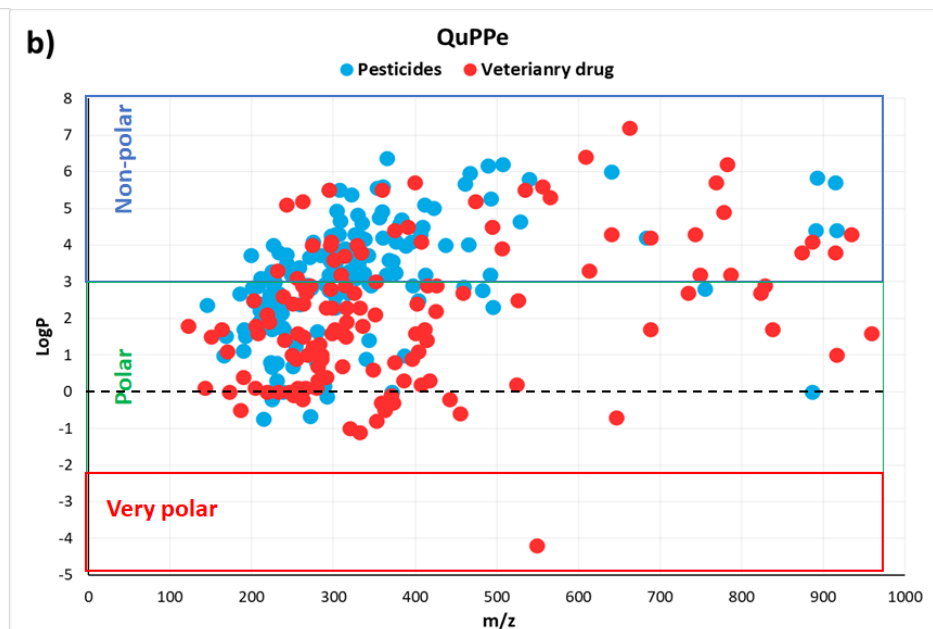
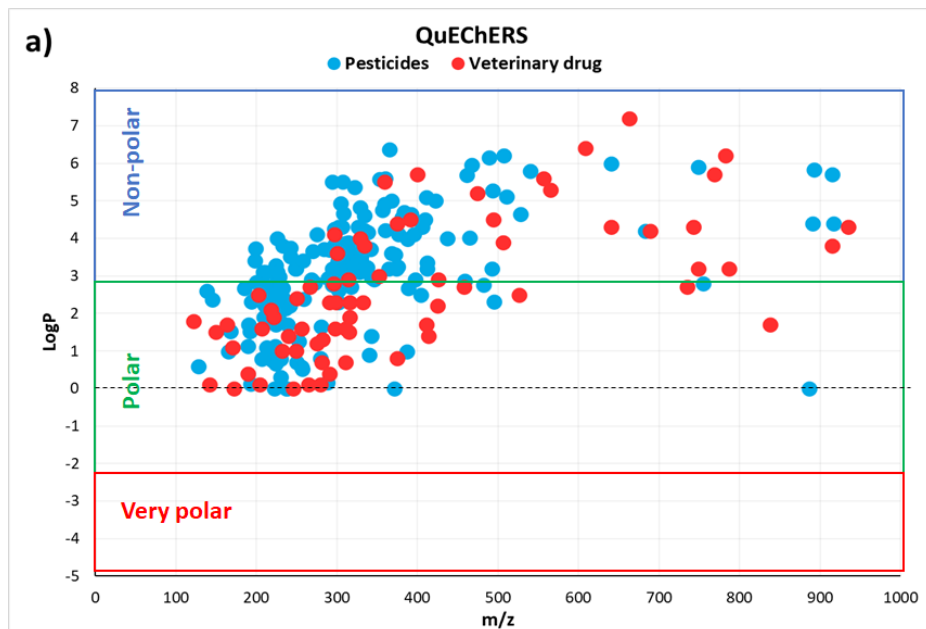




911 **Table S9.** Suspect screening results and frequency of appearance (%FoA).

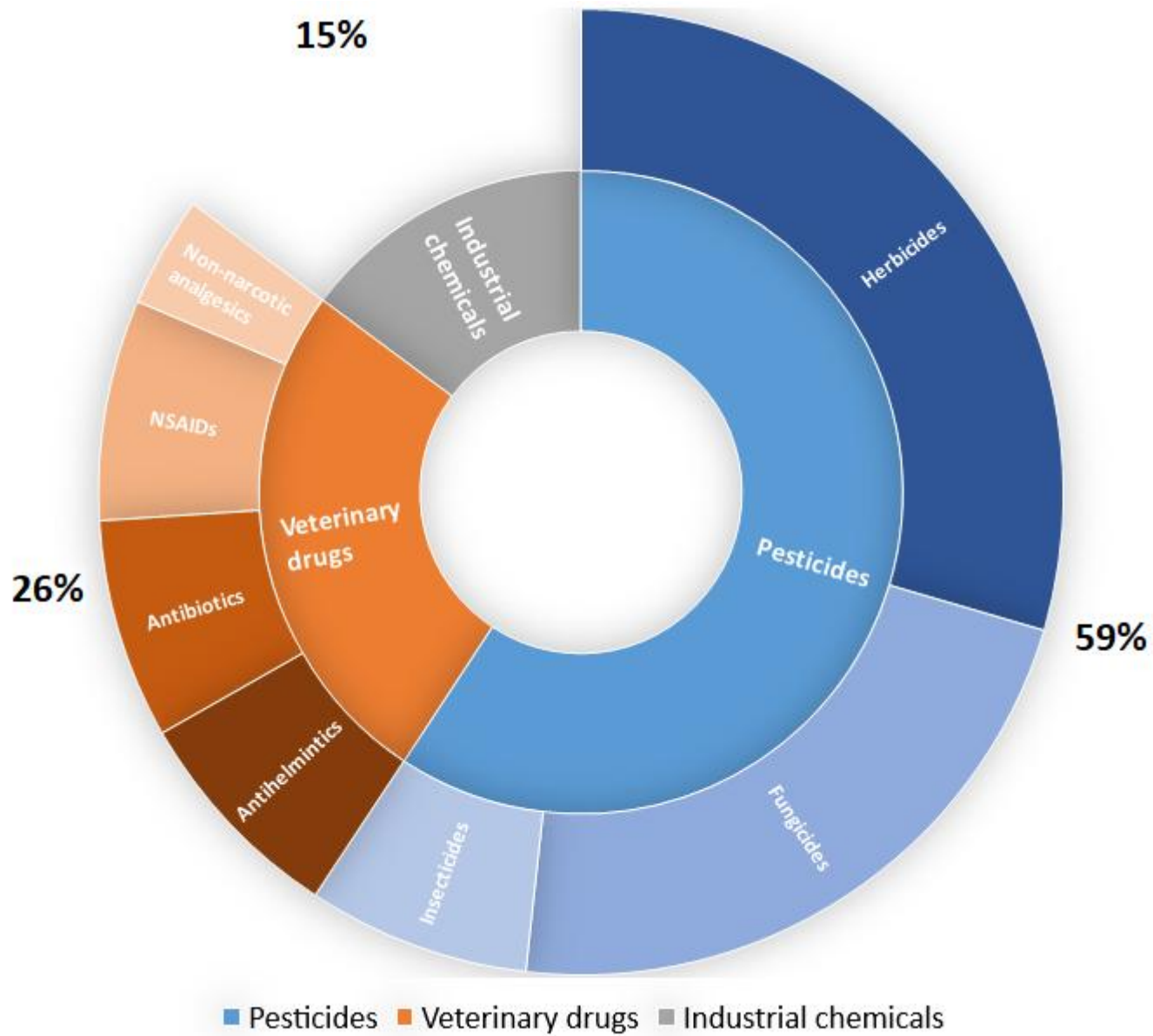
<b>Compound</b>	<b>Class</b>	<b>Positive seafood species</b>	<b>%FoA</b>
17alpha-Methyltestosterone	Antineoplastic agent	Mussels	25
2,6-Xylidine	Metabolite of lidocaine (anesthetic)	Sole	13
4-Hydroxybenzoic acid	Personal care product	Mussels	25
Allopurinol	Antigout agent	Crayfish	13
Benzocaine	Anesthetic	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 regulator	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 allopurinol (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



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

915



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

919

920 **References used in SM**

- 921 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  
922 contaminants in aquaculture products using liquid chromatography/quadrupole time-of-flight mass spectrometry. *Food Chem. X* 15,  
923 100380. <https://doi.org/10.1016/j.fochx.2022.100380>
- 924 Barbieri, M.V., Postigo, C., Guillem-Argiles, N., Monllor-Alcaraz, L.S., Simionato, J.I., Stella, E., Barceló, D., López de Alda, M., 2019.  
925 Analysis of 52 pesticides in fresh fish muscle by QuEChERS extraction followed by LC-MS/MS determination. *Sci. Total Environ.* 653,  
926 958–967. <https://doi.org/10.1016/j.scitotenv.2018.10.289>
- 927 Castilla-Fernández, D., Moreno-González, D., Bouza, M., Saez-Gómez, A., Ballesteros, E., García-Reyes, J.F., Molina-Díaz, A., 2021.  
928 Assessment of a specific sample cleanup for the multiresidue determination of veterinary drugs and pesticides in salmon using liquid  
929 chromatography/tandem mass spectrometry. *Food Control* 130, 108311. <https://doi.org/10.1016/j.foodcont.2021.108311>
- 930 Chang, G.-R., Chen, H.-S., Lin, F.-Y., 2016. Analysis of banned veterinary drugs and herbicide residues in shellfish by liquid chromatography-  
931 tandem mass spectrometry (LC/MS/MS) and gas chromatography-tandem mass spectrometry (GC/MS/MS). *Mar. Pollut. Bull.* 113, 579–  
932 584. <https://doi.org/10.1016/j.marpolbul.2016.08.080>
- 933 Diallo, T., Makni, Y., Lerebours, A., Thomas, H., Guérin, T., Parinet, J., 2022. Development and validation according to the SANTE guidelines of  
934 a QuEChERS-UHPLC-QTOF-MS method for the screening of 204 pesticides in bivalves. *Food Chem.* 386, 132871.  
935 <https://doi.org/10.1016/j.foodchem.2022.132871>
- 936 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-  
937 assisted dispersive solid-phase extraction clean-up for multi-residue pesticide analysis in fatty foods of animal origin. *LWT* 137, 110448.  
938 <https://doi.org/10.1016/j.lwt.2020.110448>
- 939 Munaretto, J.S., May, M.M., Saibt, N., Zanella, R., 2016. Liquid chromatography with high resolution mass spectrometry for identification of  
940 organic contaminants in fish fillet: screening and quantification assessment using two scan modes for data acquisition. *J. Chromatogr. A*  
941 1456, 205–216. <https://doi.org/10.1016/j.chroma.2016.06.018>
- 942 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  
943 products in South Korea. *Aquaculture* 553, 738064. <https://doi.org/10.1016/j.aquaculture.2022.738064>
- 944 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  
945 with accelerated solvent extraction and gel permeation chromatography cleanup. *Food Chem.* 126, 646–654.  
946 <https://doi.org/10.1016/j.foodchem.2010.10.105>
- 947 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  
948 drugs in *Oplegnathus punctatus* by liquid chromatography coupled to quadrupole Orbitrap mass spectrometry. *J. Chromatogr. B* 1065–  
949 1066, 20–28. <https://doi.org/10.1016/j.jchromb.2017.09.013>
- 950



